

Instituto de Física Teórica
Universidade Estadual Paulista

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Numerical study of the Ginzburg-Landau-Langevin equation:
Coherent structures and noise perturbation theory

Felipe Attanasio

Orientador

Gastão I. Krein

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Resumo

Nesta Dissertação apresentamos um estudo numérico em uma dimensão espacial da equação de Ginzburg-Landau-Langevin (GLL), com ênfase na aplicabilidade de um método de perturbação estocástico e na mecânica estatística de defeitos topológicos em modelos de campos escalares reais. Revisamos brevemente conceitos de mecânica estatística de sistemas em equilíbrio e próximos a ele e apresentamos como a equação de GLL pode ser usada em sistemas que exibem transições de fase, na quantização estocástica e no estudo da interação de estruturas coerentes com fônons de origem térmica. Também apresentamos um método perturbativo, denominado teoria de perturbação no ruído (TPR), adequado para situações onde a intensidade do ruído estocástico é fraca. Através de simulações numéricas, investigamos a restauração de uma simetria Z_2 quebrada, a aplicabilidade da TPR em uma dimensão e efeitos de temperatura finita numa solução topológica do tipo ‘‘kink’’ - onde apresentamos novos resultados sobre defeitos de dois kinks.

Palavras Chaves:

Transições de fase; Equações de Ginzburg-Landau; Quantização estocástica; Defeitos topológicos

Áreas do conhecimento:

Teoria de campos; Mecânica estatística; Física computacional

Abstract

In this Dissertation we present a numerical study of the Ginzburg-Landau-Langevin (GLL) equation in one spatial dimension, with emphasis on the applicability of a stochastic perturbative method and the statistical mechanics of topological defect structures in field-theoretic models of real scalar fields. We briefly review concepts of equilibrium and near-equilibrium statistical mechanics and present how the GLL equation can be used in systems that exhibit phase transitions, in stochastic quantization and in the study of the interaction of coherent structures with thermal phonons. We also present a perturbative method, named noise perturbation theory (NPT), suitable for situations where the stochastic noise intensity is weak. Through numerical simulations we investigate the restoration of a broken Z_2 symmetry, the applicability of the NPT in one dimension and finite temperature effects on a topological ‘‘kink’’ solution - where we present new results on two-kink defects.

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Chapter 1

Introduction

The Langevin equation [1] finds applications in various fields of physics: statistical mechanics, stochastic cosmological inflation, phase transitions, stochastic quantization, to name a few, and in other areas like biology, engineering and financial markets. The Ginzburg-Landau-Langevin (GLL) equation [2] is a kind of Langevin equation in which the time evolution is governed by forces originated from a phenomenological Hamiltonian, known as Ginzburg-Landau free energy. As we will see here, it arises in contexts like equilibrium and non-equilibrium statistical mechanics, phase transitions, kinks and domain walls, and stochastic quantization - a good text book on the subject is the one of Parisi [3].

One of the first uses of the Langevin equation was motivated by the Brownian motion, the apparently random motion of pollen grains suspended in water. This motion is counterbalanced by viscous friction in such a way that the Brownian particle has a non-zero average kinetic energy. This fact points to the direction that the friction deceleration must be related to the intensity of the force caused by the collision with the molecules. The position of the grain over time can be thought of as the continuous limit of a random walk with zero mean, since there is no preferred direction for the collisions, and finite variance. This suggests the use of a Langevin equation for the particle's velocity, where a suitable noise field effectively models the bombardment by the water molecules.

Another application of the Langevin equation arises in the modeling of the near equilibrium state of a system composed by a large number of particles, such as the molecules of a gas or dust in a galaxy, where it can be employed as equation of motion for physical observables. The complete description of such physical ensembles when in thermal equilibrium

is possible using well-known methods from classical or quantum mechanics, quantum field theory or general relativity together with those from statistical mechanics. This approach consists in taking the average over phase space variables of a Boltzmann-weighted static probability distribution. However, non-equilibrium states evolve in time and the great number of degrees of freedom interacting renders the differential equations intractable. By modeling the evolution of macroscopic variables such as temperature and pressure with suitable Langevin equations it is possible to study their behavior close to the equilibrium. The stochastic noise is essential to guarantee the fluctuations around the equilibrium values characteristic of such systems - a recent textbook on the subject is the one of Onuki [4].

Interesting examples of close to equilibrium situations are systems in the vicinity of a phase transition [5]. A physical system is said to exhibit a phase transition if some of its properties, like order parameters, change their analytical behavior at a given value of the external parameters. This point in parameter space is called a critical point and marks where the system changes its physical properties. At the critical point the order parameter, or its n -th order derivative for some n , is divergent. Common examples are the fusion and boiling temperatures and pressures for water, the Curie temperature of a ferromagnetic material and even the deconfinement temperature of quantum chromodynamics (QCD). At the phase transition the range of the microscopical effects within the system, called correlation length, diverges. This means that in a vicinity of the transition the large wavelength excitations dominate and an effective model can be used. The most famous example is the Landau theory of phase transitions: it is a mean-field theory that gives the critical exponents of physical quantities, i.e., their behavior near the critical point, using a phenomenological Hamiltonian. This theory can be augmented to take into account environmental effects of random nature (e.g. of thermal origin) by the addition of a noise field, and thus becoming a Ginzburg-Landau-Langevin equation.

A special kind of physical systems that exhibit phase transitions are those in which a spontaneously broken continuous (like $SO(3)$) or discrete (such as Z_2) symmetry is restored at a critical temperature [6]. Spontaneous breakdown of a symmetry occurs when the potential has degenerate minimum energy states and the system must "choose" one of them. The minima are usually separated by a potential barrier and for energies

above a certain value the system becomes insensitive to the barrier, thus restoring the symmetry. For discrete symmetries the equations of motion support non-perturbative solutions that interpolate between the minima called kinks, in one dimension, or domain walls, for higher dimensions. Contact with a heat bath will induce thermal fluctuations that change the kink structure and may even destroy the kinks if the temperature is sufficiently high to restore the symmetry, a situation where there is, effectively, only one minimum energy state.

Another situation where Ginzburg-Landau-Langevin equations are used is Parisi and Wu's method of stochastic quantization [7], in which the noise plays the role of the quantum fluctuations. This method is equivalent to the well-known methods of canonical, using Schrödinger or Heisenberg equations of motion, or path-integral quantization, where the classical Lagrangian is the central quantity. The key to this stochastic method is to view imaginary-time (Euclidean) quantum systems as the equilibrium limit of a statistical system coupled to a thermal reservoir. The system evolves in a new fictitious time direction according to a Langevin equation, where the coupling to the heat reservoir is simulated by a stochastic noise field. In equilibrium, at the infinite fictitious time limit, stochastic averages become identical to imaginary-time vacuum-to-vacuum transition amplitudes. This is particularly useful in numerical simulations of quantum systems, especially when the chemical potential is non-zero and particles may be exchanged with the environment, as the Euclidean Action becomes complex-valued and not suitable for Monte Carlo simulations - a recent discussion on the subject is Ref. [8].

Unfortunately, in practical situations the Ginzburg-Landau-Langevin equation can be too complicated for analytical evaluation or even numerical computations, where it may be too time consuming, restricting its range of applicability. In these situations some kind of perturbative expansion has to be employed. Besides the usual weak and strong coupling expansions or semi-classical methods in the context of GLL equations it is also possible to perform an expansion in powers of the noise intensity. This method, known as Noise Perturbation Theory (NPT), provides a set of linear stochastic differential equations for the noise corrections to the unperturbed (noise-free) solution. It has been used in the past years mainly in the context of stochastic cosmological inflation [9, 10, 11], an effective theory that models quantum fluctuations

to the early expanding universe. This theory has a multiplicative noise field, instead of an additive one. Nevertheless, noise perturbation theory enables analytical solutions to be obtained for fields subject to arbitrary potentials, and motivates studies of its applicability in other contexts.

Summarizing, Langevin equations arise mainly when:

- we are only interested in, or can only deal with, a subset of the degrees of freedom of a system and the influence of the remaining ones are taken into account via a stochastic noise term, such as the time evolution of a Brownian particle;
- there is a certain degree of randomness or lack of sufficient information to make a deterministic prediction, like in financial markets;
- we are dealing with macroscopic or collective behavior, where the exact microscopic dynamics is not relevant, as in near equilibrium statistical mechanics.

The main objective of the present Dissertation is to present a review of the different subjects discussed above. Our aim is to present an introductory text where the different pieces are presented in a coherent and didactic manner. We are particularly interested in presenting the appearing of Ginzburg-Landau-Langevin type of equations in the theory of phase transitions, stochastic quantization and noise effects of statistical and quantum origin on coherent structures of topological nature of field-theoretic models. We focus on field-theoretic models involving a scalar field in one space dimension, since such models present topological solutions of the classical equations of motion at zero temperature. A second objective of the Dissertation is the discussion of numerical methods for treating Ginzburg-Landau-Langevin equations. In particular, we discuss the applicability of a method based on a perturbative expansion in the strength of the noise correlation function [12]. Although our discussion of the applicability of the method focus on simple models, for which comparison with the numerical solution of the full equation is feasible, we expect that the method finds its full power in problems with complicated actions that are non-local in space and time. Such actions arise in the context of quantum field theories [6] - one example of such an action recently discussed in the literature can be

found in Ref. [13]. Finally, we present a numerical algorithm to solve Ginzburg-Landau-Langevin equations on a spatial grid.

The Dissertation is organized as follows: in Chapter 2 we review the methods of equilibrium statistical mechanics, introduce the Langevin equation for the Brownian motion and study a model for situations near thermodynamic equilibrium. In Chapter 3 we investigate some applications of the Langevin equation: critical phenomena, stochastic quantization and defect structures like kinks and domain walls. In Chapter 4 we present a perturbative method to obtain simpler Ginzburg-Landau-Langevin equations when the phenomenological Hamiltonian is too complicated for analytical solutions or numerical computations. In Chapter 5 we show the results of numerical simulations of the GLL equation and analyze how finite lattice size effects may lead to non-zero order parameters in one dimension, whether or not the noise perturbation theory gives good results in one dimension and the interaction of thermal phonons with one-kink and two-kink solutions. Conclusions and future perspectives are presented in Chapter 6. This work also has four appendices where some complementary topics are discussed.

Chapter 2

Equilibrium Statistical Mechanics

Statistical mechanics studies systems with a large number of constituents ($N \sim 10^{23}$) through its macroscopic/thermodynamical properties, such as temperature, pressure, volume, etc. Those variables are usually not independent, as they are related to each other via a *thermodynamic equation of state*

$$f(p, V, T, S, \dots) = 0. \quad (2.1)$$

Given a microscopic Hamiltonian, i.e., from which a complete description of the system could in principle be obtained, we can construct a generating function for all thermodynamic quantities, their respective statistical moments (mean, variance, etc) and also the equations of state.

It is known that the entropy of a thermodynamical system always increases or remains constant and reaches its maximum value at the equilibrium state, i.e., when the fluxes of particles, energy, etc with the environment are stationary. The concept of entropy is used to explain why certain processes, although permitted by conservation laws, do not happen, e.g., heat flowing from a cold body to a hot one or a perpetual machine. From the statistical mechanics point of view, entropy is related to the number of microscopic states (e.g., position and momenta) of the components of the system that lead to the same macrostates, i.e., thermodynamical variables satisfying the same equations of state. Everyday experience then tells us that there is a lower number of microscopic configurations in which two bodies in contact are at different temperatures than if they were in thermal equilibrium.

2.1 Mathematical formulation

Assuming our system is in contact with a heat bath at temperature T its thermodynamical properties can be deduced from the *partition function*

$$Z = \int d\rho e^{-\beta H} \quad (2.2)$$

where $d\rho$ is a volume element in the phase space, $H(\vec{p}, \vec{q})$ is the Hamiltonian governing its dynamics and $\beta = (k_B T)^{-1}$, k_B is the Boltzmann constant (which we take equal to unity). This partition function is called the *canonical* partition function* and can be deduced by applying the *principle of maximum entropy* to the Shannon information entropy [14] functional $\mathcal{H}[p]$ (not to be confused with the Hamiltonian), given by

$$\mathcal{H}[p] = - \int d\rho p \ln p \quad (2.3)$$

where p is the probability that the system may be found at a given region of the phase space. Imposing via Lagrange multipliers that the system has a definite average energy E gives

$$\delta \mathcal{H}[p] = \delta \left\{ - \int d\rho p \ln p + \lambda_0 \left[\int d\rho p - 1 \right] + \lambda_1 \left[\int d\rho H(\vec{p}, \vec{q}) p - E \right] \right\} = 0, \quad (2.4)$$

which has

$$p = \exp[-\lambda_0 - \lambda_1 H - 1] \equiv \frac{e^{-\lambda_1 H}}{Z} \quad (2.5)$$

as solution. Imposing the normalization constraint we have

$$\int d\rho p = 1 \Rightarrow Z = \int d\rho e^{-\lambda_1 H} \quad (2.6)$$

Now, denoting by $S(\langle H \rangle)$ the maximum of $\mathcal{H}[p]$ subject to the given constraints

$$S(\langle H \rangle) = - \int d\rho p \ln p = - \frac{1}{Z} \int d\rho e^{-\lambda_1 H} (-\ln Z - \lambda_1 H) = \ln Z + \lambda_1 \langle H \rangle \quad (2.7)$$

we see the resemblance with the thermodynamical relation $F = E - TS$, where F is the Helmholtz free energy, E is the internal energy and S is

*If the system was in contact with a particle reservoir we would use the *grand canonical* partition function. In general, Z is defined according to the experimental setup.

the Boltzmann-Gibbs entropy, if we identify $\lambda_1 = \beta$ and $F = \beta^{-1} \ln Z$. Thus we arrive at eq (2.2) and it becomes clear that

$$\langle H \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = \frac{1}{Z} \int d\rho H e^{-\beta H} = E, \quad (2.8)$$

that is, β and E are conjugated variables in the sense that a system with a definite temperature has its energy fluctuating around a well-defined average value, and vice-versa. We come back to this point shortly.

Other experimental constraints will lead to different partition functions. A few well-known examples follow: If the system is isolated and may not exchange heat or particles with the environment its energy should remain fixed at a value E , but experimentally it's very difficult to have the system with a sharp value for the energy. Thus we allow $E \leq H(\vec{p}, \vec{q}) \leq E + \Delta E$, with $\Delta E \ll E$. In this case

$$\mathcal{H}[p] = - \int_D d\rho p \ln p + \lambda_0 \left[\int_D d\rho p - 1 \right] \quad (2.9)$$

where D is the region of the phase space that satisfies our energy constraint. The maximum of $\mathcal{H}[p]$ lies at $p = \exp[-\lambda_0 - 1] = Z^{-1}$. Normalization gives

$$Z = \int_D d\rho = \Omega. \quad (2.10)$$

Denoting again the maximum of $\mathcal{H}[p]$ by S we have

$$S = - \int_D d\rho \frac{1}{\Omega} \ln (\Omega^{-1}) = \ln \Omega \quad (2.11)$$

and we recover the famous Boltzmann relation. Namely, the entropy of a system in the so-called microcanonical ensemble is the logarithm of the number of accessible states in the phase space. The equilibrium temperature $T = \beta^{-1}$ is

$$\beta = \frac{\partial S}{\partial E}. \quad (2.12)$$

Another experimental setup consists in a system in contact with both a heat and a particle reservoirs. In this situation the equilibrium state will have definite average energy and particle number values, so

$$\begin{aligned} \mathcal{H}[p] = & - \int d\rho p \ln p + \lambda_0 \left[\int d\rho p - 1 \right] + \lambda_1 \left[\int d\rho H p - \langle H \rangle \right] \\ & + \lambda_2 \left[\int d\rho N p - \langle N \rangle \right] \end{aligned} \quad (2.13)$$

and, upon extremization,

$$p = \frac{e^{-\lambda_1 H - \lambda_2 N}}{Z}. \quad (2.14)$$

The maximum of the entropy in this case reads

$$S = \ln Z + \lambda_1 \langle H \rangle + \lambda_2 \langle N \rangle, \quad (2.15)$$

and using the thermodynamical relation $S = -\beta G + \beta U - \beta \mu \langle N \rangle$ we can identify

$$-\beta^{-1} \ln Z = G \quad (2.16)$$

$$\lambda_1 = \beta \quad (2.17)$$

$$\lambda_2 = -\beta \mu \quad (2.18)$$

where G is the Gibbs free energy, $\beta = T^{-1}$ and μ is called chemical potential.

2.1.1 Simple example

As a simple example we consider an ideal gas of particles of mass m in a box of volume V at temperature $T = \beta^{-1}$. The Hamiltonian in this case is

$$H = \frac{1}{2m} \sum_{i=1}^N (p_{x_i}^2 + p_{y_i}^2 + p_{z_i}^2) = \frac{1}{2m} \sum_{i=1}^{3N} p_i^2 \equiv \sum_{i=1}^{3N} H_i \quad (2.19)$$

and the partition function can be easily evaluated

$$\begin{aligned} Z &= \int d\rho e^{-\beta H} = \int \prod_{i=1}^{3N} \frac{dp_i dq_i}{N!} e^{-\beta H_i} = \frac{1}{N!} \prod_{i=1}^{3N} \left[\int dp_i dq_i e^{-\beta H_i} \right] \\ &= \frac{V^N}{N!} \left(2\pi \frac{m}{\beta} \right)^{\frac{3N}{2}}, \end{aligned} \quad (2.20)$$

where we have factorized the $6N$ -dimensional integral in $3N$ 2-dimensional integrals and the factor $N!^{-1}$ accounts for the indistinguishability of the particles considered[†]. From it we obtain an expression for the internal energy of the system

$$E = -\frac{\partial}{\partial \beta} \ln Z = \frac{3N}{2\beta} = \frac{3N}{2} T, \quad (2.21)$$

in accordance with the equipartition theorem. Also, we may write an equation of state using the thermodynamic identity

$$p = \frac{\partial F}{\partial V} = \beta^{-1} \frac{\partial}{\partial V} \ln Z = \frac{N}{V} T \quad (2.22)$$

[†]The factor $N!$ is of quantum origin - if absent, it leads to the Gibbs paradox.

which relates the pressure, volume, number of particles and the temperature. In summary Z , or rather $\ln Z$ is the central quantity in statistical mechanics.

2.2 Langevin equation

Langevin equation is a stochastic differential equation used to describe the time evolution of a subset of the degrees of freedom of a physical system. In situations where the number of phase space variables is too large it is impossible, in practice, to solve all the equations of motion. We will show that the Langevin equation can be used to model the effective macroscopic behavior of a system given its microscopic dynamics or to describe the evolution of a few degrees of freedom that vary in time slower than the rest, which may be taken into account via a noise field.

2.2.1 Background

Parts of this section are based on Ref. [15]. The Langevin equation first arose in the context of Brownian motion, in order to model the apparently random motion of a particle in a fluid due to collisions with the molecules of the fluid. The equation of motion is

$$\frac{dv}{dt}(t) = -\gamma v(t) + \xi(t) \quad (2.23)$$

where γ is a macroscopic dissipation coefficient and ξ , which represents the collisions of the Brownian particle with fluid molecules, is a Gaussian white noise, i.e.,

$$\langle \xi(t) \rangle = 0 \quad (2.24)$$

$$\langle \xi(t)\xi(t') \rangle = 2\Gamma \delta(t - t'). \quad (2.25)$$

Where $\langle \dots \rangle$ means an average over noise realizations, i.e.,

$$\langle \xi(t) \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \xi_i(t) = 0, \quad (2.26)$$

$$\langle \xi(t)\xi(t') \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \xi_i(t)\xi_i(t') = 2\Gamma \delta(t - t'). \quad (2.27)$$

That is, ξ represents a force that acts uniformly with intensity $\sqrt{2\Gamma}$ in all directions. Moreover, due to eq (2.25) a force acting on $t = t'$ does not depend on what happened for $t < t'$, as the autocorrelation $\langle \xi(t)\xi(t') \rangle = 0$ for $t \neq t'$.

We write the Langevin equation as a Stochastic Differential Equation (SDE)

$$dv = -\gamma v dt + \Gamma d\omega \quad (2.28)$$

where $d\omega(t) = \xi(t) dt$ is a Wiener Process, i.e.,

$$\langle d\omega(t) \rangle = 0, \quad (2.29)$$

$$\langle d\omega(t)d\omega(t) \rangle = dt, \quad (2.30)$$

$$\langle d\omega(t)^n \rangle = 0, \text{ for } n \geq 3. \quad (2.31)$$

The above properties are heuristically derived in the appendix A. Considering a (well-behaved) arbitrary function $f[v]$. Ito's lemma, also derived in appendix A, tells us that $f[v]$ satisfies the SDE

$$df[v] = -\gamma v \frac{df}{dv} dt + \sqrt{2\Gamma} \frac{df}{dv} d\omega + \Gamma \frac{d^2 f}{dv^2} dt. \quad (2.32)$$

The noise average of $f[v]$ can be written as

$$\langle f[v(t)] \rangle \equiv \int dv f(v) P(v, t), \quad (2.33)$$

where $P(v, t)$ is a probability density function from which the statistical properties can be obtained, and obeys the SDE

$$\langle df[v] \rangle = -\gamma \left\langle v \frac{df}{dv} \right\rangle dt + \Gamma \left\langle \frac{d^2 f}{dv^2} \right\rangle dt \quad (2.34)$$

$$\left\langle \frac{df}{dt} \right\rangle = -\gamma \left\langle v \frac{\partial f}{\partial v} \right\rangle + \Gamma \left\langle \frac{\partial^2 f}{\partial v^2} \right\rangle. \quad (2.35)$$

Using eq. (2.33) and doing a few partial integrations

$$\begin{aligned} \int dv f(v) \frac{\partial P}{\partial t} &= -\gamma \int dv v \frac{\partial f}{\partial v} P + \Gamma \int dv \frac{\partial^2 f}{\partial v^2} P \\ &= \int dv \left[\gamma \frac{\partial v P}{\partial v} + \Gamma \frac{\partial^2 P}{\partial v^2} \right] f(v) \end{aligned} \quad (2.36)$$

we find the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \gamma \frac{\partial v P}{\partial v} + \Gamma \frac{\partial^2 P}{\partial v^2} \quad (2.37)$$

associated to the Langevin equation eq (2.23), since $f(v)$ is arbitrary by assumption.

For long times ($t \rightarrow \infty$) the system will reach an equilibrium state, i.e., $\partial_t P = 0$. The dissipative factor $-\gamma v$ and the random driving force $\xi(t)$ compensate each other so that $\langle v \rangle$ is constant in time. Therefore we have

$$\frac{\partial}{\partial v} \left[\gamma v P + \Gamma \frac{\partial P}{\partial v} \right] = 0 \Rightarrow \Gamma \frac{\partial P}{\partial v} + \gamma v P = C, \quad (2.38)$$

with C being a constant which will be fixed later. To solve the above equation we look for an integrating factor $g(v)$ such that

$$g \frac{\partial P}{\partial v} + \frac{\gamma v g}{\Gamma} P = \frac{\partial}{\partial v} [gP] = \frac{gC}{\Gamma}. \quad (2.39)$$

Thus $g(v)$ must satisfy

$$\frac{\partial g}{\partial v} = \frac{\gamma v}{\Gamma} g \Rightarrow g(v) = \exp \left[\frac{\gamma (v^2 - v_0^2)}{2\Gamma} \right], \quad (2.40)$$

where v_0 is an integration constant. We then have that

$$P(v) = \frac{g(v_0)P(v_0)}{g(v)} + \frac{C}{\Gamma g(v)} \int_{v_0}^v dv' g(v'). \quad (2.41)$$

Substituting it back on eq. (2.38) we find that $C = 0$, and imposing normalization we finally arrive at

$$P(v) = \sqrt{\frac{\gamma}{2\pi\Gamma}} \exp \left[-\frac{\gamma v^2}{2\Gamma} \right]. \quad (2.42)$$

Combining the above result with the equipartition theorem $\langle E \rangle = T/2$ (for a 1-dimensional motion)

$$\frac{1}{2} m \langle v^2 \rangle = \frac{m}{2} \frac{1}{2} \frac{2\Gamma}{\gamma} = \frac{1}{2} T \quad (2.43)$$

we see that the dissipation γ and diffusion Γ coefficients are related to each other in the equilibrium state by $m\Gamma = T\gamma$. This is known as the Fluctuation-Dissipation Theorem (FDT). It gives the relation between the external (random) and dissipative forces that will drive the system to a non-trivial stationary state: if $m\Gamma < T\gamma$, that is, if the dissipative force were stronger than the external one the brownian particle would eventually come to rest. On the other hand, if $m\Gamma > T\gamma$ the particle velocity would increase indefinitely.

2.2.2 Approach to equilibrium

In this section we discuss how a system slightly out of equilibrium evolves in time to an equilibrium state. The aim here is to motivate how Langevin-type of equations are useful to describe evolution to equilibrium of a thermodynamic system. The discussion here is based on Ref. [6]. As we have seen earlier the equilibrium state of a thermodynamical system lies at the maximum of the Boltzmann-Gibbs entropy function $S(X_i)$, where X_i stand for all the relevant variables (e.g. energy, volume, number of particles, etc). In a situation close to equilibrium the system will experience some *thermodynamic forces*, i.e. quantities related to gradients of the entropy (like mechanical forces are related to gradients of a potential energy). Let's denote the components of the thermodynamic forces by L_i , so that $L_i = -\partial_{X_i} S$, i.e., they are the components of minus the gradient of S [6]. A possible model for the thermodynamical variables would be $\dot{X}_i = \Gamma_{ij} L_j$ (repeated indices are summed over), where the Γ_{ij} are called ‘‘kinetic coefficients’’ [4]. However, this dynamics would be too efficient: the system would just relax to the equilibrium state and stay there. There would be no thermal fluctuations, as will be shown further below.

On the other hand, the Fluctuation-Dissipation Theorem tells us that a white noise with the right properties will model a system *fluctuating* around the equilibrium state. We then look for an appropriate generalization of the FDT for the present case. As the equilibrium state distribution for the system is $p_{eq} = e^{-S} = Z^{-1} e^{-\beta H}$ for a system in contact with a heat bath, $p_{eq} = \Omega^{-1}$ for an isolated system, etc, we have that

$$\langle X_i L_j \rangle = - \int d\rho X_i \frac{\partial S}{\partial X_j} e^{-S} = \int d\rho X_i \frac{\partial e^{-S}}{\partial X_j} = - \int d\rho \frac{\partial X_i}{\partial X_j} e^{-S} = -\delta_{ij}. \quad (2.44)$$

Now, let

$$\dot{X}_i(t) = \Gamma_{ij} L_j(t) + \xi_i(t) \quad (2.45)$$

be the Langevin equation for the variable X_i , with $\langle \xi_i(t) \xi_j(t') \rangle = 2\sigma_{ij} \delta(t - t')$. Correlation functions should be time-independent in equilibrium, in particular

$$\begin{aligned} \frac{d}{dt} \langle X_i X_j \rangle &= \langle \dot{X}_i X_j + X_i \dot{X}_j \rangle \\ &= \langle \Gamma_{ik} L_k X_j \rangle + \langle \xi_i X_j \rangle + \langle X_i \Gamma_{jl} L_l \rangle + \langle X_i \xi_j \rangle = 0. \end{aligned} \quad (2.46)$$

Therefore

$$\langle \xi_i X_j \rangle + \langle X_i \xi_j \rangle = \Gamma_{ik} \delta_{kj} + \Gamma_{jl} \delta_{il} = \Gamma_{ij} + \Gamma_{ji}. \quad (2.47)$$

Invoking the Novikov identity [16] for a Gaussian white noise we can write

$$\langle X_i(t) \xi_j(t') \rangle = \int dt'' \frac{\delta X_i(t)}{\delta \xi_k(t'')} \langle \xi_k(t'') \xi_j(t') \rangle \quad (2.48)$$

which in our case becomes

$$\langle X_i(t) \xi_j(t') \rangle = 2\sigma_{kj} \frac{\delta X_i(t)}{\delta \xi_k(t')}. \quad (2.49)$$

A general solution for eq. (2.45) is

$$X_i(t) = X_i^{(h)}(t) + \int^t dt' G_{ij}(t-t') \xi_j(t') \quad (2.50)$$

where $X_i^{(h)}(t)$ is the homogeneous solution (noise-independent) and G_{ij} is the Green's function. From eq. (2.45) we see that $G_{ij}(0) = \delta_{ij}$ and thus

$$\frac{\delta X_i(t)}{\delta \xi_j(t')} = \int^t dt' G_{ik}(t-t') \delta_{jk} \delta(t-t') = \frac{1}{2} \delta_{ij}. \quad (2.51)$$

Our generalized version of the FDT then reads

$$\sigma_{ij} = \frac{1}{2} [\Gamma_{ij} + \Gamma_{ji}]. \quad (2.52)$$

A Gaussian white noise with intensity $\frac{1}{2} [\Gamma_{ij} + \Gamma_{ji}]$ in the Langevin equation then correctly models the thermal fluctuations of the system near its equilibrium state. A purely conservative dynamics, as will be shown below, leads to an anti-symmetric Γ matrix, that is, the dynamics is deterministic as the noises have zero correlation.

Let us consider a Hamiltonian system and take our variables X_i to be the position q_i and momenta p_i , $i = 1, \dots, N$, of the particles of a system whose dynamics obeys the Hamilton equations of motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad (2.53)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}. \quad (2.54)$$

Writing those in the form of eq. (2.45) we find that

$$\Gamma_{q_i q_j} = 0, \quad \Gamma_{p_i q_j} = 1, \quad (2.55)$$

$$\Gamma_{q_i p_j} = -1, \quad \Gamma_{p_i p_j} = 0, \quad (2.56)$$

for $i, j = 0, \dots, N$, in other words, Γ is the canonical symplectic matrix. The fluctuation-dissipation theorem then gives us $\sigma_{ij} = 0$. Thus, for a classical non-dissipative system at zero temperature there is no need for noise sources.

Furthermore, let us consider the Fokker-Planck equation associated with eq. (2.45)

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial X_i} (\Gamma_{ij} L_j P) + \frac{\partial}{\partial X_i} \left(\sigma_{ij} \frac{\partial}{\partial X_j} P \right) \equiv -\frac{\partial}{\partial X_i} J_i, \quad (2.57)$$

where we interpret J_i as a probability current generated by X_i and the Fokker-Planck equation as a law of conservation of probability. If we neglect fluctuations, that is, if the X_i evolve according to $\dot{X}_i = \Gamma_{ij} L_j$ the associated Fokker-Planck would be

$$\partial_t P = -\partial_i (\Gamma_{ij} L_j P). \quad (2.58)$$

For the stationary distribution we must have $\Gamma_{ij} L_j = 0$, and so X_i will be constant, as they are taken to be the independent variables. This proves our earlier assertion that the X_i 's would just relax to their equilibrium value and stay there. When the thermal fluctuations modelled by the white noise are taken into account it is straightforward to see that $P_{eq} = e^{-S}$ satisfies

$$J_i^{eq} = \Gamma_{ij} (\partial_j P_{eq} - L_j P_{eq}) = 0. \quad (2.59)$$

Equilibrium expectation values are computed according to

$$\langle F(\{X_i(t)\}) \rangle \equiv \int [dX] F(\{X_i\}) e^{-S}. \quad (2.60)$$

For the sake of completeness let us look at a time-dependent entropy for the system defined in terms of the macroscopic variables, given by [17]

$$\mathcal{S}(t) = -\int \prod_i dX_i P \ln P \equiv -\int [dX] P \ln P = -\langle \ln P \rangle. \quad (2.61)$$

Its rate of change with time is

$$\begin{aligned}
\dot{S} &= - \int [dX] (\ln P + 1) \dot{P} = \int [dX] (\ln P + 1) \partial_i J_i = - \int [dX] J_i \partial_i \ln P \\
&= - \int [dX] J_i \partial_i P \frac{1}{P} = \int [dX] (L_j P - \partial_j P) (J_j - \Gamma_{ij} L_i P) \frac{1}{P} \\
&= \int [dX] (L_i P - \partial_i P) \Gamma_{ij} (L_j P - \partial_j P) \frac{1}{P} - \int [dX] J_i L_i P \frac{1}{P} \\
&= \int [dX] (L_i - \partial_i \ln P) \Gamma_{ij} (L_j - \partial_j \ln P) P - \int [dX] J_i L_i \\
&\equiv \Pi - \Phi.
\end{aligned} \tag{2.62}$$

Where in the first line we have used a partial integration and assumed that the boundary term vanishes and $\partial_i = \frac{\partial}{\partial X_i}$. We can identify the first term with the entropy production Π , as it is the expectation value of a positive-semidefinite quantity

$$\begin{aligned}
\Pi &= \int [dX] (L_i - \partial_i \ln P) \Gamma_{ij} (L_j - \partial_j \ln P) \\
&= \langle (L_i - \partial_i \ln P) \Gamma_{ij} (L_j - \partial_j \ln P) \rangle \geq 0.
\end{aligned} \tag{2.63}$$

At equilibrium we have seen that $P = e^{-S}$, so

$$\Pi_{eq} = \langle (L_i + \partial_i S) \Gamma_{ij} (L_j + \partial_j S) \rangle = 0, \tag{2.64}$$

as expected. The second term, identified with the flow of the relevant thermodynamic potential (entropy, free energy, etc) from the system to the environment, can be written as

$$\begin{aligned}
\Phi &= \int [dX] J_i L_i = - \int [dX] J_i \partial_i S = \int [dX] \partial_i J_i S \\
&= - \int [dX] \dot{P} = - \frac{\partial}{\partial t} \int [dX] S P = - \frac{\partial}{\partial t} \langle S \rangle.
\end{aligned} \tag{2.65}$$

If we consider the time evolution of the total entropy, of the system and the environment together we get

$$\dot{S}_{total} = \dot{S}_{system} + \dot{S}_{environment} = \Pi_{system} + \Pi_{environment} \geq 0, \tag{2.66}$$

since, by definition,

$$\Phi_{system} = -\Phi_{environment}. \tag{2.67}$$

This makes explicit the fact that the total entropy is non-decreasing, even though it may *locally* decrease if some parts of the system ‘‘throw away’’ their entropy into the other parts.

Chapter 3

Applications of the Langevin equation

After using the Brownian motion as a prototype we present here three applications of the Langevin equation: the Ginzburg-Landau theory, Parisi and Wu's method of stochastic quantization and the statistical mechanics of defect structures.

Systems that exhibit phase transitions may be described near the critical point, the region in parameter space where the transition occurs, by the Ginzburg-Landau theory. It gives a mean-field description of the order parameters in terms of an effective Hamiltonian from which the critical exponents, the critical behavior of the thermodynamical quantities, may be obtained. In order to take fluctuations near the critical point into account a Langevin equation can be used generate configurations of the order parameters according to a certain partition function.

Quantum systems often follow one of the two classic prescriptions: canonical quantization, where dynamic variables are promoted to operators and the dynamics is given by the Schrödinger or Heisenberg equations of motion, or path-integral quantization, in which correlation functions are evaluated as a functional integral of the classical Lagrangian. Parisi and Wu proposed a method where a N dimensional system is embedded in a $N + 1$ dimensional space and evolve in this extra dimension following a Langevin equation.

Defect structures, namely kinks and domain walls, are non-dispersive solutions of the equations of motion of a field subject to potentials that exhibit degenerate minima, if such minima cannot be continuously rotated into one another. Quantum and thermal fluctuations, however, may destroy such coherent structures as they enable the field to tunnel from one minimum to the others. Such interactions may be studied with Langevin equations to simulate the contact with a heat bath.

3.1 Ginzburg-Landau-Langevin equation

3.1.1 Critical phenomena

A given state of some physical system is determined by specifying the values of its intensive and extensive parameters. If we divide our system in n parts some of its properties, like temperature and mass density, will be the same for each subsystem: $x = x_1 = x_2 = \dots = x_n$. Those are called intensive parameters. Quantities like total mass and total volume of each of the n subsystems are to be added in order to retrieve the ones characterising the whole system $y = y_1 + y_2 + \dots + y_n$, and are called extensive variables. The latter ones have the interesting property that the ratio of two extensive variables results in an intensive variable usually called *mechanical variable*.

Often, the mechanical variables are uniquely defined in a given system. But if the system is undergoing a phase transition this will not be the case: Consider the $2D$ Ising model. It is a simple model for ferromagnetic interactions of a lattice of spin variables $\sigma_i \in \{-1, 1\}$ whose dynamics follow from the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \sum_i B_i \sigma_i, \quad (3.1)$$

where $J > 0$ is the interaction strength, $\sum_{\langle i,j \rangle}$ represents a sum over first-neighbors and B is an external magnetic field. The thermodynamics of a large Ising system in contact with a heat reservoir is obtained from the partition function

$$Z = \sum_{\{\sigma\}} e^{-\beta H} \quad (3.2)$$

where we sum over all possible spin configurations (2^N for a system of N spins). The average site magnetization at zero external field is given by

$$\begin{aligned} \langle \sigma \rangle &\equiv \sum_i \frac{\langle \sigma_i \rangle}{N} = \sum_i \frac{1}{N} \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i e^{-\beta H} \Bigg|_{B_i=0} = - \sum_i \frac{1}{N} \frac{1}{\beta} \frac{\partial}{\partial B_i} \ln Z \Bigg|_{B_i=0} \\ &= \sum_i \frac{1}{N} \frac{\partial F}{\partial B_i} \Bigg|_{B_i=0} \end{aligned} \quad (3.3)$$

with F being the Helmholtz free energy. For high temperatures $e^{-\beta H} \approx 1$ and $\langle \sigma \rangle$, a mechanical variable, is equal to zero. However, if the tem-

perature falls below a certain value called the Curie (or critical) temperature T_c the system exhibits spontaneous magnetization, i.e., $\langle \sigma \rangle \neq 0$ [18]. In the case of $B_i = 0$, for all i , the system is likely to magnetize in either direction, $+1$ or -1 , as shown in Fig 3.1. That is, the average

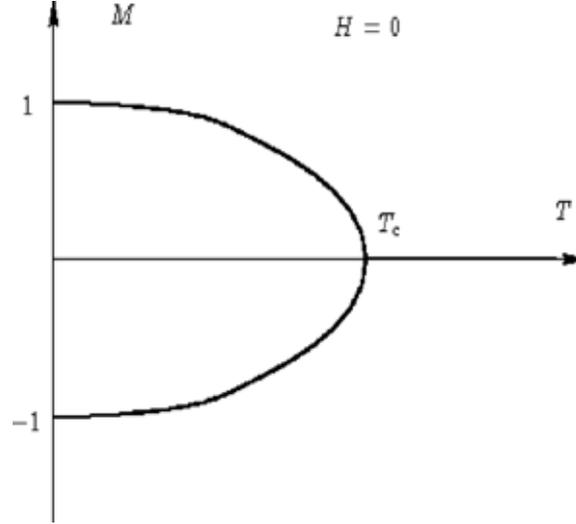


Figure 3.1: Phase diagram for the 2D Ising model.

site magnetization becomes double-valued for $T < T_c$.

This is typical of system that undergo a phase transition when certain external parameters reach so-called critical values. The mechanical variables that cease to be single-valued are called the *order parameters* and serve as indicative that a phase transition occurred. Another example of this phenomenon is water when the external pressure and temperature are such that its liquid and vapour states coexist (Fig 3.2) and the density is double-valued. At the critical point and beyond it there is no distinction between liquid and vapor and the density has a unique value.

Phase transitions can be classified by looking at the free energy and its derivatives. In the Ising case we have that $\langle \sigma \rangle = 0$ at $T = T_c$ but the magnetic susceptibility at zero external field

$$\chi_B = \sum_i \frac{\langle \sigma_i^2 \rangle - \langle \sigma_i \rangle^2}{T} = \sum_i \left. \frac{1}{N} \frac{\partial^2 F}{\partial B_i^2} \right|_{B_i=0} \quad (3.4)$$

and heat capacity

$$c = \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2} = \beta^2 \frac{\partial^2 (\beta F)}{\partial \beta^2} \quad (3.5)$$

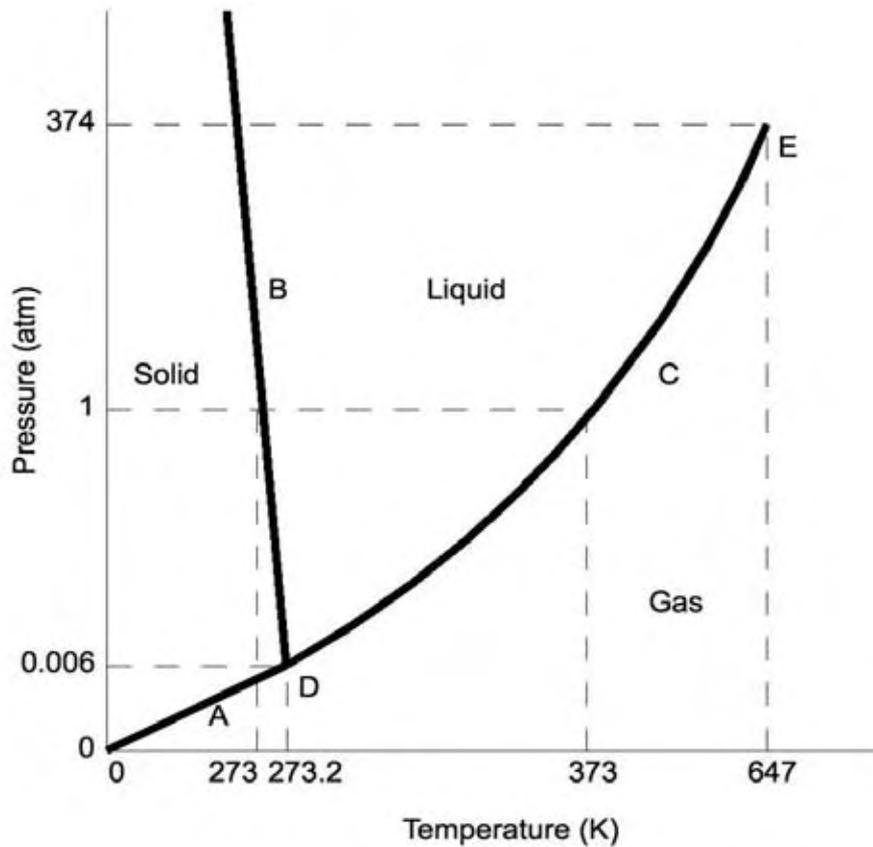


Figure 3.2: Phase diagram for the water.

are infinite. It is said that the Ising model exhibits a second order phase transition, as the second order derivative of the free energy is discontinuous. This is known as the Ehrenfest classification: the order of the phase transition is the same as the lowest derivative of the free energy that has a discontinuity.

An important parameter in the theory of phase transitions is the correlation length, usually denoted by ξ . It measures the range of the microscopic effects within a system. In other words, if we were to perform a coarse-graining and approximate the microscopic degrees of freedom by macroscopic spatial averages, the cluster size a has to be greater than ξ . If $a \lesssim \xi$ the effective macroscopic model would be a poor approximation as the effects from the microdynamics cannot be neglected. At the critical point the correlation length diverges, meaning that the whole system consists of clusters of all possible sizes.

To illustrate this point, we have implemented a Monte Carlo simulation of the two-dimensional Ising model. We used the Metropolis algorithm

for a square lattice with sides $L = 200$. Typical configurations for different temperatures are shown below, in the Figs. 3.3 and 3.4.

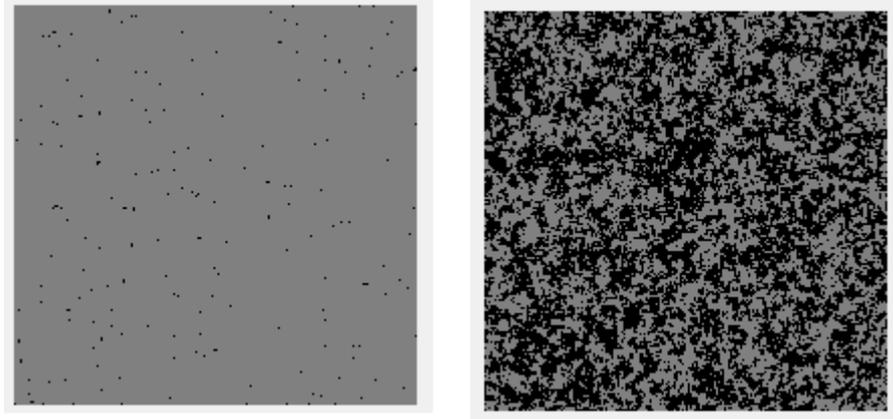


Figure 3.3: Typical configurations of the $2D$ Ising model. *Left*: for $T \ll T_c$ there are a few, spaced, flipped spins; *Right*: at $T \lesssim T_c$ we see a large number of domains with various sizes.

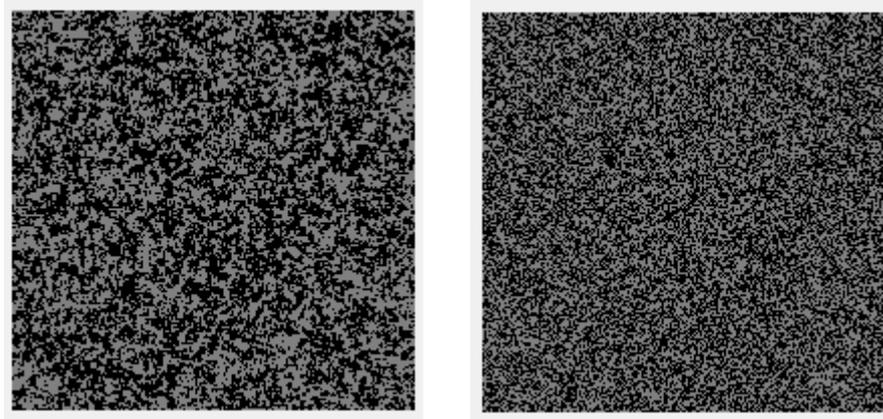


Figure 3.4: Typical configurations of the $2D$ Ising model. *Left*: at $T \gtrsim T_c$ the domains start to break down; *Right*: for $T \gg T_c$ there are no domains and the spins are randomly aligned.

Near the critical point the large wavelength excitations dominate, and thus the dynamics of the order parameter can be modelled by an effective model. A very well-known model for this situation is the Landau theory of phase transitions. Landau proposed that the order parameter, here assumed to be a scalar field $\phi(\mathbf{x})$, in the presence of an external source $J(\mathbf{x})$ obeys the Ginzburg-Landau Hamiltonian

$$H_{GL}[\phi, J] = \int d\mathbf{x} \left[\frac{1}{2} (\nabla\phi(\mathbf{x}))^2 + \frac{1}{2} r_0 \phi^2(\mathbf{x}) + \frac{1}{4!} u_0 \phi^4(\mathbf{x}) - J(\mathbf{x})\phi(\mathbf{x}) \right], \quad (3.6)$$

where $u_0 > 0$ and $r_0 = r_0(T)$, with $r_0(T_c) = 0$ for some T_c . This phenomenological Hamiltonian is constructed based on the following assumptions:

- i: The Hamiltonian should be symmetric under parity reversal $H_{GL}[\phi, J] \rightarrow H_{GL}[-\phi, -J]$. If we were dealing with vector or tensor fields group theoretical arguments should be taken into account;
- ii: Since we are interested only in the long wave-length fluctuations, $\phi(\mathbf{x})$ is slowly varying with respect to \mathbf{x} and we only keep the gradient term;
- iii: Near the critical point the order parameter is small, so quadratic and quartic powers should suffice to describe its behavior.

The partition function within this scheme is given by a functional integral

$$Z[J] = \int \mathcal{D}\phi e^{-\beta H_{GL}}, \quad (3.7)$$

which is usually impossible to evaluate analytically. Landau proposed it should be approximated by its most probable value using the saddle-point method:

$$Z[J] \approx e^{-\beta F_{GL}}, \quad F_{GL} = \min_{\phi} \{H_{GL}[\phi, J]\} \quad (3.8)$$

where F_{GL} is called the Landau free energy. The Landau theory, being a mean-field theory, only works in a small vicinity of the critical point because it neglects fluctuations. Despite this fact, it can still be used to obtain the critical behavior of the thermodynamical quantities, i.e., their critical exponents: near the phase transition physical quantities vary with the temperature as $|T - T_c|^\alpha$, for some real constant α .

3.1.2 Real time evolution

Let us now consider a system described by variables $\varphi_j(t)$, $j = 1, \dots, N$ that evolve according to

$$\Gamma \frac{\partial \varphi_j}{\partial t} = \frac{\partial F}{\partial \varphi_j} + \xi_j(t) \quad (3.9)$$

where $\langle \xi_i(t) \xi_j(t') \rangle = 2\Gamma T \delta(t - t')$ and Γ is a transport coefficient. Such a configuration of dynamical variables is equivalent to a thermodynamical system, close to equilibrium, at temperature T whose independent variables are the φ_j , $\Gamma_{ij} = 1/\Gamma \delta_{ij}$ and the forces L_j come from the gradient of

the Free Energy function $F = F(\{\varphi_j\})$,

$$dF = \frac{\partial F}{\partial \varphi_1} d\varphi_1 + \cdots + \frac{\partial F}{\partial \varphi_n} d\varphi_n. \quad (3.10)$$

This description can be used to model a n -dimensional lattice, or even a field, of ‘‘slow’’ varying variables [4], that is, when we are only interested in the long wavelength components. The Ginzburg-Landau-Langevin equation governing the evolution of a field usually comes from a coarse-graining of lattice variables or approximations for an order parameter in non-equilibrium quantum field theory, where the free energy function $F(\{\varphi_j(t)\})$ and the gradient $\partial/\partial\varphi_j$ are replaced by a functional $F = F[\varphi(\vec{x}, t)]$ and a functional derivative $\delta/\delta\varphi(\vec{x}, t)$,

$$\Gamma \frac{\partial \varphi}{\partial t} = \frac{\delta F}{\delta \varphi} + \xi(\vec{x}, t). \quad (3.11)$$

Where now the noise correlation is given by $\langle \xi(\vec{x}, t) \xi(\vec{x}', t') \rangle = 2\Gamma T \delta(t - t') \delta^n(\vec{x} - \vec{x}')$. Examples of active fields of study are effective models for the QCD phase transition. It is generally believed that the chiral symmetry is an approximate, spontaneously broken, symmetry of the strong interactions that would be restored at high temperatures and baryon densities [19]. Due to the non-zero masses of the light quarks, *up* and *down*, the chiral symmetry can not be exact, but since they are small, $1.7\text{MeV}/c^2 \leq m_u \leq 3.1\text{MeV}/c^2$ and $4.1\text{MeV}/c^2 \leq m_d \leq 5.7\text{MeV}/c^2$, it may be considered as an approximate symmetry of QCD.

Goldstone [20, 21], based on a previous work of Nambu [22], proved that when a continuous symmetry is spontaneously broken there must be a massless boson for each of the symmetry’s infinitesimal generators. If we restrict ourselves to the light quark sector and take $m_u = m_d = 0$ then chiral symmetry is exact in QCD and we may identify the Goldstone bosons with the π mesons. As $0 < m_u \approx m_d \ll \Lambda_{QCD}$, with Λ_{QCD} being the QCD energy scale, the chiral symmetry is inexact and the Goldstone bosons have a non-zero, but very small, mass $m_\pi \approx 0$.

In the pre-QCD era, Gell-Mann and Levy introduced [23] a model, called *linear sigma model*, to effectively describe the dynamical chiral symmetry breaking of the strong interactions. It consisted of a nucleon doublet coupled to one scalar (σ) and three pseudo-scalar fields. After QCD was established the model was changed: the nucleons were replaced by the light quarks u and d , the pseudo-scalar fields were identified

with the π mesons and $\sigma = \langle \bar{\psi}\psi \rangle = \langle 0|\bar{\psi}\psi|0 \rangle$ represents the vacuum quark condensate.

Experimental results show that high-energy heavy ion collisions produce a strongly interacting hadronic matter, known as quark-gluon plasma (QGP), that evolves like a low-viscosity fluid [24, 25, 26, 27, 28, 29]. A first approach for this phenomenon is to take the quarks and gluons to constitute a relativistic fluid in which the chiral fields σ and π^i , $i = 1, 2, 3$, propagate [30]. However, this formulation neglects quantum and thermal fluctuations of the chiral fields. Those act as noise sources and turn the field equations into stochastic differential equations in the form of Ginzburg-Landau-Langevin equations [31].

Applying the Schwinger-Keldysh closed-time-path effective action formalism to the linear sigma model [6] it is possible to obtain, after a few approximations, the GLL equations describing the evolution of the σ and $\vec{\pi}$ fields.

3.1.3 Fictitious time evolution

A system described by n variables or fields whose probability distribution has the Boltzmann form

$$P(\{\varphi\}) = \frac{1}{Z} \exp[-\alpha H(\{\varphi\})], \quad (3.12)$$

where Z is a normalization constant, α is a control parameter and H is a Hamiltonian, in which average values and correlation functions are given by

$$\langle \varphi_1 \cdots \varphi_m \rangle = \int [d\varphi] (\varphi_1 \cdots \varphi_m) P(\{\varphi\}) \quad (3.13)$$

can in principle be numerically simulated by generating a large number N of random configurations of the φ and sampling eq. (3.13) as

$$\langle \varphi_1 \cdots \varphi_m \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N (\varphi_1^n \cdots \varphi_m^n) P(\{\varphi^n\}), \quad (3.14)$$

where the superscript n indicates the n -th configuration generated. This is known as the Monte Carlo method. It is employed in a wide range of applications where it is not possible or too time consuming to evaluate the average values exactly.

An alternative way to numerically simulate eq. (3.13) is to consider it as the equilibrium distribution of a system evolving via a Ginzburg-

Landau-Langevin equation

$$\Gamma \frac{\partial \varphi_j}{\partial \tau} = \frac{\partial H}{\partial \varphi_j} + \xi_j(\tau), \quad (3.15)$$

in the case of a finite number variables or

$$\Gamma \frac{\partial \varphi}{\partial \tau} = \frac{\delta H}{\delta \varphi} + \xi(\vec{x}, \tau), \quad (3.16)$$

if the system is described by fields. The noise correlations are the same as in the real time evolution, except that we replace t by τ and T by α^{-1} . Here the name ‘‘fictitious time’’ evolution will be justified: τ is a dummy variable that used to generate the distribution $P(\{\varphi\})$ as limiting ($\tau \rightarrow \infty$) case. Since we have implicitly used the Fluctuation-Dissipation theorem by choosing $T = 1/\alpha$ the equilibrium distribution for the Fokker-Planck equation associated with, e.g., eq. (3.15) will have the equilibrium distribution

$$P_{eq}(\{\varphi_j\}) = \frac{1}{Z} \exp[-\alpha H(\{\varphi_j\})]. \quad (3.17)$$

Now, to simulate the correlation functions all we need to do is numerically solve the GLL equation (3.15) or (3.16) and look at its infinite-time limit:

$$\langle \varphi_1 \cdots \varphi_m \rangle = \lim_{\tau \rightarrow \infty} \langle \varphi_1(\tau) \cdots \varphi_m(\tau) \rangle. \quad (3.18)$$

The GLL equations (3.15) and (3.16) can also be used to study fluctuations around a phase transition using the Landau theory. We once again model the noise correlation proportional to the temperature T and identify H with the Ginzburg-Landau Hamiltonian H_{GL} .

3.2 Stochastic quantization

Stochastic quantization presents an alternative method to quantize non-relativistic and relativistic Euclidean (imaginary time) physical systems. The central idea is to embed the system into a higher dimensional space with an additional, fictitious, time dimension and postulate an evolution in this extra time obeying a Langevin equation. At the infinite fictitious time limit, stochastic averages coincide with quantum correlation functions [15]. We present here a review of the path integral quantization for quantum mechanics and quantum field theory and then show the equivalence with the stochastic quantization method.

3.2.1 Review of quantum mechanics

Let us take a look at non-relativistic quantum mechanics of a single particle in a one-dimensional space. Its state vector $|\psi(t)\rangle$ evolves according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad (3.19)$$

where \hat{H} is the Hamiltonian operator. If \hat{H} is time-independent then we may formally write, for $t > t_0$,

$$|\psi(t)\rangle = \exp \left[-\frac{i(t-t_0)\hat{H}}{\hbar} \right] |\psi(t_0)\rangle \equiv \hat{U}(t, t_0) |\psi(t_0)\rangle \quad (3.20)$$

in which we defined the time-evolution operator \hat{U} , and $|\psi(t_0)\rangle$ is an initial condition.

We wish to calculate the matrix elements of \hat{U} in the coordinate basis $|x\rangle$,

$$U(x, t; x_0, t_0) \equiv \langle x | \hat{U}(t, t_0) | x_0 \rangle \quad (3.21)$$

so the evolution of the wave function can be written as

$$\begin{aligned} \psi(x, t) &= \langle x | \psi(t) \rangle = \langle x | \hat{U}(t, t_0) | \psi(t_0) \rangle = \int dx_0 \langle x | \hat{U}(t, t_0) | x_0 \rangle \langle x_0 | \psi(t_0) \rangle \\ &= \int dx_0 U(x, t; x_0, t_0) \psi(x_0, t_0). \end{aligned} \quad (3.22)$$

However, in order to do computer simulations we must switch to Euclidean (imaginary) time $\tau = it$. In this context we have

$$\hat{U}(\tau, \tau_0) = \exp \left[-\frac{(\tau - \tau_0)\hat{H}}{\hbar} \right], \quad (3.23)$$

and

$$\begin{aligned} U(x, \tau; x_0, \tau_0) &= \langle x | \hat{U}(\tau, \tau_0) | x_0 \rangle = \langle x | e^{-(\tau - \tau_0)\hat{H}/\hbar} | x_0 \rangle \\ &= \langle x | e^{-\tau\hat{H}/\hbar} e^{\tau_0\hat{H}/\hbar} | x_0 \rangle = {}_H \langle x, \tau | x_0, \tau_0 \rangle_H \end{aligned} \quad (3.24)$$

where $|x, \tau\rangle_H$ is the eigenvector of the (Euclidean time) Heisenberg operator $\hat{X}(\tau)$

$$\hat{X}(\tau) |x, \tau\rangle_H = x |x, \tau\rangle_H. \quad (3.25)$$

Let us return to the evolution of the matrix elements of \hat{U} . We split the time interval $\tau - \tau_0$ in N equal slices $\varepsilon = (\tau - \tau_0)/N \ll (\tau - \tau_0)$, so that

$$U(x, \tau; x_0, \tau_0) = \langle x | \underbrace{e^{-\varepsilon\hat{H}/\hbar} \dots e^{-\varepsilon\hat{H}/\hbar}}_{N \text{ times}} | x_0 \rangle, \quad (3.26)$$

and insert $N - 1$ complete sets of states $\int dx' |x'\rangle \langle x'| = \mathbf{1}$ as

$$\begin{aligned} U(x, \tau; x_0, \tau_0) &= \int dx_1 \cdots dx_{N-1} \langle x | e^{-\varepsilon \hat{H}/\hbar} | x_{N-1} \rangle \times \\ &\quad \langle x_{N-1} | e^{-\varepsilon \hat{H}/\hbar} | x_{N-2} \rangle \cdots \langle x_1 | e^{-\varepsilon \hat{H}/\hbar} | x_0 \rangle \\ &= \int dx_1 \cdots dx_{N-1} U(x, \tau; x_{N-1}, \tau_{N-1}) \cdots U(x_1, \tau_1; x_0, \tau_0), \end{aligned} \quad (3.27)$$

where $\tau_n = \tau_0 + n\varepsilon$. We see that each of the above factors has the same structure, namely the probability amplitude for the particle to go from the position x_i to x_{i+1} over the small time interval ε . In particular, if the Hamiltonian operator has the usual form

$$\hat{H} = \frac{1}{2m} \hat{P}^2 + V(\hat{X}) \quad (3.28)$$

the matrix element $U(x_i, \tau_i; x_{i-1}, \tau_{i-1})$ can be written as

$$U(x_i, \tau_i; x_{i-1}, \tau_{i-1}) = \langle x_i | \exp\left(-\varepsilon \frac{\hat{P}^2}{2m\hbar}\right) | x_{i-1} \rangle \exp\left[-\varepsilon \frac{1}{\hbar} V\left(\frac{x_i + x_{i-1}}{2}\right)\right] \quad (3.29)$$

where we have used the Weyl ordering for the operator $V(\hat{X})$, i.e.,

$$\langle x | V^n(\hat{X}) | y \rangle = V^n\left(\frac{x+y}{2}\right) \langle x | y \rangle. \quad (3.30)$$

To deal with the remaining inner product we introduce a complete set of momentum states and use the relation $\langle p | x \rangle = (2\pi\hbar)^{-1/2} e^{-ipx/\hbar}$

$$\begin{aligned} U(x_i, \tau_i; x_{i-1}, \tau_{i-1}) &= \int dp_i \langle x_i | p_i \rangle \langle p_i | x_{i-1} \rangle e^{-\varepsilon \frac{p_i^2}{2m\hbar}} e^{-\varepsilon \frac{1}{\hbar} V\left(\frac{x_i + x_{i-1}}{2}\right)} \\ &= \frac{1}{2\pi\hbar} e^{-\varepsilon \frac{1}{\hbar} V\left(\frac{x_i + x_{i-1}}{2}\right)} \int dp_i e^{-\varepsilon \frac{p_i^2}{2m\hbar} + i \frac{p_i(x_i - x_{i-1})}{\hbar}} \\ &= \frac{1}{2\pi\hbar} \sqrt{\frac{2m\pi\hbar}{\varepsilon}} e^{-\frac{(x_i - x_{i-1})^2}{\hbar^2} \frac{2m\hbar}{4\varepsilon} - \varepsilon \frac{1}{\hbar} V\left(\frac{x_i + x_{i-1}}{2}\right)} \\ &= \sqrt{\frac{m}{2\pi\hbar\varepsilon}} e^{-\frac{\varepsilon}{\hbar} \left[\frac{m}{2} \left(\frac{x_i - x_{i-1}}{\varepsilon}\right)^2 + V\left(\frac{x_i + x_{i-1}}{2}\right) \right]}. \end{aligned} \quad (3.31)$$

Finally,

$$\begin{aligned} U(x, \tau; x_0, \tau_0) &= \int \prod_{i=1}^N dx_i U(x_i, \tau_i; x_{i-1}, \tau_{i-1}) \\ &= \left[\frac{m}{2\pi\hbar\varepsilon} \right]^{N/2} \int \prod_{i=1}^N dx_i e^{-\frac{\varepsilon}{\hbar} \sum_{i=1}^N \left[\frac{m}{2} \left(\frac{x_i - x_{i-1}}{\varepsilon}\right)^2 + V\left(\frac{x_i + x_{i-1}}{2}\right) \right]}, \end{aligned} \quad (3.32)$$

in which we made the identification $x_N \equiv x$. If we let $N \rightarrow \infty$ and $\varepsilon \rightarrow 0$ as to keep $N\varepsilon = \tau - \tau_0$ we can identify the term inside the exponential with minus the classical Euclidean Action functional, divided by \hbar

$$\frac{S_E}{\hbar} = \int_{\tau_0}^{\tau} d\tau' L_E = \int_{\tau_0}^{\tau} d\tau' \left[\frac{m}{2} \left(\frac{dx}{d\tau'} \right)^2 + V(x) \right], \quad (3.33)$$

where

$$\frac{x_i - x_{i-1}}{\varepsilon} \rightarrow \frac{dx}{d\tau'}$$

and

$$\sum_i \varepsilon L_E \left(\frac{x_i - x_{i-1}}{\varepsilon}, \frac{x_i + x_{i-1}}{2} \right) \rightarrow \int d\tau L_E(\dot{x}, x).$$

Thus we find that the propagator $U(x, \tau; x_0, \tau_0)$ is given by the famous Feynman path integral formula

$$\begin{aligned} U(x, \tau; x_0, \tau_0) &= \lim_{\substack{\varepsilon \rightarrow 0 \\ N \rightarrow \infty}} \left[\frac{m}{2\pi\hbar\varepsilon} \right]^{N/2} \int \prod_{i=1}^N dx_i e^{-\frac{\varepsilon}{\hbar} \sum_{i=1}^N \left[\frac{m}{2} \left(\frac{x_i - x_{i-1}}{\varepsilon} \right)^2 + V\left(\frac{x_i + x_{i-1}}{2} \right) \right]} \\ &\equiv A \int_{x_0, \tau_0}^{x, \tau} \mathcal{D}x e^{-\frac{1}{\hbar} S_E}. \end{aligned} \quad (3.34)$$

This formula not only says that the evolution of the particle from x_0 to x is a weighted sum of all possible histories with endpoints x_0 and x , but also makes explicit use of the *classical* action in quantum mechanics.

Expectation values may, within this framework, be evaluated as

$$\begin{aligned} &\langle \psi | \hat{X}(\tau_N) \cdots \hat{X}(\tau_1) | \psi \rangle \\ &= \int dx_1 \cdots dx_N dx_i dx_f \langle \psi | x_f, \tau_f \rangle \langle x_f, \tau_f | \hat{X}(\tau_N) | x_N, \tau_N \rangle \cdots \langle x_i, \tau_i | \psi \rangle \\ &= \int dx_1 \cdots dx_N dx_i dx_f x_1 \cdots x_N \psi^*(x_f, \tau_f) \psi(x_i, \tau_i) \langle x_f, \tau_f | x_N, \tau_N \rangle \cdots \langle x_1, \tau_1 | x_i, \tau_i \rangle \\ &= \int dx_1 \cdots dx_N dx_i dx_f x_1 \cdots x_N \psi^*(x_f, \tau_f) \psi(x_i, \tau_i) \\ &\quad \times \left[A \int_{x_i, \tau_i}^{x_1, \tau_1} \mathcal{D}x e^{-\frac{1}{\hbar} S_E} \right] \left[A \int_{x_1, \tau_1}^{x_2, \tau_2} \mathcal{D}x e^{-\frac{1}{\hbar} S_E} \right] \cdots \left[A \int_{x_N, \tau_N}^{x_f, \tau_f} \mathcal{D}x e^{-\frac{1}{\hbar} S_E} \right], \end{aligned} \quad (3.35)$$

for $\tau_N > \tau_{N-1} > \cdots > \tau_1$, where the above expression consists of a path integral (PI) from the initial position x_0 to an arbitrary point x_1 and a series of PI's from an arbitrary point to another and finally to x_N . In other words, we are integrating over paths that start at x_0 , go through all x_i 's, $i = 1, \dots, N-1$, and end at x_N and then integrate over all

intermediate points. So, in fact, we are integrating over *all* paths. Writing this out explicitly,

$$\begin{aligned}
& \langle \psi | \hat{X}(\tau_N) \cdots \hat{X}(\tau_1) | \psi \rangle = \\
& \lim_{\substack{\varepsilon \rightarrow 0 \\ N' \rightarrow \infty}} \left[\frac{m}{2\pi\hbar\varepsilon} \right]^{NN'/2} \int dx_i dx_f dx_1 \cdots dx_N x_1 \cdots x_N \psi^*(x_f, \tau_f) \psi(x_i, \tau_i) \\
& \times \int dx_1^1 \cdots dx_1^{N'} \exp \left[-\frac{\varepsilon}{\hbar} \sum_{\tau_i}^{\tau_1} L_E \right] \times \int dx_2^1 \cdots dx_2^{N'} \exp \left[-\frac{\varepsilon}{\hbar} \sum_{\tau_1}^{\tau_2} L_E \right] \\
& \times \cdots \times \int dx_N^1 \cdots dx_N^{N'} \exp \left[-\frac{\varepsilon}{\hbar} \sum_{\tau_N}^{\tau_f} L_E \right] \tag{3.36}
\end{aligned}$$

$$\begin{aligned}
& \langle \psi | \hat{X}(\tau_N) \cdots \hat{X}(\tau_1) | \psi \rangle = \\
& = \lim_{\substack{\varepsilon \rightarrow 0 \\ N' \rightarrow \infty}} \left[\frac{m}{2\pi\hbar\varepsilon} \right]^{NN'/2} \int dx_i dx_f \psi^*(x_f, \tau_f) \psi(x_i, \tau_i) \\
& \times \int [dx_1^0 \cdots dx_1^{N'}] [dx_2^0 \cdots dx_2^{N'}] \cdots [dx_N^0 \cdots dx_N^{N'}] x_1 \cdots x_N \\
& \times \exp \left[-\frac{\varepsilon}{\hbar} \sum_{\tau_i}^{\tau_f} L_E \right] \\
& = A \int dx_i dx_f \psi^*(x_f, \tau_f) \psi(x_i, \tau_i) \int_{x_i, \tau_i}^{x_f, \tau_f} \mathcal{D}x x(\tau_1) \cdots x(\tau_N) e^{-\frac{1}{\hbar} S_E}. \tag{3.37}
\end{aligned}$$

Thus, the factor $x_1 \cdots x_{N-1}$ can be incorporated into the PI by including the term $x(\tau_1) \cdots x(\tau_{N-1})$. The normalization constant N reads

$$\begin{aligned}
N^{-1} &= \langle \psi | \psi \rangle = \int dx \langle \psi | x, \tau \rangle \langle x, \tau | \psi \rangle = \int dx dx' \langle \psi | x, \tau \rangle \langle x, \tau | x', \tau' \rangle \langle x', \tau' | \psi \rangle \\
&= A \int dx dx' \psi^*(x) \psi(x') \int_{x', \tau'}^{x, \tau} \mathcal{D}x e^{-\frac{1}{\hbar} S_E}. \tag{3.38}
\end{aligned}$$

Differently from canonical quantization where we promote classical dynamic variables to operators and postulate the Schrödinger or Heisenberg equations of motion, in the Path Integral formulation expectation values can be computed from the classical Lagrangian making no reference to operators.

Generalization to n dimensions is straightforward: the Heisenberg position and momentum operators are $\hat{\mathbf{X}}(\tau)$ and $\hat{\mathbf{P}}(\tau)$, with eigenvectors $|\mathbf{x}, \tau\rangle$ and $|\mathbf{p}, \tau\rangle$, respectively. Their commutation relation is

$$[\hat{\mathbf{X}}, \hat{\mathbf{P}}] = i\hbar \mathbf{1}_n, \tag{3.39}$$

where $\mathbf{1}_n$ is the $n \times n$ identity matrix, and $\langle \mathbf{p} | \mathbf{x} \rangle = (2\pi\hbar)^{-n/2} e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}$. With these considerations the algebra that led to the Path Integral formulation gives for the n -dimensional evolution operator

$$U(\mathbf{x}, \tau; \mathbf{x}_0, \tau_0) = A \int_{\mathbf{x}_0, \tau_0}^{\mathbf{x}, \tau} \mathcal{D}\mathbf{x} e^{-\frac{i}{\hbar} S_E}. \quad (3.40)$$

3.2.2 Quantum Field Theory

The necessity of fields came up when quantum mechanics and special relativity were combined to give a correct quantum treatment of the electromagnetic field. Photons arose as the excitations of the EM field that mediate the interaction between electric charges and served as prototype to describe the other elementary particles using fields. Through the years the strong and the weak interactions were also put in the language of quantum fields and consolidated in the Standard Model of Elementary Particles.

At each space-time point \mathbf{x} the field $\phi(\mathbf{x})$ assumes a definite value. We call this a field configuration. Let us start with a classical field in Euclidean space. Following Hamilton's principle, the field evolves according to the Euler-Lagrange equation

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} - \frac{\partial \mathcal{L}}{\partial \phi} = 0, \quad (3.41)$$

where repeated indices are summed from 1 to $n+1$, n being the number of space dimensions, and $\mathcal{L}(\phi, \partial_\mu \phi)$ is the Lagrangian density for the field, i.e., $L = \int d^n x \mathcal{L}$. The momentum field conjugated to $\phi(\mathbf{x})$ is defined as

$$\pi(\mathbf{x}) = \frac{\partial \mathcal{L}}{\partial(\partial_t \phi)}.$$

The Hamiltonian density is defined as the Legendre transform of the Lagrangian density

$$\mathcal{H}(\pi, \phi) = \sup_{\partial_t \phi} [\pi \partial_t \phi - \mathcal{L}], \quad (3.42)$$

from which we define the Hamiltonian as $H = \int d^n x \mathcal{H}$. Following the non-relativistic canonical quantization we promote the field and its conjugated momentum field to operators $\Phi(\mathbf{x}, t)$ and $\Pi(\mathbf{x}, t)$, respectively, obeying Heisenberg equations of motion

$$-i\hbar \dot{\Phi} = [H, \Phi], \text{ and} \quad (3.43)$$

$$-i\hbar \dot{\Pi} = [H, \Pi], \quad (3.44)$$

and the equal-time canonical commutation relations

$$[\Phi(\mathbf{x}, t), \Pi(\mathbf{y}, t)] = i\hbar\delta^n(\mathbf{x} - \mathbf{y}) \quad (3.45)$$

$$[\Phi(\mathbf{x}, t), \Phi(\mathbf{y}, t)] = 0 \quad (3.46)$$

$$[\Pi(\mathbf{x}, t), \Pi(\mathbf{y}, t)] = 0. \quad (3.47)$$

The field operators eigenstates and eigenvalues are

$$\Phi(\mathbf{x}, t)|\phi(\mathbf{x}), t\rangle = \phi(\mathbf{x})|\phi(\mathbf{x}), t\rangle \quad (3.48)$$

$$\Pi(\mathbf{x}, t)|\pi(\mathbf{x}), t\rangle = \pi(\mathbf{x})|\pi(\mathbf{x}), t\rangle. \quad (3.49)$$

The formal solution to eq. (3.43) is

$$\Phi(\mathbf{x}, t) = e^{iH(t-t_0)/\hbar}\Phi(\mathbf{x}, t_0)e^{-iH(t-t_0)/\hbar} \equiv U^\dagger(t, t_0)\Phi(\mathbf{x}, t_0)U(t, t_0) \quad (3.50)$$

where $\Phi(\mathbf{x}, t_0)$ is some initial condition, and U is again the time evolution operator.

The probability amplitude for a given field eigenstate $|\phi', t'\rangle$ to evolve to another state $|\phi, t\rangle$ is similar to the non-relativistic case

$$\langle\phi(\mathbf{x}), t|\phi'(\mathbf{x}), t'\rangle = \langle\phi(\mathbf{x})|e^{-iH(t-t_0)/\hbar}|\phi'(\mathbf{x})\rangle = \langle\phi(\mathbf{x})|U(t, t')|\phi'(\mathbf{x})\rangle. \quad (3.51)$$

In order to make the similarity clearer and facilitate the calculations, we discretize the space-time in a hypercubic lattice. The field operators $\Phi(\mathbf{x}, t)$ and $\Pi(\mathbf{x}, t)$ become $\Phi_{\mathbf{m}}(t)$ and $\Pi_{\mathbf{m}}(t)$, respectively, where $\mathbf{m} = a\mathbf{x}$ indicates the lattice point and a is the lattice spacing. The above relations now read

$$[\Phi_{\mathbf{m}}(t), \Pi_{\mathbf{m}'}(t)] = i\hbar a^{-n}\delta_{\mathbf{m}\mathbf{m}'} \quad (3.52)$$

$$[\Phi_{\mathbf{m}}(t), \Phi_{\mathbf{m}'}(t)] = 0 \quad (3.53)$$

$$[\Pi_{\mathbf{m}}(t), \Pi_{\mathbf{m}'}(t)] = 0 \quad (3.54)$$

$$\Phi_{\mathbf{m}}(t)|\phi_{\mathbf{m}}, t\rangle = \phi_{\mathbf{m}}|\phi_{\mathbf{m}}, t\rangle \quad (3.55)$$

$$\Pi_{\mathbf{m}}(t)|\pi_{\mathbf{m}}, t\rangle = \pi_{\mathbf{m}}|\pi_{\mathbf{m}}, t\rangle \quad (3.56)$$

$$\langle\phi_{\mathbf{m}}, t|\phi'_{\mathbf{m}}, t'\rangle = \langle\phi_{\mathbf{m}}|U(t, t')|\phi'_{\mathbf{m}}\rangle. \quad (3.57)$$

From here on we once again switch to imaginary time $\tau = it$. For each lattice point \mathbf{m}_0 the field operator $\Phi_{\mathbf{m}_0}(\tau)$ is analogous to the position operator $\hat{X}(\tau)$, such that we can interpret $\Phi_{\mathbf{m}}(\tau)$ as $\hat{\mathbf{X}}(\tau)$ and the similarity is now obvious. Using

$$\langle\phi_{\mathbf{m}}, \tau|\pi_{\mathbf{m}}, \tau\rangle = (2\pi\hbar)^{n/2} \exp\left[\frac{i}{\hbar} \sum_{\mathbf{m}} \pi_{\mathbf{m}}\phi_{\mathbf{m}}\right] \quad (3.58)$$

the transition amplitude for field states is

$$\langle \phi_{\mathbf{m}}, \tau | \phi'_{\mathbf{m}}, \tau' \rangle = A \int \prod_{\mathbf{m}} \mathcal{D}\phi_{\mathbf{m}} \exp \left[-\frac{a^n}{\hbar} \sum_{\mathbf{m}} \mathcal{L}_{\mathbf{m}} \right] \quad (3.59)$$

where $\mathcal{L}_{\mathbf{m}}$ is the discretized version of the Lagrangian density. Turning back to the continuum limit we have

$$\langle \phi(\mathbf{x}, \tau | \phi'(\mathbf{x}), \tau' \rangle = A' \int \mathcal{D}\phi e^{-S_E/\hbar}, \quad (3.60)$$

$$S_E = \int_{\tau'}^{\tau} d\tau'' \int d^n x \mathcal{L}_E. \quad (3.61)$$

Proceeding with the analogy we may write for the correlation functions

$$\begin{aligned} & \langle \phi(\mathbf{x}), \tau | \Phi(\mathbf{x}_{N-1}, \tau_{N-1}) \cdots \Phi(\mathbf{x}_1, \tau_1) | \phi'(\mathbf{x}), \tau' \rangle \\ &= A' \int \mathcal{D}\phi \phi(\mathbf{x}_{N-1}) \cdots \phi(\mathbf{x}_1) e^{-S_E/\hbar}. \end{aligned} \quad (3.62)$$

Now, in quantum field theory we are usually interested in vacuum-to-vacuum transition amplitudes, i.e., no particles in the infinite past, then particles are created, interact, and are later annihilated. To evaluate such amplitudes, let us assume the Hamiltonian has a discrete spectrum, for simplicity, with E_m being the eigenvalues corresponding to the eigenstates $|m\rangle$, $m \geq 0$, and insert complete sets of energy eigenstates on eq. (3.62)

$$\begin{aligned} & \sum_{m, m' \geq 0} \langle \phi(x), \tau | m \rangle \langle m | \Phi(x_{N-1}, \tau_{N-1}) \cdots \Phi(x_1, \tau_1) | m' \rangle \langle m' | \phi'(x), \tau' \rangle \\ &= \sum_{m, m' \geq 0} \langle m | \Phi(x_{N-1}, \tau_{N-1}) \cdots \Phi(x_1, \tau_1) | m' \rangle \\ & \quad \times \langle \phi(x), \tau_0 | e^{-H(\tau-\tau_0)/\hbar} | m \rangle \langle m' | e^{H(\tau'-\tau_0)/\hbar} | \phi'(x), \tau_0 \rangle \\ &= \sum_{m, m' \geq 0} \langle m | \Phi(x_{N-1}, \tau_{N-1}) \cdots \Phi(x_1, \tau_1) | m' \rangle \\ & \quad \times \langle \phi(x), \tau_0 | m \rangle \langle m' | \phi'(x), \tau_0 \rangle e^{-E_m(\tau-\tau_0)/\hbar} e^{E_{m'}(\tau'-\tau_0)/\hbar} \end{aligned} \quad (3.63)$$

Due to Lorentz invariance the vacuum state energy E_0 must be zero, since it is annihilated by the momentum operator $P_\mu |0\rangle = 0$, with $P_{n+1} = H$. So, in the infinite time limit, $\tau \rightarrow \infty$, $\tau' \rightarrow -\infty$, only the ground state will contribute

$$\begin{aligned} & \lim_{\substack{\tau \rightarrow \infty \\ \tau' \rightarrow -\infty}} \langle \phi(\mathbf{x}), \tau | \Phi(\mathbf{x}_{N-1}, \tau_{N-1}) \cdots \Phi(\mathbf{x}_1, \tau_1) | \phi'(\mathbf{x}), \tau' \rangle \\ &= \langle \phi(x), \tau_0 | 0 \rangle \langle 0 | \phi'(x), \tau_0 \rangle \langle 0 | \Phi(x_{N-1}, \tau_{N-1}) \cdots \Phi(x_1, \tau_1) | 0 \rangle. \end{aligned} \quad (3.64)$$

Thus, vacuum correlation functions may be written using Path Integrals as

$$\begin{aligned}
& \langle 0 | \Phi(x_{N-1}, \tau_{N-1}) \cdots \Phi(x_1, \tau_1) | 0 \rangle \\
&= \lim_{\substack{\tau' \rightarrow \infty \\ \tau' \rightarrow -\infty}} \frac{\langle \phi(\mathbf{x}), \tau | \Phi(\mathbf{x}_{N-1}, \tau_{N-1}) \cdots \Phi(\mathbf{x}_1, \tau_1) | \phi'(\mathbf{x}), \tau' \rangle}{\langle \phi(\mathbf{x}), \tau | \phi'(\mathbf{x}), \tau' \rangle} \\
&= \frac{\int \mathcal{D}\phi \phi(\mathbf{x}_{N-1}) \cdots \phi(\mathbf{x}_1) \exp \left[-\frac{1}{\hbar} \int_{-\infty}^{\infty} dt L \right]}{\int \mathcal{D}\phi \exp \left[-\frac{1}{\hbar} \int_{-\infty}^{\infty} dt L \right]}, \tag{3.65}
\end{aligned}$$

and we see that the (infinite) normalization constant cancels out.

It is possible to define a generating functional for the vacuum correlation functions as follows: we introduce a classical source field $J(x)$ to our Lagrangian density

$$\mathcal{L} \rightarrow \mathcal{L} + J(x)\phi(x) \equiv \mathcal{L}[J] \tag{3.66}$$

and define

$$Z[J] \equiv \langle 0 | 0 \rangle_J \equiv A \int \mathcal{D}\phi \exp \left[-\frac{1}{\hbar} \int_{-\infty}^{\infty} dt \int d^n x \mathcal{L}[J] \right]. \tag{3.67}$$

Then the vacuum-to-vacuum transition amplitudes are calculated as

$$\begin{aligned}
& \langle 0 | \Phi(x_{N-1}, \tau_{N-1}) \cdots \Phi(x_1, \tau_1) | 0 \rangle \\
&= \frac{(-\hbar)^n}{Z[J]} \frac{\delta^n}{\delta J(x_{N-1}, \tau_{N-1}) \cdots \delta J(x_1, \tau_1)} Z[J] \Big|_{J=0} \tag{3.68}
\end{aligned}$$

where each functional derivative brings down a factor $(-\hbar\phi)$.

3.2.3 Parisi and Wu's method

Vacuum transition amplitudes are similar to statistical averages of a given probability distribution,

$$\langle f(x) \rangle = \int d^n x f(x) P(x), \tag{3.69}$$

for a finite number n of variables or

$$\langle f(x) \rangle = \int \mathcal{D}x f(x) P(x), \tag{3.70}$$

if we have an infinite number of degrees of freedom. Correlation functions in QFT have the probability distribution

$$P = \exp \left[-\frac{1}{\hbar} \int_{-\infty}^{\infty} dt L \right] = \exp \left[-\frac{1}{\hbar} S_E \right], \tag{3.71}$$

i.e., a Boltzmann-weighted distribution. Recalling from section 3.1.3 such distribution can be thought of as the equilibrium distribution for the Fokker-Planck equation

$$\frac{\partial P}{\partial T} = \int d^n x \frac{\delta}{\delta \phi} \left[-\frac{\delta S_E}{\delta \phi} P + \hbar \frac{\delta P}{\delta \phi} \right] \quad (3.72)$$

as $T \rightarrow \infty$. Parisi and Wu [7] proposed that vacuum amplitudes could be calculated as

$$\langle \phi(x_1) \cdots \phi(x_n) \rangle = \lim_{T \rightarrow \infty} \langle \phi(x_1, T) \cdots \phi(x_n, T) \rangle \quad (3.73)$$

if $\phi(x, T)$ obeyed the Ginzburg-Landau-Langevin SDE

$$\frac{\partial \phi}{\partial T} = -\frac{\delta S_E}{\delta \phi} + \xi(x, T) \quad (3.74)$$

with

$$\langle \xi(x, T) \rangle = 0, \quad (3.75)$$

and

$$\langle \xi(x, T) \xi(x', T') \rangle = 2\hbar \delta(x - x') \delta(T - T'). \quad (3.76)$$

This, as in section 3.1.3 makes use of a fictitious time variable to obtain correlation functions, which may be used numerically as an alternative to Monte Carlo methods. It should be stressed that despite the noise intensity being proportional to \hbar this method does not use the noise to model unknown ‘‘hidden variables’’ - it just accounts for the inherent randomness of quantum mechanics.

To illustrate the method of stochastic quantization we calculate the energy gap $\Delta E = E_1 - E_0$ between the ground state and first excited state of the harmonic oscillator using canonical, path-integral and stochastic quantization and compare them. We will show that

$$\Delta(t, t') = \langle 0 | T \left\{ \hat{X}(t) \hat{X}(t') \right\} | 0 \rangle \propto e^{-i\Delta E |t - t'| / \hbar}, \quad (3.77)$$

or, in imaginary time,

$$\Delta(\tau, \tau') = \langle 0 | T \left\{ \hat{X}(\tau) \hat{X}(\tau') \right\} | 0 \rangle \propto e^{-\Delta E |\tau - \tau'| / \hbar}, \quad (3.78)$$

where T represents the time-ordering operator. For simplicity we will derive the correlation function Δ in Fourier space,

$$\Delta(\omega, \omega') \propto \frac{1}{(\Delta E)^2 + (\hbar\omega)^2} \delta(\omega + \omega'). \quad (3.79)$$

Canonical quantization

By using standard methods [32] we can write the harmonic oscillator hamiltonian, in real time, with ladder operators \hat{a} and \hat{a}^\dagger ,

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\bar{\omega}^2\hat{X}^2 = \hbar\bar{\omega}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \quad (3.80)$$

with eigenstates $|n\rangle$ such that

$$\hat{H}|n\rangle = \hbar\bar{\omega}\left(n + \frac{1}{2}\right)|n\rangle. \quad (3.81)$$

For $t > t'$ we may write

$$\begin{aligned} \Delta(t, t') &= \langle 0|\hat{X}(t)\hat{X}(t')|0\rangle = e^{iE_0(t-t')/\hbar}\langle 0|\hat{X}e^{-i\hat{H}(t-t')/\hbar}\hat{X}|0\rangle \\ &= e^{iE_0(t-t')/\hbar}\sum_n\left|\langle n|\hat{X}|0\rangle\right|^2 e^{-iE_n(t-t')/\hbar} \\ &= \frac{\hbar e^{iE_0(t-t')/\hbar}}{2m\bar{\omega}}\sum_n\left|\langle n|(\hat{a} + \hat{a}^\dagger)|0\rangle\right|^2 e^{-iE_n(t-t')/\hbar} \end{aligned} \quad (3.82)$$

where we have used a complete set of eigenstates $\sum_n|n\rangle\langle n| = \mathbf{1}$. Since $\hat{a}|0\rangle = 0$ and $\hat{a}^\dagger|0\rangle = |1\rangle$ only the $n = 1$ term contributes to the above sum and

$$\Delta(t, t') = \frac{\hbar}{2m\bar{\omega}}e^{iE_0(t-t')/\hbar}e^{-iE_1(t-t')/\hbar} = \frac{\hbar}{2m\bar{\omega}}e^{-i\bar{\omega}(t-t')}. \quad (3.83)$$

Equivalently, for $t' > t$

$$\Delta(t, t') = \frac{\hbar}{2m\bar{\omega}}e^{-i\bar{\omega}(t'-t)}, \quad (3.84)$$

and so

$$\Delta(t, t') = \frac{\hbar}{2m\bar{\omega}}e^{-i\bar{\omega}|t-t'|} = \frac{\hbar}{2m\bar{\omega}}\begin{cases} e^{-i\bar{\omega}(t-t')}, & \text{for } t > t' \\ e^{-i\bar{\omega}(t'-t)}, & \text{for } t' > t \end{cases}. \quad (3.85)$$

Switching to imaginary time $\tau = it$ we have

$$\Delta(\tau, \tau') = \frac{\hbar}{2m\bar{\omega}}e^{-\bar{\omega}|\tau-\tau'|} = \frac{\hbar}{2m\bar{\omega}}e^{-\Delta E|\tau-\tau'|}, \quad (3.86)$$

and performing the double Fourier in τ and τ' transform gives

$$\Delta(\omega, \omega') = \frac{2\pi\hbar}{m}\frac{1}{(\bar{\omega}^2 + \omega^2)}\delta(\omega + \omega'), \quad (3.87)$$

as expected, from which we extract $\Delta E = \hbar\bar{\omega}$.

Path-integral quantization

By following the same steps that lead to the vacuum-to-vacuum correlation functions in quantum field theory we may write for the quantum harmonic oscillator

$$\langle 0|T \left\{ \hat{X}(\tau_N) \cdots \hat{X}(\tau_1) \right\} |0\rangle = \frac{\int \mathcal{D}x x(\tau_N) \cdots x(\tau_1) e^{-S_E/\hbar}}{\int \mathcal{D}x e^{-S_E/\hbar}}, \quad (3.88)$$

or, for $N = 2$,

$$\Delta(\tau, \tau') = \frac{\int \mathcal{D}x x(\tau)x(\tau') e^{-S_E/\hbar}}{\int \mathcal{D}x e^{-S_E/\hbar}}, \quad (3.89)$$

with the imaginary time classical action

$$S_E = \int d\tau'' x(\tau) \left[\frac{m}{2} \frac{d^2}{d\tau''^2} + \frac{m}{2} \bar{\omega}^2 \right] x(\tau). \quad (3.90)$$

Adding to S_E a source term J

$$S_E[J] = S_E - \int d\tau'' J(\tau'')x(\tau'') \quad (3.91)$$

we write the correlation function as

$$\begin{aligned} \Delta(\tau, \tau') &= \frac{(-\hbar)^2}{Z[J]} \frac{\delta^n}{\delta J(\tau)\delta J(\tau')} Z[J] \Big|_{J=0} \\ &= \frac{(-\hbar)^2}{Z[0]} \frac{\delta^n}{\delta J(\tau)\delta J(\tau')} \int \mathcal{D}x e^{-S_E[J]/\hbar} \Big|_{J=0}, \end{aligned} \quad (3.92)$$

Writing $x(\tau)$ and $J(\tau)$ as the Fourier transforms of $\tilde{x}(\omega)$ and $\tilde{J}(\omega)$, respectively,

$$\begin{pmatrix} x(\tau) \\ J(\tau) \end{pmatrix} = \int d\omega e^{-i\omega\tau} \begin{pmatrix} \tilde{J}(\omega) \\ \tilde{x}(\omega) \end{pmatrix}, \quad (3.93)$$

we have

$$S_E = \int d\omega'' \tilde{x}(\omega'') \left[\frac{m}{2} \omega''^2 + \frac{m}{2} \bar{\omega}^2 \right] \tilde{x}(-\omega'') - \int d\omega'' \tilde{J}(\omega'') \tilde{x}(-\omega''). \quad (3.94)$$

Since the action is quadratic in \tilde{x} we may easily evaluate $Z[\tilde{J}]$ to be

$$Z[\tilde{J}] = N \exp \left[-\frac{\pi}{m\hbar} \int d\omega'' \frac{\tilde{J}(\omega'')\tilde{J}(-\omega'')}{\omega''^2 + \bar{\omega}^2} \right], \quad (3.95)$$

which gives for $\Delta(\omega, \omega')$

$$\Delta(\omega, \omega') = \frac{2\pi\hbar}{m} \frac{1}{\omega^2 + \bar{\omega}^2} \delta(\omega + \omega') \quad (3.96)$$

Stochastic quantization

Next, we evaluate $\Delta(\tau, \tau')$ by solving the Langevin equation

$$\frac{\partial x}{\partial T} = -\frac{\delta S_E}{\delta x} + \xi(T, \tau) = m\frac{\partial^2 x}{\partial \tau^2} - m\bar{\omega}^2 x + \xi \quad (3.97)$$

for $x = x(T, \tau)$ and then taking the limit $T \rightarrow \infty$ of the noise averaged correlation function $\langle x(T, \tau)x(T, \tau') \rangle$, that is,

$$\Delta(\tau, \tau') = \lim_{T \rightarrow \infty} \langle x(T, \tau)x(T, \tau') \rangle. \quad (3.98)$$

We work in Fourier space, i.e.,

$$\begin{pmatrix} x(T, \tau) \\ \xi(T, \tau) \end{pmatrix} = \int d\omega e^{-i\omega\tau} \begin{pmatrix} \tilde{x}(T, \omega) \\ \tilde{\xi}(T, \omega) \end{pmatrix}, \quad (3.99)$$

which gives us

$$\frac{\partial \tilde{x}}{\partial T} = -m(\omega^2 + \bar{\omega}^2) \tilde{x} + \tilde{\xi} \quad (3.100)$$

and has

$$\tilde{x}(T, \omega) = \tilde{x}_0 e^{-pT} + e^{-pT} \int_0^T dT' e^{pT'} \tilde{\xi}(T', \omega), \quad (3.101)$$

with $p = m(\omega^2 + \bar{\omega}^2)$, as solution for some initial condition \tilde{x}_0 . The correlation function $\langle \tilde{x}(T, \omega)\tilde{x}(T, \omega') \rangle$ is calculated as

$$\begin{aligned} \langle \tilde{x}(T, \omega)\tilde{x}(T, \omega') \rangle &= \tilde{x}_0^2 e^{-(p+p')T} + 4\pi\hbar e^{-(p+p')T} \\ &\quad \times \int_0^T dT' \int_0^T dT'' e^{pT'} e^{p'T''} \delta(T' - T'') \delta(\omega + \omega') \\ &= \tilde{x}_0^2 e^{-(p+p')T} + 4\pi\hbar e^{-(p+p')T} \int_0^T dT' e^{(p+p')T'} \delta(\omega + \omega') \\ &= \tilde{x}_0^2 e^{-(p+p')T} + 4\pi\hbar e^{-(p+p')T} \frac{e^{(p+p')T} - 1}{p + p'} \delta(\omega + \omega'), \end{aligned} \quad (3.102)$$

where we have used

$$\langle \tilde{\xi}(T, \omega)\tilde{\xi}(T', \omega') \rangle = 4\pi\hbar \delta(T - T') \delta(\omega + \omega'). \quad (3.103)$$

We make the identification $p' \rightarrow p$ since the delta function forces $\omega' = -\omega$ and $p' = p'(\omega'^2)$. In the large fictitious time T limit we finally have that

$$\Delta(\omega, \omega') = \lim_{T \rightarrow \infty} \langle \tilde{x}(T, \omega)\tilde{x}(T, \omega') \rangle = \frac{2\pi\hbar}{m(\omega^2 + \bar{\omega}^2)} \delta(\omega + \omega'). \quad (3.104)$$

3.3 Defect structures

There has been some interest in the equilibrium and non-equilibrium statistical mechanics of solitons, solitary waves and other coherent structures for quite some time. Recent applications arose in condensed-matter physics, particle physics, cosmology, displacive phase transitions and magnetic spin chains.

Kinks, in 1 dimension, or domain walls, in more than one dimension, usually arise when the potential has degenerate minima that cannot be continuously rotated into one another. Due to quantum or thermal effects the field at each point may ‘‘jump’’, or tunnel, from one minimum to the other. For high temperatures the field excitations (phonons) can be such that it may freely tunnel between the minima. On the other hand, for low temperatures the phonon intensity is small and the field will be likely to sit at a given minimum. In this situation we see the formation of domains, regions of space where the field has the same value, separated by walls.

We study here two related defect structures: the statistical mechanics of static classical kinks in 1+1 and $D+1$ dimensions. In the former case the kink solution arises naturally from a quartic potential, where in the latter a deformity in the potential has to be introduced so that the kink becomes stable.

3.3.1 Classical kinks in 1+1 dimensions

Here we study the same model found in [33], the equilibrium statistical mechanics of ‘‘kinks’’, solitary waves, of a (1+1) dimensional field $\phi(x, t)$ subject to a double-well potential,

$$V = -\frac{1}{2}m^2\phi^2 + \frac{1}{4}\lambda\phi^4, \quad (3.105)$$

with $m^2 > 0$ and $\lambda > 0$. The corresponding Lagrangian density is

$$\mathcal{L} = \frac{1}{2} \left(\frac{\partial\phi}{\partial t} \right)^2 - \frac{1}{2} \left(\frac{\partial\phi}{\partial x} \right)^2 + \frac{1}{2}m^2\phi^2 - \frac{1}{4}\lambda\phi^4 \quad (3.106)$$

which gives the equation of motion

$$\frac{\partial^2\phi}{\partial t^2} = \frac{\partial^2\phi}{\partial x^2} + m^2\phi - \lambda\phi^3. \quad (3.107)$$

The potential energy has its minima at

$$\phi = \pm\phi_0 = \pm\frac{m}{\sqrt{\lambda}}. \quad (3.108)$$

A possible solution to eq. (3.107) is one that interpolates between $-\phi_0$ and ϕ_0 and is localized in space, i.e., non-dispersive. Such a solution is called a kink and is inaccessible to perturbation theory. The static kink solution centered at $x = x_0$ is

$$\phi_{kink}(x) = \frac{m}{\sqrt{\lambda}} \tanh \left[\frac{m(x - x_0)}{\sqrt{2}} \right] \quad (3.109)$$

and the $\phi_{kink'} = -\phi_{kink}$ is called an antikink. Time dependent solutions may be obtained by Lorentz transforming the static solutions,

$$\phi_{kink}(x, t) = \frac{m}{\sqrt{\lambda}} \tanh \left[\frac{m}{\sqrt{2}} \gamma (x - x_0 + vt) \right], \quad (3.110)$$

where v is the kink velocity and $\gamma^{-1} = \sqrt{1 - v^2/c^2}$. The energy density of the kink or antikink is evaluated from the Hamiltonian density

$$\mathcal{H} = \frac{1}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 + \frac{1}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 - \frac{1}{2} m^2 \phi^2 + \frac{1}{4} \lambda \phi^4 + \frac{1}{4} \frac{m^4}{\lambda}, \quad (3.111)$$

where we added a constant term to make $V(\phi_0) = 0$, and we find

$$\varepsilon_{kink}(x, t) = \mathcal{H}[\phi = \phi_{kink}] = \frac{m^4}{4\lambda} (1 + \gamma^2 + \gamma^2 v^2) \operatorname{sech}^4 \left[\frac{m}{\sqrt{2}} \gamma (x - x_0 + vt) \right], \quad (3.112)$$

for the time-dependent solution, and

$$\varepsilon_{kink}(x) = \frac{m^4}{2\lambda} \operatorname{sech}^4 \left[\frac{m(x - x_0)}{\sqrt{2}} \right], \quad (3.113)$$

for the static solution. The kink mass, i.e., rest energy is

$$m_{kink} = \int_{-\infty}^{+\infty} \varepsilon_k(x) dx = \sqrt{\frac{8}{9}} \frac{m^3}{\lambda}. \quad (3.114)$$

In general, the solution to eq. (3.107) can be written in terms of the Jacobi elliptic sine function $\operatorname{sn}(a|b)$ [34],

$$\phi_k(x, t) = u \operatorname{sn}(\kappa \gamma (x - vt) + \delta | k) \quad (3.115)$$

as shown in the appendix B, where

$$k = \left[\frac{2m^2}{\lambda u} - 1 \right]^{-1/2}, \quad (3.116)$$

$$\kappa = \sqrt{\frac{m^2}{1 + k^2}}. \quad (3.117)$$

The parameter k , $0 \leq k \leq 1$, is called the *modulus* of the Jacobi function, and $0 < u \leq m^2/\lambda$ and δ are integration constants. The Jacobi elliptic sine function is a double-periodic function of period $4K(k^2)$, where K stands for the Complete Elliptic Integral [35]. We discuss two limiting cases of the Jacobi function: $k = 0$ and $k = 1$. The situation where $k = 0$ corresponds to the limit of $\lambda \rightarrow 0$, i.e., the equation of motion becomes

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial x^2} = m^2 \phi, \quad (3.118)$$

and has $\phi = u \sin(m\gamma(x - vt) + \delta)$ as solution. As can be noted from the above, this solution is periodic of quarter period $K(k^2 = 0) = \pi/2$. On the other hand, in the limit $k \rightarrow 1$ the non-linearity is essential: the quarter period becomes infinite since [34, 35]

$$\lim_{k \rightarrow 1} K(k^2) = \frac{1}{2} \ln \left(\frac{16}{1 - k^2} \right) \quad (3.119)$$

and the kink solution approaches that of (3.109). In a sense, we can say that the $k \rightarrow 1$ solution gives a lower bound to the kink energy as the number of nodes of $\phi_k(x, t)$ increases with decreasing period.

In numerical simulations it is customary to use dimensionless quantities

$$\bar{\phi} = \phi/a \quad (3.120)$$

$$\bar{x} = mx \quad (3.121)$$

$$\bar{t} = mt \quad (3.122)$$

where $a^2 = m^2/\lambda$. This rescaling restricts $0 < u \leq 1$ and the modulus k now reads

$$k = \left[\frac{2}{u} - 1 \right]^{-1/2} \quad (3.123)$$

The transformed Lagrangian can be obtained from

$$L = ma^2 \bar{L} = ma^2 \int d\bar{t} \left[\left(\frac{\partial \bar{\phi}}{\partial \bar{t}} \right)^2 - \left(\frac{\partial \bar{\phi}}{\partial \bar{x}} \right)^2 + \frac{1}{2} \bar{\phi}^2 - \frac{1}{4} \bar{\phi}^4 \right] \quad (3.124)$$

and the equation of motion,

$$\frac{\partial^2 \bar{\phi}}{\partial \bar{t}^2} = \frac{\partial^2 \bar{\phi}}{\partial \bar{x}^2} - \bar{\phi} (\bar{\phi}^2 - 1). \quad (3.125)$$

The classical equilibrium statistical mechanics of the field ϕ follows from the canonical partition function

$$Z = \int \mathcal{D}\bar{\pi} \mathcal{D}\bar{\phi} e^{-\bar{\beta} \bar{H}} \quad (3.126)$$

where $\bar{\beta} = \beta/ma^2$, with β being the inverse temperature and \bar{H} is the Hamiltonian corresponding to our rescaled Lagrangian \bar{L} . The above partition function factorises as

$$Z = Z_\pi Z_\phi = \int \mathcal{D}\pi e^{-\beta \int dx \pi^2/2} \int \mathcal{D}\phi e^{-\beta \int dx V(\phi)}. \quad (3.127)$$

From this equation on we are dropping the bar over the rescaled quantities since there is no risk of ambiguity. The momentum term does not contribute to the equilibrium dynamics we shall ignore it and focus on Z_ϕ . Field configurations with a probability distribution given the Boltzmann weight in eq. (3.127) can be generated from the Langevin equation for fictitious time τ

$$\eta \frac{\partial \phi}{\partial \tau} = \frac{\partial^2 \phi}{\partial x^2} - \phi(\phi^2 - 1) + \xi(x, \tau), \quad (3.128)$$

with

$$\langle \xi(x, \tau) \rangle = 0, \quad \langle \xi(x, \tau) \xi(x', \tau') \rangle = 2\eta\beta^{-1} \delta(x - x') \delta(\tau - \tau'). \quad (3.129)$$

Numerical results obtained by simulating eq. (3.128) will be shown later in this work.

3.3.2 Deformed potentials

High energy physics, in particular string theory, brings a wide range of situations where a system in D spatial dimensions supports defect structures of topological nature. However, a theorem by Hobart [36] and Derrick [37] states that real scalar fields can only have stable defect structures in 1+1 dimensions. By enriching the model to support vortexes [38] or monopoles [39] static coherent structures become stable.

In D spatial dimensions we study potentials of the form [40]

$$V(\phi; x) = \frac{1}{2} \frac{1}{r^{2D-2}} W_\phi^2, \quad (3.130)$$

where W is a smooth function of the field ϕ and $W_\phi = \partial W / \partial \phi$, which support static radial defect solutions. A simple derivation of eq. (3.130) is found in appendix C, in the context of a color dielectric model. The equation of motion for a radially symmetric field $\phi = \phi(r)$ is

$$\frac{1}{r^{D-1}} \frac{d}{dr} \left(r^{D-1} \frac{d\phi}{dr} \right) = \frac{1}{r^{2D-2}} W_\phi W_{\phi\phi}. \quad (3.131)$$

By using the map

$$dx = \pm r^{1-D} dr \quad (3.132)$$

we have

$$\frac{d^2\phi}{dx^2} = W_\phi W_{\phi\phi}, \quad (3.133)$$

i.e., we have mapped the equation of motion for the field in D dimensions into the one-dimensional problem. The solutions to the above equation also satisfy the first order equations

$$\frac{d\phi}{dr} = \pm \frac{1}{r^{D-1}} W_\phi, \quad \text{or} \quad \frac{d\phi}{dx} = \pm W_\phi, \quad (3.134)$$

where we have used the above map, if they also obey the boundary conditions

$$\lim_{x \rightarrow -\infty} \phi(x) = \bar{\phi}, \quad \lim_{x \rightarrow -\infty} \frac{d\phi}{dx} = 0, \quad (3.135)$$

with $\bar{\phi}$ being such that

$$\left. \frac{dV}{d\phi} \right|_{\bar{\phi}} = 0. \quad (3.136)$$

From here on we shall concentrate on the $D = 1$ field solutions and use the inverse map to study them in an arbitrary number of dimensions. The Hamiltonian density corresponding to eq. (3.133) and eq. (3.134) has the form

$$\mathcal{H} = \frac{1}{2} \left[\left(\frac{d\phi}{dx} \right)^2 + W_\phi^2 \right] = \pm \frac{dW}{dx} + \frac{1}{2} \left(\frac{d\phi}{dx} \mp W_\phi \right)^2 \quad (3.137)$$

and is minimized by field configurations that solve eq. (3.134). The energy for such configurations is $E = |\Delta W| = |W[\phi(\infty)] - W[\phi(-\infty)]|$ and they are linearly stable [40, 41].

We are going to study the case $D = 1$ for the family of potentials

$$V_p(\phi) = \frac{1}{2} \phi^2 (\phi^{-1/p} - \phi^{1/p})^2. \quad (3.138)$$

The parameter p , taken to be an odd integer, is related to the way the field self-interacts: $p = 1$ is the usual ϕ^4 theory, $p = 3, 5, \dots$ present new potentials that support minima at $\phi = 0$ and $\phi = \pm 1$. The equation of motion for ϕ has the family of static kinks

$$\phi_\pm^{(p)}(x) = \pm \tanh^p(x/p) \quad (3.139)$$

as solution, where we took the kinks to be centered at $x_0 = 0$. We sketch some of the solutions in Fig. 3.5.

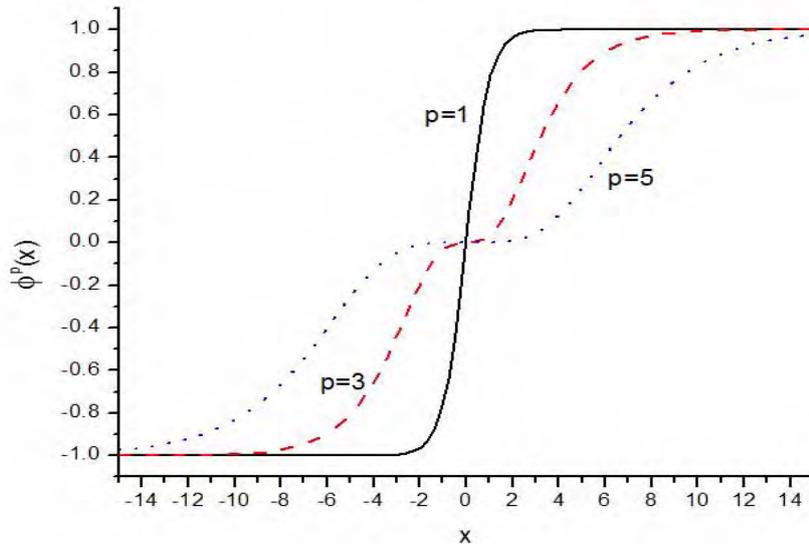


Figure 3.5: Graphs of the kink solutions for $p = 1$, $p = 3$ and $p = 5$.

For $p \geq 3$ we can see that it has a vanishing derivative at the symmetric minimum $\phi = 0$. These structures are called two-kink defects, because they look like they are composed by two standard kinks separated by a distance that increases with p . This kind of defect structures is similar to the ones studied in $Z(3)$ symmetric models [42] and also in supersymmetric theories [43]. Bazeia *et al* have also studied the $V_p(\phi)$ coupled to gravity in warped spacetime [44]. Magnetic domain walls, found in constricted ferromagnetic systems, also have profiles that can be well described by solutions like $\phi_{\pm}^{(p)}$ [45].

In $D = 2$ dimensions the map given in eq. (3.132) gives $x = \pm \ln r$ and the kink solutions become domain walls whose profile behaves like

$$\phi_{\pm}^{(p)} = \pm \tanh^p(\ln r^{1/p}) = \pm \left(\frac{r^{2/p} - 1}{r^{2/p} + 1} \right)^p. \quad (3.140)$$

For $D \geq 3$ we have that $x = \mp r^{2-D}/(D-2)$. In this case we see that x either belongs to $(-\infty, 0]$ or $[0, \infty)$ and we should use the minus sign for $x \leq 0$ and the plus sign for $x \geq 0$. We show some plots of $\phi_{\pm}^{(p)}(r)$ for $D = 2$ and $D = 3$ in Figs. 3.6 and 3.7.

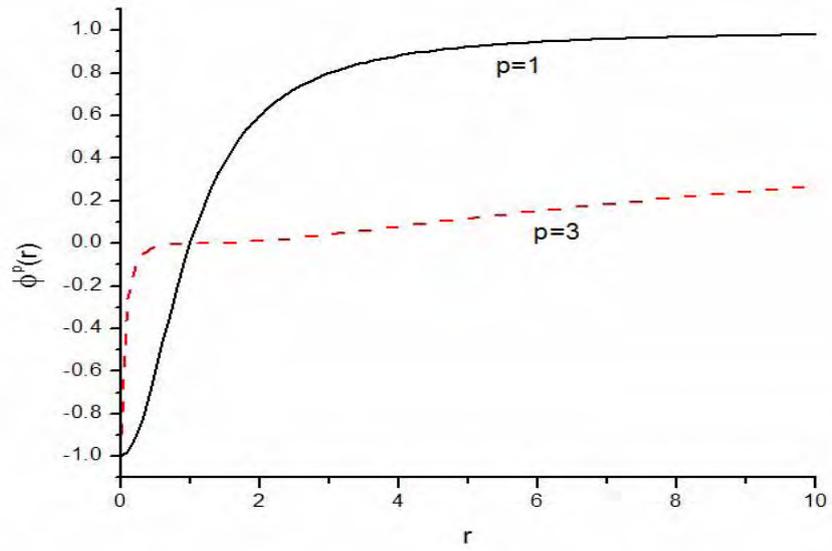


Figure 3.6: Graphs of the kink solutions for $p = 1$ and $p = 3$ in two dimensions.

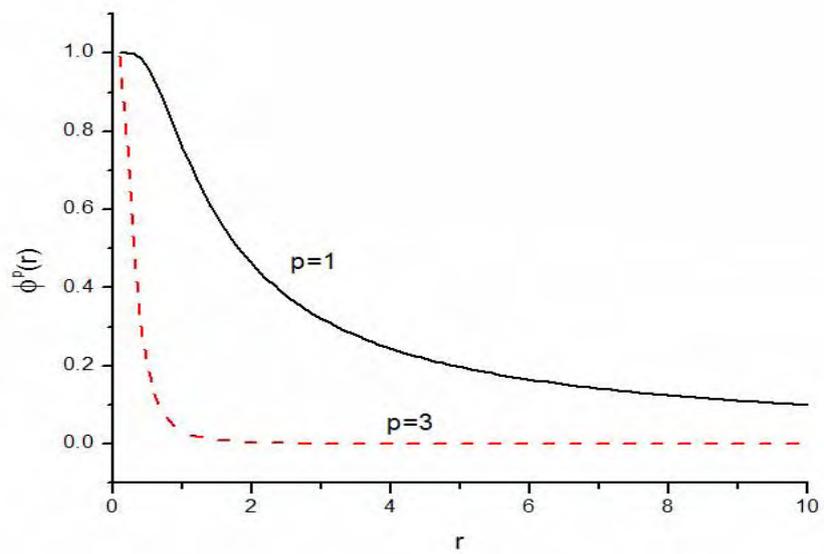


Figure 3.7: Graphs of the kink solutions for $p = 1$ and $p = 3$ in three dimensions.

Chapter 4

Noise Perturbation Theory

Ginzburg-Landau-Langevin equations arise in a variety of contexts, like physics, engineering, chemistry, biology and medicine. However, in many of those situations the Ginzburg-Landau Hamiltonian H or Action S is a very complicated function or functional of the dynamical variables or fields,

$$\frac{\partial \phi}{\partial t}(x, t) = K[\phi; x, t] + \xi(x, t), \quad (4.1)$$

where $K[\phi; x, t]$, is an arbitrary function of ϕ or even a nonlocal functional of space and time, and ξ can be a colored noise functional

$$\langle \xi(x, t) \rangle = 0, \quad \langle \xi(x, t) \xi(x', t') \rangle = \gamma F(x - x', t - t'), \quad (4.2)$$

with γ being the noise intensity.

We will discuss here a perturbation method that can be used to handle equations like eq. (4.1) when the noise intensity γ is weak. An example of such situation occurs when a system which exhibits a phase transition at a temperature $T = T_c$ in contact with a heat bath at $T \gg T_c$ is submitted to a deep temperature quench into broken-symmetric phase, $T \gg T_c \rightarrow T' \ll T_c$. At low temperatures the thermal noise is weak since usually $\xi \sim \sqrt{T}$, and we may expand the field $\phi(x, t)$ in powers of $\gamma^{n/2}$ to study weak thermal effects over a broken-symmetric system. Another example comes from cosmology: in the inflationary phase of the universe both general relativity and quantum mechanics effects must be taken into account. Stochastic inflation aims to describe a homogeneous scalar field, coarse-grained over a Hubble patch, where the quantum fluctuations are modelled by a stochastic noise originating from the small-scale Fourier effects [9, 10]. The size of the coarse-graining is such that the dynamics can be described by a Langevin equation and the quantum fluctuations modelled by a white noise field (section 4.3). The statistical mechanics

of coherent structures, such as kinks and instantons, present one last example. These so-called defect structures can interact with phonons generated by thermal fluctuations. At low temperatures this interaction is small and we may treat the phonons as perturbation to the kink solution (section 4.4).

4.1 Outline of the method

Closely following [12], let us write the solution of eq. (4.1) as

$$\phi(x, t) = \phi_0(x, t) + \bar{\phi}(x, t) \equiv \phi_0(x, t) + \sum_{n=1}^{\infty} \phi_n(x, t), \quad (4.3)$$

where $\phi_0(x, t)$ is the solution to the noise-free equation

$$\frac{\partial \phi_0}{\partial t}(x, t) = K[\phi_0; x, t], \quad (4.4)$$

and the $\phi_n(x, t)$ are the perturbations, in the sense that $\phi_n(x, t) \sim \gamma^{n/2}$. The functional Taylor expansion of K around $\phi_0(x, t)$ can be written as

$$K[\phi] = K[\phi_0] + K^{(1)}[\phi_0] * \bar{\phi} + K^{(2)}[\phi_0] * \bar{\phi} * \bar{\phi} + \dots, \quad (4.5)$$

where the schematic notation means

$$K^{(1)}[\phi_0] * \bar{\phi} = \int dx_1 dt_1 \left. \frac{\delta K[\phi; x, t]}{\delta \phi(x_1, t_1)} \right|_{\phi=\phi_0} \bar{\phi}(x_1, t_1), \quad (4.6)$$

$$K^{(2)}[\phi_0] * \bar{\phi} * \bar{\phi} = \frac{1}{2!} \int dx_1 dt_1 dx_2 dt_2 \left. \frac{\delta^2 K[\phi; x, t]}{\delta \phi(x_1, t_1) \delta \phi(x_2, t_2)} \right|_{\phi=\phi_0} \\ \times \bar{\phi}(x_1, t_1) \bar{\phi}(x_2, t_2), \quad (4.7)$$

and so on. Using both ϕ and K expansions and equating powers of γ on both sides, keeping in mind that $\xi \sim \sqrt{\gamma}$, we obtain a set of *linear* Ginzburg-Landau-Langevin equations for the ϕ_n fields. For $n \leq 2$ we have

$$\frac{\partial \phi_1}{\partial t} = K^{(1)}[\phi_0] * \phi_1 + \xi, \quad (4.8)$$

$$\frac{\partial \phi_2}{\partial t} = K^{(1)}[\phi_0] * \phi_2 + K^{(2)}[\phi_0] * \phi_1 * \phi_1. \quad (4.9)$$

It is worthwhile noting that the above equations might still be very complicated to simulate because the ϕ_n on the right-hand side of the equations are integrated over space and time. One way to circumvent this is to use a mean-field approximation in which products of the fields

are replaced by average values. However, care must be taken since the noise-dependent equations may exhibit divergences at high momenta (or small lattice spacing, for discretized theories), as pointed in [12] and sketched in the next section.

4.2 Expansion in powers of γ

As an example for the expansion we calculate the 2–point connected correlation function of the quantum $\lambda\phi^4$ theory in Euclidean space up to order $\gamma(\sim \hbar)$. To do this we expand the field $\phi(x, \tau)$ as

$$\phi(x, \tau) = \phi_0(x, \tau) + \phi_1(x, \tau) + \phi_2(x, \tau) + \dots, \quad (4.10)$$

where the fields satisfy

$$\frac{\partial\phi_0}{\partial\tau} = \nabla^2\phi_0 - m^2\phi_0 - \lambda\phi_0^3, \quad (4.11)$$

$$\frac{\partial\phi_1}{\partial\tau} = \nabla^2\phi_1 - m^2\phi_1 - 3\lambda\phi_0^2\phi_1 + \xi, \quad (4.12)$$

$$\frac{\partial\phi_2}{\partial\tau} = \nabla^2\phi_2 - m^2\phi_2 - 3\lambda\phi_0^2\phi_2 - 3\lambda\phi_0\phi_1^2, \quad (4.13)$$

$$\frac{\partial\phi_3}{\partial\tau} = \nabla^2\phi_3 - m^2\phi_3 - \lambda[3\phi_0^2\phi_3 + \phi_1^3 + 6\phi_0\phi_1\phi_2], \quad (4.14)$$

with $\phi_n = \phi_n(x, \tau)$ and

$$\langle\xi(x, \tau)\xi(x', \tau')\rangle = 2\hbar\delta(x - x')\delta(\tau - \tau'). \quad (4.15)$$

The equations for ϕ_n , $n > 0$, have the same structure, namely,

$$\frac{\partial\phi_n}{\partial\tau} = F\phi_n + P_n, \quad (4.16)$$

where

$$F = \nabla^2 - m^2 - 3\lambda\phi_0^2 \quad (4.17)$$

is a linear differential operator and

$$P_n = \begin{cases} \xi & \text{for } n = 1, \\ 3\lambda\phi_0\phi_1^2 & \text{for } n = 2, \end{cases} \quad (4.18)$$

is a source term. The general solution to eq. (4.16) reads

$$\phi_n(x, \tau) = \phi_n^h(x, \tau) + \int d^4x' \int_0^\tau d\tau' G(x - x', \tau - \tau') P_n(x', \tau'), \quad (4.19)$$

where ϕ_n^h is the solution to the homogeneous equation and G is the Green's function. Performing a Fourier transform on the x coordinates in eq. (4.16),

$$\phi_n(x, \tau) = \int d^4x e^{ikx} \tilde{\phi}(k, t), \quad (4.20)$$

and assuming that $\phi_0(x, \tau) = \varphi_0$, we have

$$\frac{\partial \tilde{\phi}_n^h}{\partial \tau}(k, \tau) = -(k^2 + m^2 + 3\lambda\varphi_0^2)\tilde{\phi}_n^h(k, \tau) \quad (4.21)$$

for the homogeneous part. Its solution is

$$\begin{aligned} \tilde{\phi}_n^h(k, \tau) &= e^{-(k^2+m^2+3\lambda\varphi_0^2)(\tau-\tau_0)} \tilde{\phi}_n^h(k, \tau_0) \\ &\equiv \tilde{G}(k, \tau - \tau_0) \tilde{\phi}_n^h(k, \tau_0). \end{aligned} \quad (4.22)$$

The full solution in Fourier space, then, reads

$$\tilde{\phi}_n(k, \tau) = \tilde{\phi}_n^h(k, \tau) + \int_0^\tau d\tau' \tilde{G}(k, \tau - \tau') \tilde{P}_n(k, \tau'). \quad (4.23)$$

The assumption that $\phi_0(x, \tau) = \varphi_0$ gives for the initial condition

$$\phi(x, 0) = \varphi_0 + \phi_1(x, 0) + \phi_2(x, 0) + \dots = \varphi_0, \quad (4.24)$$

or

$$\phi_1(x, 0) = \phi_2(x, 0) = \dots = \phi_n(x, 0) = \dots = 0. \quad (4.25)$$

With this in mind we may write for $\phi_1(x, t)$

$$\phi_1(x, \tau) = \int d^4y d\tau' \left[\int \frac{d^4k}{(2\pi)^4} e^{ik(x-y) - (k^2+m^2+3\lambda\varphi_0^2)(\tau-\tau')} \right] \xi(y, \tau'), \quad (4.26)$$

and for $\phi_2(x, t)$,

$$\phi_2(x, \tau) = \int d^4y d\tau' \left[\int \frac{d^4k}{(2\pi)^4} e^{ik(x-y) - (k^2+m^2+3\lambda\varphi_0^2)(\tau-\tau')} \right] 3\lambda\varphi_0\phi_1^2(y, \tau'). \quad (4.27)$$

The connected 2-point correlation function is defined as

$$\langle \phi(x)\phi(x') \rangle_c = \langle \phi(x)\phi(x') \rangle - \langle \phi(x) \rangle \langle \phi(x') \rangle, \quad (4.28)$$

where, since we are in realm of stochastic quantization,

$$\langle F[\phi(x)] \rangle = \lim_{\tau \rightarrow \infty} \langle F[\phi(x, \tau)] \rangle. \quad (4.29)$$

Expanding eq. (4.28) to order \hbar we get

$$\begin{aligned}
\langle \phi(x)\phi(x') \rangle_c &= \varphi_0^2 + \varphi_0 \langle \phi_1(x) \rangle + \varphi_0 \langle \phi_1(x') \rangle + \langle \phi_1(x)\phi_1(x') \rangle \\
&\quad + \varphi_0 \langle \phi_2(x') \rangle + \varphi_0 \langle \phi_2(x) \rangle + \dots \\
&\quad - [(\varphi_0 + \langle \phi_1(x) \rangle + \langle \phi_2(x) \rangle + \dots) \\
&\quad \times (\varphi_0 + \langle \phi_1(x') \rangle + \langle \phi_2(x') \rangle + \dots)] \\
&= \langle \phi_1(x)\phi_1(x') \rangle + \mathcal{O}(\hbar^{3/2}).
\end{aligned} \tag{4.30}$$

Thus, we only need to evaluate

$$\langle \phi_1(x)\phi_1(x') \rangle = \lim_{\tau \rightarrow \infty} \langle \phi_1(x, \tau)\phi_1(x', \tau) \rangle. \tag{4.31}$$

Using the result from eq. (4.26) we have

$$\begin{aligned}
\langle \phi_1(x, \tau)\phi_1(x', \tau) \rangle &= \int d^4y d^4y' \int_0^\tau d\tau' d\tau'' \\
&\quad \times \left[\int \frac{d^4k}{(2\pi)^4} e^{ik(x-y) - (k^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')} \right] \\
&\quad \times \left[\int \frac{d^4k'}{(2\pi)^4} e^{ik'(x'-y') - (k'^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau'')} \right] \\
&\quad \times \langle \xi(y, \tau')\xi(y', \tau'') \rangle
\end{aligned} \tag{4.32}$$

$$\begin{aligned}
&= \int d^4y d^4y' \int_0^\tau d\tau' d\tau'' \frac{d^4k}{(2\pi)^4} \frac{d^4k'}{(2\pi)^4} \\
&\quad \times \exp [ik(x-y) - (k^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')] \\
&\quad \times \exp [ik'(x'-y') - (k'^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau'')] \\
&\quad \times 2\hbar\delta(y-y')\delta(\tau' - \tau''),
\end{aligned} \tag{4.33}$$

where we have used the white noise property of ξ . Now we integrate over the delta functions

$$\begin{aligned}
\langle \phi_1(x, \tau)\phi_1(x', \tau) \rangle &= 2\hbar \int d^4y \int_0^\tau d\tau' \frac{d^4k}{(2\pi)^4} \frac{d^4k'}{(2\pi)^4} e^{-iy(k+k')} \\
&\quad \times \exp [ikx - (k^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')] \\
&\quad \times \exp [ik'x' - (k'^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')]
\end{aligned} \tag{4.34}$$

$$\begin{aligned}
&= 2\hbar \int_0^\tau d\tau' \int \frac{d^4k}{(2\pi)^4} d^4k' \delta(k+k') \\
&\quad \times \exp [ikx - (k^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')] \\
&\quad \times \exp [ik'x' - (k'^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')].
\end{aligned} \tag{4.35}$$

Again we have integrated over the delta function, since

$$\int d^4y e^{-iy(k+k')} = (2\pi)^4 \delta(k+k'). \tag{4.36}$$

Finally, we have that

$$\langle \phi_1(x, \tau) \phi_1(x', \tau) \rangle = 2\hbar \int_0^\tau d\tau' \int \frac{d^4k}{(2\pi)^4} e^{ik(x-x') - 2(k^2 + m^2 + 3\lambda\varphi_0^2)(\tau - \tau')} \quad (4.37)$$

$$= \hbar \int \frac{d^4k}{(2\pi)^4} e^{ik(x-x')} \frac{1 - e^{-2(k^2 + m^2 + 3\lambda\varphi_0^2)\tau}}{k^2 + m^2 + 3\lambda\varphi_0^2} \quad (4.38)$$

Taking the infinite fictitious time limit,

$$\langle \phi_1(x) \phi_1(x') \rangle = \int \frac{d^4k}{(2\pi)^4} e^{ik(x-x')} \frac{\hbar}{k^2 + m^2 + 3\lambda\varphi_0^2}, \quad (4.39)$$

a well-known result from canonical and path-integral quantum field theory [3, 6]. The divergence cited in the last section is now clear from the above result because the integrand behaves like k^2 for large 4-momentum.

4.3 Stochastic inflation

During the early instants of the universe after the Big-Bang (around $10^{-36}s$ to sometime between 10^{-33} and $10^{-32}s$) it experienced a period of rapid expansion, by a factor of 10^{78} in volume, called *cosmological inflation*, or just inflation. It explains why the temperatures and curvatures of different regions of the universe are so nearly equal: with exponentially expanding space, two nearby regions are separated very quickly - so much that everything becomes almost homogeneous from a local point of view. However, quantum fluctuations pose significant inhomogeneities during this period. We present here a situation where the expansion of a physical field in powers of the noise, used to model the quantum effects, enables the evaluation of correlation functions.

For a homogeneous and isotropic universe, described by the Friedmann-Robertson-Walker metric,

$$ds^2 = dt^2 - a^2(t)dx_i dx^i, \quad (4.40)$$

the inflation [11] is a phase of accelerated expansion of the scale factor $a(t)$ driven by a scalar field ϕ whose dynamics is described by the Klein-Gordon equation

$$\ddot{\phi} = 3H\dot{\phi} + V'(\phi) = 0, \quad (4.41)$$

where $\dot{\phi} = \partial\phi/\partial t$ and $V' = \delta V/\delta\phi$, coupled to the Friedmann equation for the scale factor

$$H^2(\phi) = \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi}{3m_{Pl}^2} \left[\frac{\dot{\phi}^2}{2} + V(\phi)\right] \quad (4.42)$$

with m_{Pl} being the Planck mass. The field $\phi(x)$ shows strong quantum effects and undergoes large fluctuations on large scales. Thus we split it in long and short wavelengths, compared to H^{-1} . The high frequency part contains quasi-free modes φ that can be canonically quantized. Inserting the field into the Klein-Gordon equation gives the effective equation

$$\ddot{\phi} + 3H\dot{\phi} - \frac{\nabla^2\phi}{a^2} + V'(\phi) = \dot{\xi} + 3H\xi, \quad (4.43)$$

where $\xi = \xi(x, t)$ is a source field. Long wavelength modes perturb φ similarly to a Brownian motion, so we may model it by a white noise field, as quantum fluctuations of high frequency modes act as a classical noise coupled to our coarse-grained field. We also make use of the ‘‘slow roll’’ approximation,

$$\ddot{\phi} \ll 3H\dot{\phi}, \quad \dot{\xi} \approx 0, \quad (4.44)$$

and neglect the Laplacian term since the field is homogeneous for distances smaller than H^{-1} . Thus φ satisfies

$$\dot{\varphi} + \frac{V'(\varphi)}{3H(\varphi)} = \frac{H^{3/2}(\varphi)}{2\pi}\xi, \quad (4.45)$$

with

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \delta(t - t'). \quad (4.46)$$

Equation (4.45) is a Langevin equation with *multiplicative* noise, instead of additive. Nevertheless, we may still expand φ in powers of the noise as $\varphi = \varphi_{cl} + \delta\varphi_1 + \delta\varphi_2 + \dots$, where

$$\dot{\varphi}_{cl} + \frac{V'(\varphi_{cl})}{3H(\varphi_{cl})} = 0 \quad (4.47)$$

is the classical solution, which neglects quantum fluctuations,

$$\delta\dot{\varphi}_1 + \frac{m_{Pl}^2}{4\pi}H''(\varphi_{cl})\delta\varphi_1 = \frac{H^{3/2}}{2\pi}\xi(t), \quad (4.48)$$

and

$$\delta\dot{\varphi}_2 + \frac{m_{Pl}^2}{4\pi}H''(\varphi_{cl})\delta\varphi_2 = -\frac{m_{Pl}^2H'''(\varphi_{cl})}{8\pi}\delta\varphi_1^2 + \frac{3}{4\pi}H^{1/2}(\varphi_{cl})H'(\varphi_{cl})\delta\varphi_1\xi(t) \quad (4.49)$$

are the first two quantum corrections.

Following [10] we write the solutions to the perturbation fields as

$$\delta\varphi_1(t) = \frac{H'[\varphi_{cl}(t)]}{2\pi} \int_{t_{in}}^t d\tau \frac{H^{3/2}[\varphi_{cl}(\tau)]}{H'[\varphi_{cl}(\tau)]} \xi(\tau), \quad (4.50)$$

and

$$\delta\varphi_2(t) = -\frac{m_{Pl}^2 H'}{8\pi} \int_{t_{in}}^t d\tau \frac{H'''}{H'} \delta\varphi_1^2(\tau) + \frac{3H'}{4\pi} \int_{t_{in}}^t d\tau H^{1/2} \delta\varphi_1(\tau) \xi(\tau), \quad (4.51)$$

from which the correlation functions may be evaluated. Since $\delta\varphi_1$ is linear in the noise its mean value is zero

$$\langle \delta\varphi_1 \rangle = 0. \quad (4.52)$$

The $\langle \delta\varphi_1^2 \rangle$ term reads

$$\langle \delta\varphi_1^2 \rangle = \frac{(H')^2}{\pi m_{Pl}^2} \int_{\varphi_{cl}}^{\varphi_{in}} d\psi \left(\frac{H}{H'} \right)^3, \quad (4.53)$$

while $\langle \delta\varphi_2 \rangle$ is non-zero because it is quadratic in the noise

$$\langle \delta\varphi_2 \rangle = \frac{H''}{2H'} \langle \delta\varphi_1^2 \rangle + \frac{H'}{4\pi m_{Pl}^2} \left[\frac{H_{in}^3}{(H'_{in})^2} - \frac{H^3}{(H')^2} \right]. \quad (4.54)$$

Therefore, at second order in the noise, everything can be reduced to the calculation of a single quadrature, the one in (4.53). The above perturbation method is valid regardless of the inflationary potential $V(\varphi)$ used and thus works for a wide variety of models.

4.4 Coherent structures

For low temperatures, $\beta^{-1} \ll 1$, we may expand ϕ in powers of $\beta^{-1/2}$ and analyse how small thermal effects affect the kink structure. We write the solution to eq. (3.128) as $\phi = \phi_0 + \phi_1 + \dots$, where the rescaled equilibrium noise-free (zero temperature) field obeys

$$\eta \frac{\partial \phi_0}{\partial \tau} = \frac{\partial^2 \phi_0}{\partial x^2} - (\phi_0^2 - 1) \phi_0, \quad (4.55)$$

and the first thermal phonon correction satisfies

$$\eta \frac{\partial \phi_1}{\partial \tau} = \frac{\partial^2 \phi_1}{\partial x^2} - (3\phi_0^2 - 1) \phi_1 + \xi(x, \tau). \quad (4.56)$$

For large times and suitable boundary conditions we expect that ϕ_0 will relax to a single kink or antikink solution and ϕ_1 will incorporate thermal effects that make the field fluctuate around the zero temperature solution. Further corrections can be simulated using higher order equations, e.g.,

$$\eta \frac{\partial \phi_2}{\partial \tau} = \frac{\partial^2 \phi_2}{\partial x^2} - (3\phi_0^2 - 1) \phi_2 - 3\phi_0 \phi_1^2, \quad (4.57)$$

and

$$\eta \frac{\partial \phi_3}{\partial \tau} = \frac{\partial^2 \phi_3}{\partial x^2} - (3\phi_0^2 - 1) \phi_3 - \phi_1^3 - 6\phi_0 \phi_1 \phi_2. \quad (4.58)$$

Chapter 5

Numerical simulations and results

In this Chapter we study the Ginzburg-Landau-Langevin equation numerically. After making the equation suitable for computer simulations we discuss finite-size effects in a double-well $\lambda\phi^4$ model. Then we look for the range of validity of the noise perturbation theory. Finally we study the interaction between the kink solutions and thermal fluctuations induced by the noise field.

First, we present the well-known finite differences method for simulating differential equations. The method consists in discretization of the space-time and the derivative terms and evaluation of the field over this space-time lattice. Second, we discuss issues related to lattice sizes and simulation time on symmetry restoration of a one-dimensional field with a self-interacting double-well potential. Any nonzero temperature leads to $\phi = 0$ in the thermodynamic limit: there is no phase transition in one dimension. Small lattices give rise to finite-size effects that change this behavior and may lead to wrong interpretations of the results. We discuss how dimensionality of space influences this picture.

Next, to verify the validity of the method of noise perturbation theory, we perform numerical simulations of the Ginzburg-Landau-Langevin equation for the quartic potential described above and investigate the range of validity of this expansion method in a one-dimensional theory. Finally, we investigate the effect of thermal fluctuations on a kink in the context of the deformed potentials discussed earlier. As the temperature increases the interaction of the thermal phonons with the kink becomes stronger and, after a certain critical value, destroys the kink structures, dominating the field behavior.

5.1 Finite differences method

The 1 + 1 dimensional Ginzburg-Landau-Langevin leading to the defect structures of last section have the form

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} + F[\phi(x, t), \xi(x, t)], \quad (5.1)$$

where F is some function of ϕ and the noise field ξ , and we are working with dimensionless quantities. In order to numerically simulate eq. (5.1) we discretize the space-time over an anisotropic lattice, i.e.,

$$x = na, \quad (5.2)$$

$$t = m\delta, \quad (5.3)$$

with $m, n = 0, \pm 1, \pm 2, \dots$. The derivative terms involve the difference of the field at two neighboring points as their distance gets infinitesimally small. On the lattice there are several ways to define the first derivative such as

$$f'_+(x) = \frac{f(x+a) - f(x)}{a}, \quad (5.4)$$

$$f'_-(x) = \frac{f(x) - f(x-a)}{a}, \quad (5.5)$$

$$f'_{sym}(x) = \frac{f(x+a) - f(x-a)}{2a}, \quad (5.6)$$

called forward, backward and symmetric derivatives, respectively. When compared to the exact derivative, the first two have differences of order $\mathcal{O}(a)$, while the third one is of $\mathcal{O}(a^2)$. The discretized second derivative is usually defined to be

$$f''(x) = \frac{f'_+(x) - f'_-(x)}{a} = \frac{f(x+a) + f(x-a) - 2f(x)}{a^2}. \quad (5.7)$$

Choosing the forward scheme for the time derivative we may write eq. (5.1) on the lattice, with $\phi_{n,m} \equiv \phi(x, t)$ and $\xi_{n,m} \equiv \xi(x, t)$, as

$$\frac{\phi_{n,m+1} - \phi_{n,m}}{\delta} = \frac{\phi_{n+1,m} + \phi_{n-1,m} - 2\phi_{n,m}}{a^2} + F[\phi_{n,m}, \xi_{n,m}]. \quad (5.8)$$

Rearranging the terms we have

$$\phi_{n,m+1} = \phi_{n,m} + \delta \left[\frac{\phi_{n+1,m} + \phi_{n-1,m} - 2\phi_{n,m}}{a^2} + F[\phi_{n,m}, \xi_{n,m}] \right]. \quad (5.9)$$

This approximation is numerically stable and convergent for $2\delta < a^2$. Convergence can be improved using the ‘‘LAX scheme’’ [46], where one replaces $\phi_{n,m}$ in eq. (5.8) by its space average:

$$\phi_{n,m} \rightarrow \frac{1}{2} (\phi_{n+1,m} + \phi_{n-1,m}). \quad (5.10)$$

In this scheme some numerical stabilities are averaged out by the above prescription. The white noise field $\xi_{n,m}$ scales as

$$\xi_{n,m} = \sqrt{\frac{2\gamma}{a\delta}} \zeta_{n,m}, \quad (5.11)$$

where $\zeta_{n,m}$ is another white noise field with unity autocorrelation, due to the transformation properties of the Dirac delta function, namely

$$\delta(x - x') \rightarrow \frac{1}{a} \delta_{n,n'}. \quad (5.12)$$

5.2 Numerical results

5.2.1 Symmetry restoration

We start discussing this phenomenon in arbitrary space dimensions and then present results for one dimension. The GLL equation for the field ϕ for a double-well potential (quartic self-interaction) is given by:

$$\frac{\partial \phi}{\partial \tau} = \nabla^2 \phi + m^2 \phi - \lambda \phi^3 + \xi, \quad (5.13)$$

where $m^2 \geq 0$, $\lambda > 0$ and

$$\langle \xi(x, \tau) \xi(x', \tau') \rangle = 2\gamma \delta(x - x') \delta(\tau - \tau'). \quad (5.14)$$

As stated earlier, this equation leads to the statistical mechanics of such field, for $\gamma = \beta^{-1}$, to stochastic quantization, for $\gamma = \hbar$, among other possibilities. The quartic potential

$$V(\phi) = \frac{\lambda}{4} \phi^4 - \frac{m^2}{2} \phi^2 + \frac{1}{4} \frac{m^4}{\lambda} \quad (5.15)$$

is sketched in Fig. 5.1. For low excitation energies, the field is restricted to a vicinity of one of the potential’s minima; in the language of quantum field theory, one says that the field has a nonzero expectation value $\langle \phi \rangle \neq 0$, even though the potential is symmetric under $\phi \rightarrow -\phi$. In this situation, one says that the symmetry of the potential

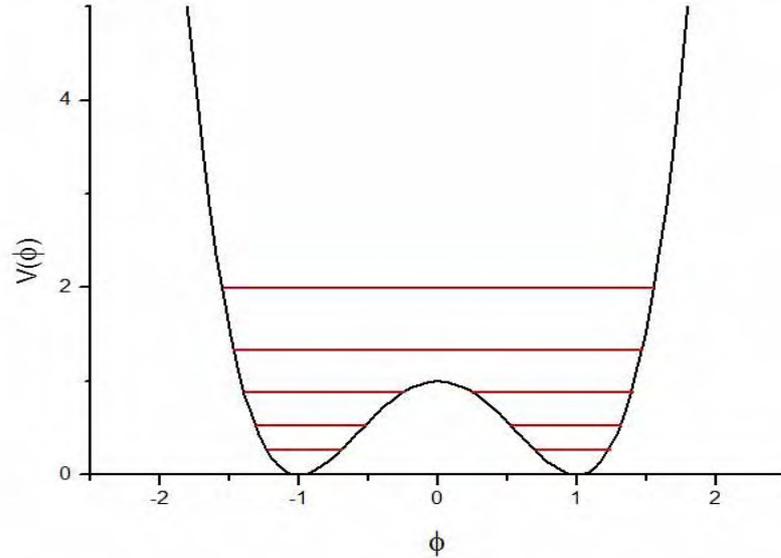


Figure 5.1: Graph of the quartic double-well potential. The horizontal lines represent schematically excitation energies.

has been broken spontaneously and one has a quantum phase transition. In the language of classical statistical mechanics, in which ϕ is an order parameter, low excitation energies means low temperatures. In this case, $\langle\phi\rangle \neq 0$ means that the thermodynamics average of order parameter is nonzero and, again, one has the situation of spontaneous symmetry breaking and the phase transition is of thermal origin. On the other hand, for high enough excitation energies (high temperatures), the field is insensitive to the potential barrier, its expectation value becomes zero and the symmetry of the system is restored. These symmetric states are related to the height of the potential barrier $V(0) = m^4/4\lambda$. In the case of quantum field theory at zero temperature, the symmetry is restored by quantum fluctuations, while in classical statistical mechanics, the symmetry is restored by thermal fluctuations. When both quantum and thermal effects are present, the situation is physically similar - usually, thermal effects overwhelm quantum effects.

The situations just described happen for space dimensions larger than one, as phase transitions are not possible in one dimension [5]. This is very easy to understand for the present model. At zero temperature, the configuration of minimum energy is one of the two minima of the potential. Now, suppose one prepares the system in a way that $\langle\phi\rangle = 1$ and bring the system in contact with a reservoir at finite temperature. In presence of a finite temperature reservoir, thermal fluctuations develop

in the system. But since in one dimension the fluctuations travel the whole system (there is no room for them to ‘‘leak’’ to other directions in the system), kinks (and antikinks) will be formed throughout the system and these give zero average for the field - there is no way to have nonzero average field at finite temperature (in the thermodynamic limit). Still easier to understand is the case of the one-dimensional Ising model: prepare the system with all spins up; bring the system in contact with the reservoir; then some spins flip (spin flip gives rise to a spin configuration that is similar to a kink) and the average of the sum of all spins is therefore zero in the thermodynamic limit. There is no way to obtain a nonzero net magnetization at nonzero temperature (and, of course, zero external magnetic field) - we give a simple argument by Landau explaining the phenomenon in appendix D.

Next, let us discuss numerical results for the one-dimensional (1+1 dimensions) case. We start examining the effect of the noise intensity on $\langle\phi\rangle$, the field averaged over the spatial dimension, for a relatively small lattice - 500 lattice sites. Working with the rescaled quantities defined in eq. (3.120) we simulated eq. (5.13) using periodic boundary conditions, for various values of the noise intensity γ . The results are shown in Fig. 5.2. We used as initial condition a field configuration as if it was subject to a single-well potential,

$$\phi_n(t=0) = \phi_0 + 0.01 * (1 - 2r_n), \quad (5.16)$$

with $\phi_0 = 0.01$, where r_n is uniformly distributed between 0 and 1. We let the field evolve up to $\tau = 4 \times 10^5$ time steps of length $\delta = 10^{-4}$ and considered the average over 30 noise realizations.

Initially, one sees that for zero noise ($\gamma = 0$), the field evolves from its initial value close to zero to the minimum of the potential, at $\phi = +1$. For a negative initial of the field, $\phi_0 = -0.01$, the final value of the evolution would be $\phi = -1$, the other minimum of the potential. As one turns on noise, we see that the barrier tunneling effects start restoring the symmetry for $\gamma \sim 10^{-3}$. For $\gamma = 0.3$ we have that $\langle\phi\rangle \approx 0$ and the symmetry is essentially restored. For this initial condition, the thermal fluctuations can rapidly restore the parity symmetry. This is not surprising: because at early times the field ϕ fluctuates around the initial average of 0.01, very close to zero, it can be easily forced to either side of the barrier by the thermal fluctuations. On averaging over many noise realizations, since the noise term has zero mean, the average

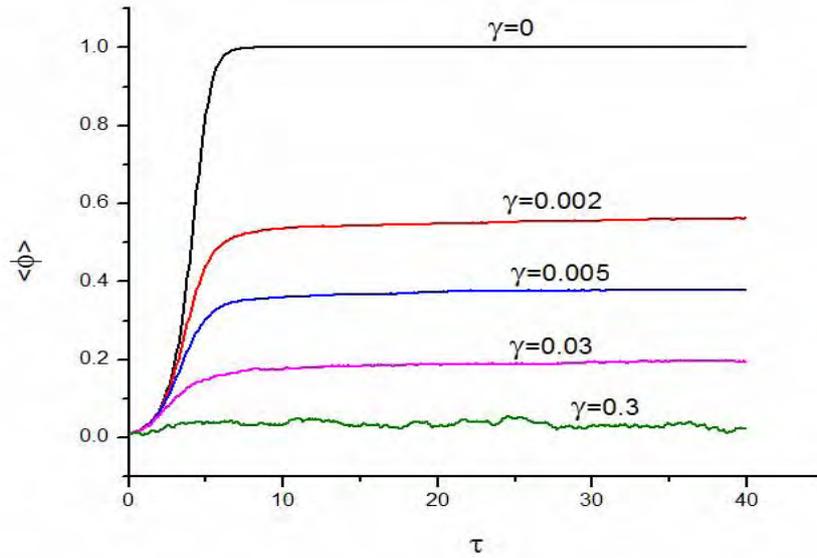


Figure 5.2: Plot of the expectation value of the field over time for different values of the noise intensity, for an initial condition $\phi_0 = 0.01$.

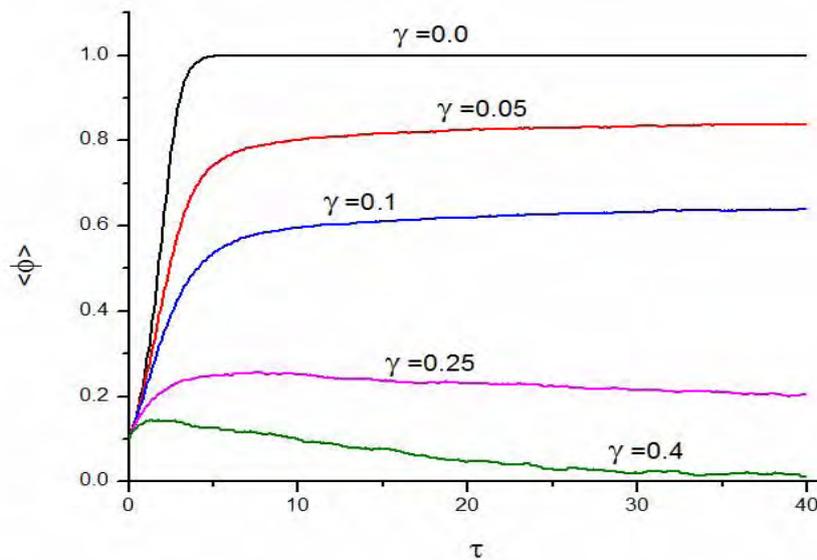


Figure 5.3: Plot of the expectation value of the field over time for different values of the noise intensity, for an initial condition $\phi_0 = 0.1$.

ϕ is obviously zero. Obviously, for any finite value of the noise, the average of the field is zero *in the thermodynamic limit* - here it is nonzero essentially because of the finite extent of the system.

For an initial condition with $\phi_0 = 0.1$ in eq. (5.16), the situation is different and one can clearly see in Fig. 5.3 that the field “thermalizes” to a positive value. We see here that the symmetry is

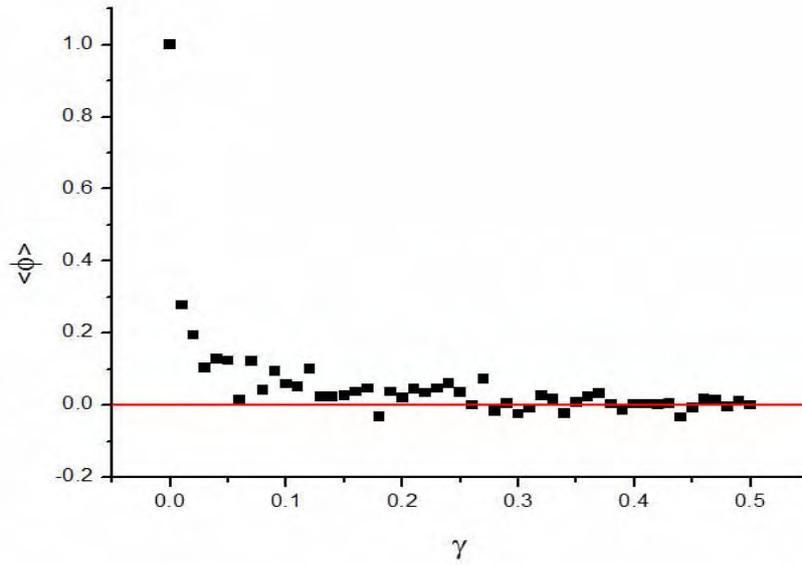


Figure 5.4: Expectation value of the field for different values of the noise intensity. The horizontal line shows $\langle \phi \rangle = 0$. The initial conditions was centered at $\phi_0 = 0.01$.

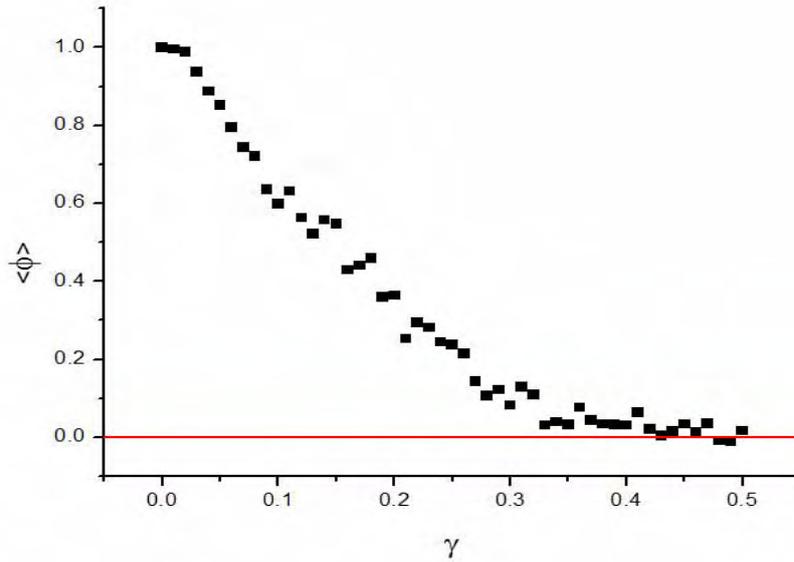


Figure 5.5: Expectation value of the field for different values of the noise intensity. The horizontal line shows $\langle \phi \rangle = 0$. The initial conditions was centered at $\phi_0 = 0.1$.

essentially restored for $\gamma \gtrsim 0.4$. To further investigate this phenomenon we performed simulations of the double-well potential using the aforementioned numerical parameters for 50 values of γ between 0 and 0.5. The

results are shown in Figs. 5.4 and 5.5. Again, we stress the nonzero value of the ‘‘thermalized’’ field is due to the relatively small lattice size. In addition, for the present case with $\phi_0 = 0.1$, the value of $\tau_{max} = 40$ is relatively small.

The aim of the discussion here was to stress that in one dimension one must be very careful with the lattice size and τ_{max} . Although we will not make an exhaustive study here, it is known that to have reliable predictions one must use a large lattice - to be effectively close to the thermodynamic limit. To illustrate this point, we follow Ref. [33] and use a lattice of 16,384 sites, with $h = 0.125$ and $\delta = 0.001$, $\tau_{max} = 50$ and noise intensity $\gamma = 1$. This gives a lattice extent of $L = 2,048$. For such a large lattice, surface/volume effects become negligible, so that one is practically in the thermodynamic limit [5]. Results are shown in Fig. 5.6 - we choose to show results in the interval $-20 \leq x \leq 20$. Clearly, although we have started from a symmetry-broken initial configuration, $\phi_0 = +1$, the equilibrium value has (volume) average zero - the solution is a train of kinks and antikinks (to obtain geometrically better-defined kinks and antikinks, τ_{max} must be increased). On the other side, for three dimensions, the use of relatively small lattice sizes, of the order of $L = 100$, is enough to study symmetry breaking/restoration [12, 31].

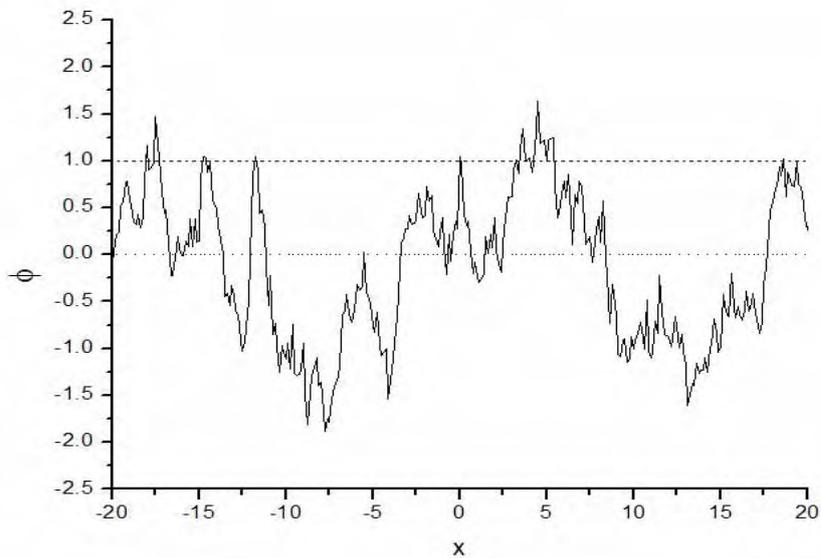


Figure 5.6: The solution $\phi(x, \tau = 50)$ of the GLL equation in the interval $-20 \leq x \leq 20$ for a lattice with 16,384 sites and one noise realization. The dashed line indicates the initial condition $\phi_0 = 1$.

5.2.2 Noise perturbation theory

The aim in this subsection is to investigate numerically the solution of the GLL equation using noise perturbation theory described in Chapter 4. We start discussing the behavior of the perturbative series for the small lattice case presented in the previous section. We start with the situation with $\phi_0 = 0.1$, i.e., where the noise intensity is not strong enough to change sensibly the effective minimum. We examined this initial condition for $\gamma = 0.005$ and $\gamma = 0.015$, with the same number of time and spatial steps as the previous simulations. The results are shown in Figs. 5.7 and 5.8.

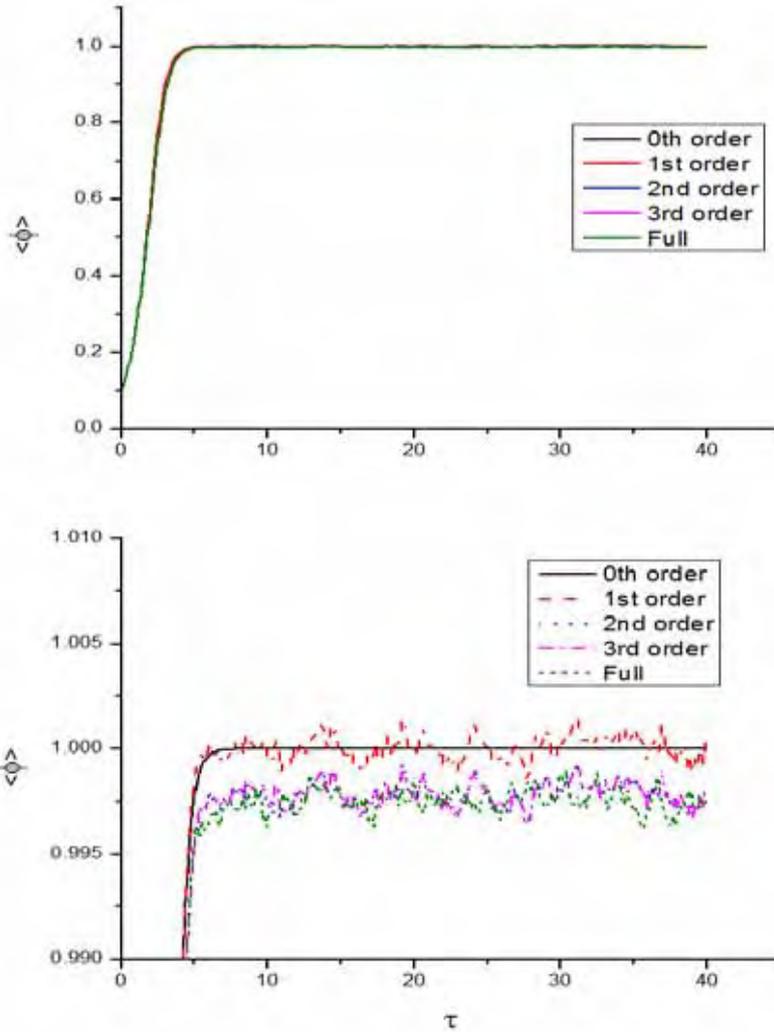


Figure 5.7: Time dependence of $\langle \phi \rangle$ for $\gamma = 0.005$, for $\phi_0 = 0.1$.

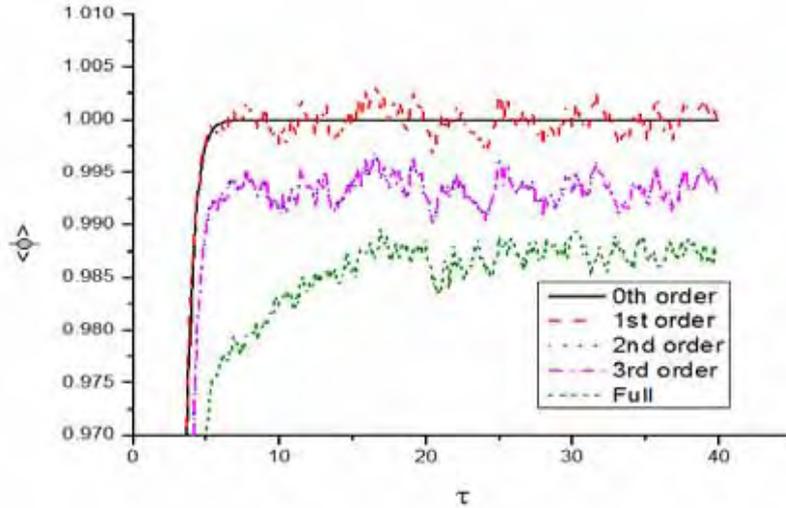
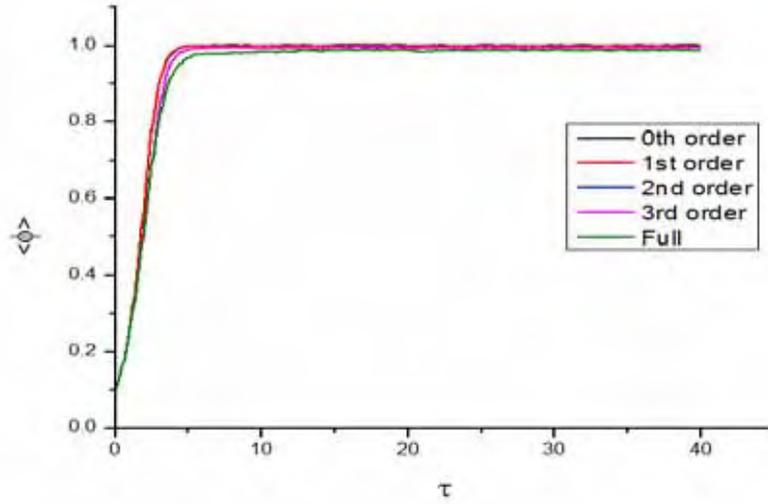


Figure 5.8: Plot of $\langle \phi \rangle$ over time for $\gamma = 0.015$, for $\phi_0 = 0.1$.

In the graphs, the third order correction was very small compared to the second order one and can not be seen on the plots. It is clear that in Fig. 5.7 the second order correction was enough to perfectly account for all thermal effects and the perturbed solution agreed with the full one. However, in Fig. 5.8 we see that the fluctuations are already sufficiently strong so that not even the third order correction gave results in perfect agreement with the complete solution, although the difference is less than 1% for the equilibrium value.

As a stress test to this method, we have applied it to an uniform initial solution, namely $\phi_0 = 1$, in a lattice of length $L = 2,048$ (16,384

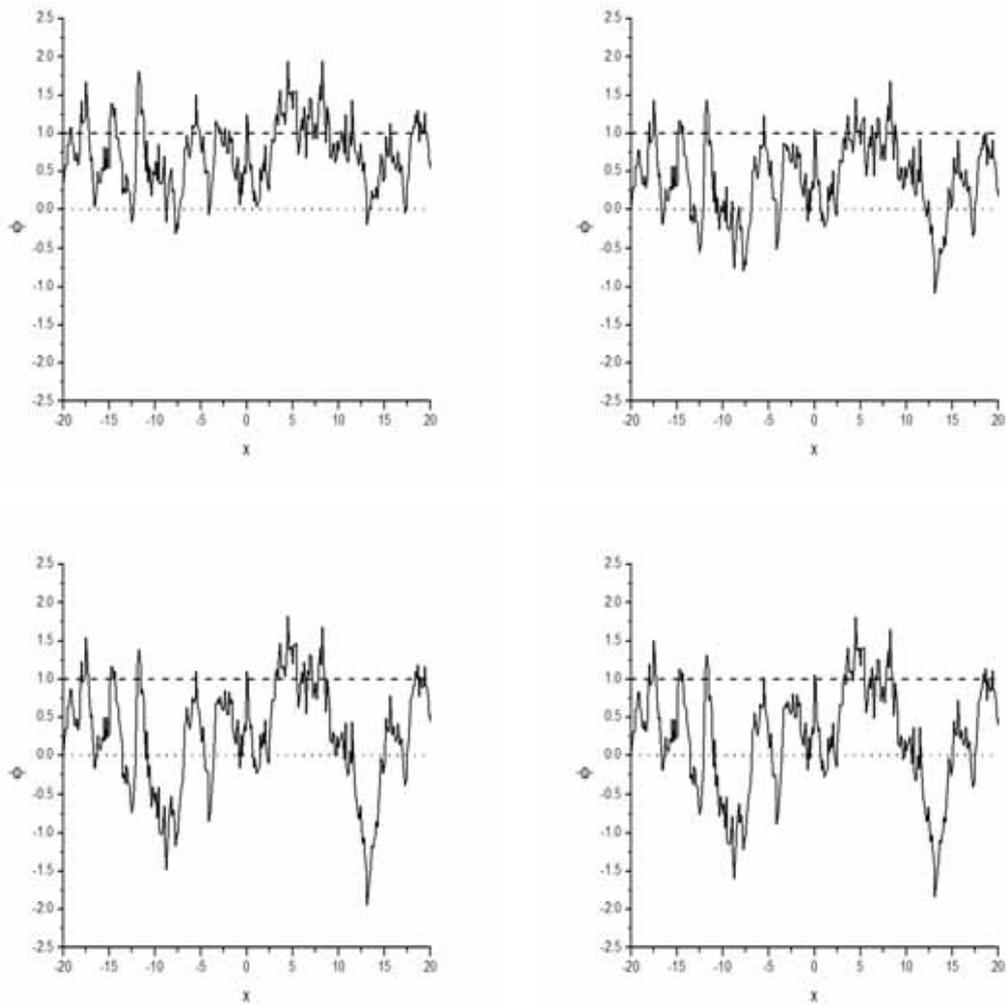


Figure 5.9: 1st and 2nd (top) and 3rd and 4th (bottom) order noise perturbations with the kink solution as the 0th order solution. In all figures the dashed lines represent the noise-free solution $\phi = 1$ and the dotted lines represent $\phi = 0$. The field is sampled in the region $-20 \leq \phi \leq 20$ for a lattice of length $L = 2,048$.

sites of size $h = 0.125$) with $\tau_{max} = 50$ and $\gamma = 1$. In this situation the initial condition is very far from the equilibrium configuration with zero (volume) average. We see in Fig. 5.9 that at increasing order in the perturbative series the field fluctuations increase in amplitude and its mean value seems to move towards zero. The fourth order correction seems to have a non-zero average value, unlike the full solution, Fig 5.6. We conclude here that the size of the lattice affects crucially the

behavior of the long-time solutions of a one-dimensional GLL equation. We also see that the perturbative method worked quite well with a sufficiently large lattice, in the sense that as contributions of higher order are incorporated, the respective solutions tend to create kinks and antikinks as the complete solution does.

5.2.3 Kinks

To study how thermal fluctuations affect the kink solutions we once again simulated a scalar field, this time subject to the double-well potential $V_p(\phi)$ of section 3.3.2 for $p = 1$ under suitable boundary conditions, namely $\phi_{0,m} = -1$ and $\phi_{n+1,m} = 1$ for all m , and let the noise-free field evolve for $T = 10^6$ time steps of length $\delta = 10^{-3}$ on a lattice of 2000 points until equilibrium. Then we turned on the noise field for different values of the intensity γ for another 3×10^6 time steps. The results were averaged over 15 noise realizations and are shown in Fig. 5.10.

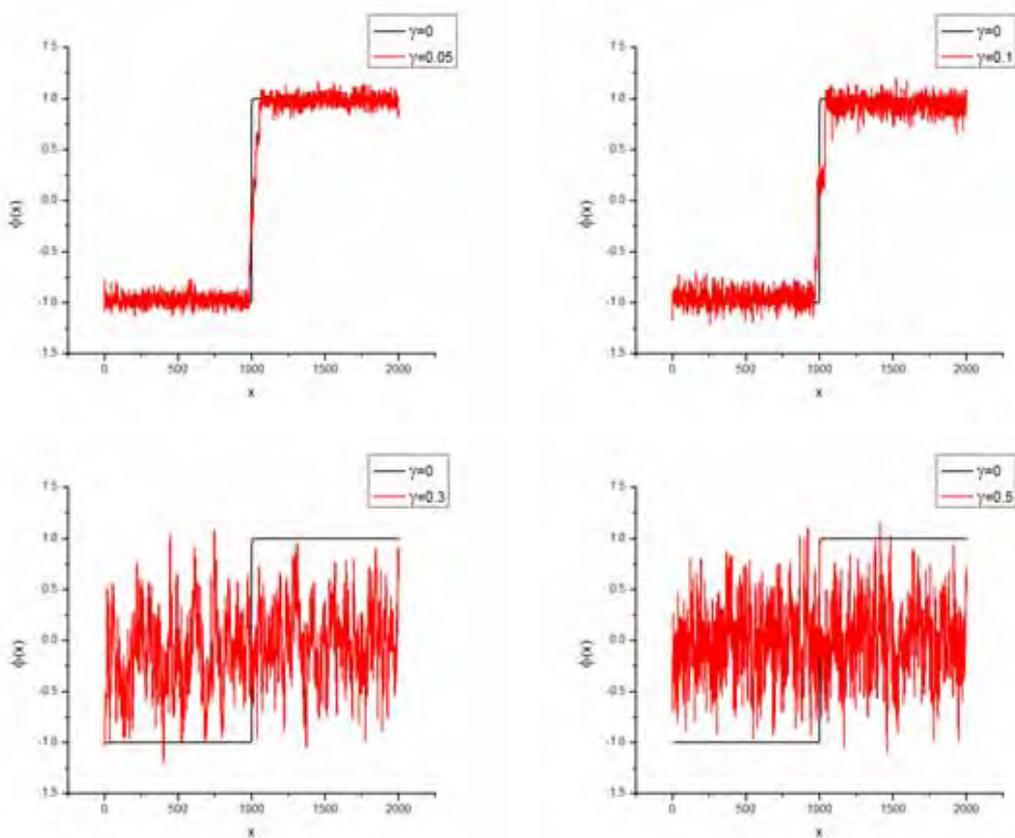


Figure 5.10: Solutions for different noise intensities γ with initial condition given by the kink.

We can see that for $\gamma \lesssim 0.1$ the interaction with the thermal phonons makes the kink fluctuate around the minima but still maintains its characteristic shape. Nevertheless, for slightly higher intensities, $\gamma = 0.3$ and 0.5 , the noise fluctuations are strong enough to destroy the single kink. Again the order of magnitude of γ where the kink solution is disrupted below the value calculated in [33].

We have conducted the same study using a lattice with 16,384 sites to minimize finite size effects. The results are plotted in Fig. 5.11 - the results shown are for a single noise realization. Clearly, at $\gamma = 0.5$ the solution still has a kink-like shape, in the sense that one still sees a background kink superimposed by noisy disturbances, although a few solutions with $\phi(x) = 0$ for $x \neq 0$ are already visible. We stress that although we have shown the solution in a restricted interval only, it should be clear the figure extends in both directions of the lattice maintaining the same overall shape. For $\gamma = 0.75$, one cannot notice a background kink anymore. Ref. [33] claims that $\gamma \simeq 0.6$ for the critical value. This value is clearly consistent with the results we obtain, although ours seem to be closer to $\gamma \simeq 0.5$. We stress once more that this transition is not a true phase transition; what is seen here is the dominance of thermal phonons over topology.

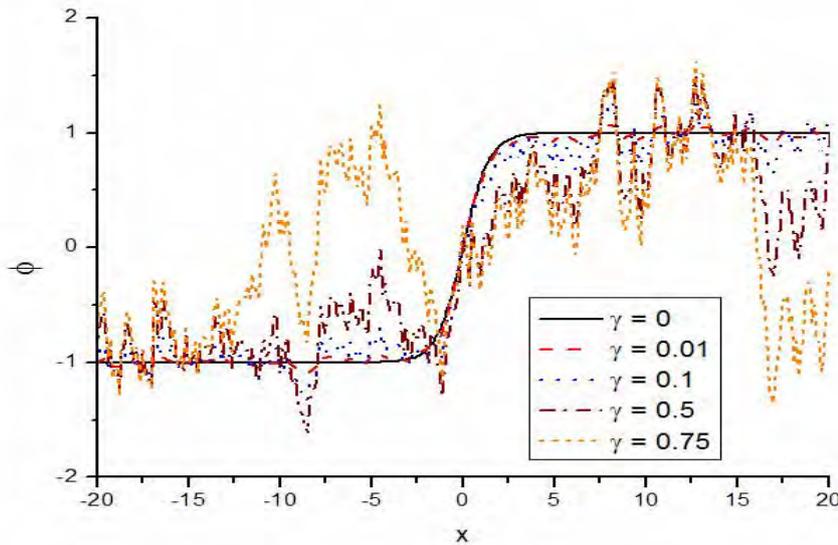


Figure 5.11: Plot of the equilibrium kink solutions in the interval $-20 \leq x \leq 20$ for various values of γ in a lattice of 16,384 sites.

Based on the previous results we were able to study two-kink structures in contact with a thermal reservoir - these had only been analyzed at zero temperature before. Kink solutions for the V_p family of potentials of section 3.3.2 with $p \geq 3$ are more sensitive to the noise since the height of the potential barrier is lower. To make this point clear, we have plotted in Fig. 5.12 the potentials $V_p(\phi)$ defined in eq. (3.138). One sees that the barriers separating the minima of the $p = 3$ potential are much lower than the barrier separating the minima of the double well - for higher values of p the height of the barriers is even lower. For lower barriers, low-intensity noises are able to disturb the $p \neq 1$ kinks very easily. One consequence is the easy destruction of the plateau around $x = 0$ - seen in Fig. 3.5 - of the ϕ_p kinks given by eq. (3.139).

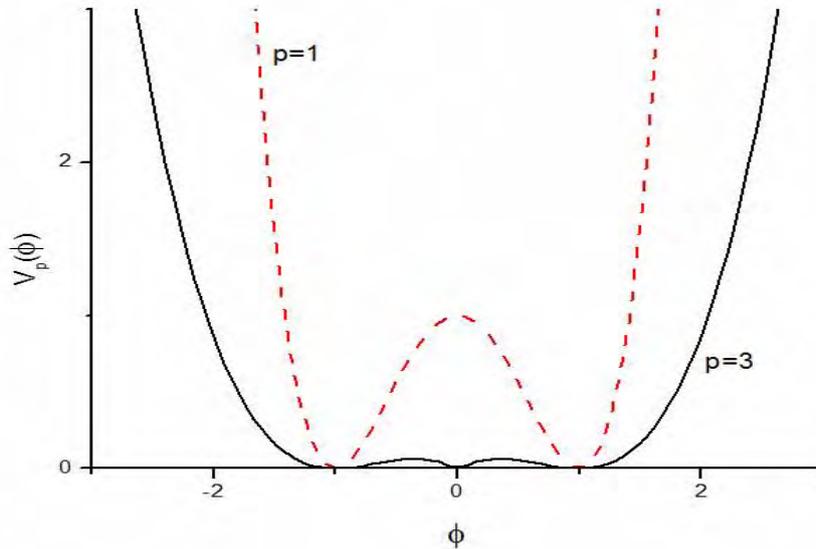


Figure 5.12: Potentials $V_p(\phi)$ defined in eq. (3.138) for $p = 1$ and $p = 3$.

The search for the critical value of γ for such potentials is much more difficult than for the double well, since one is now dealing with very small numbers. We have made an exploratory study of the effect of noise on such structures. We have solved the GLL equation with the potential $p = 3$:

$$\frac{\partial \phi}{\partial \tau} = \nabla^2 \phi + 2\phi - \frac{2}{3} \phi^{1/3} - \frac{4}{3} \phi^{5/3} + \xi, \quad (5.17)$$

on a lattice of 16,384 sites, with $h = 0.125$, $\delta = 0.001$ and $\tau_{max} = 50$, for various values of noise intensity. The results are collected in

Fig. 5.13.

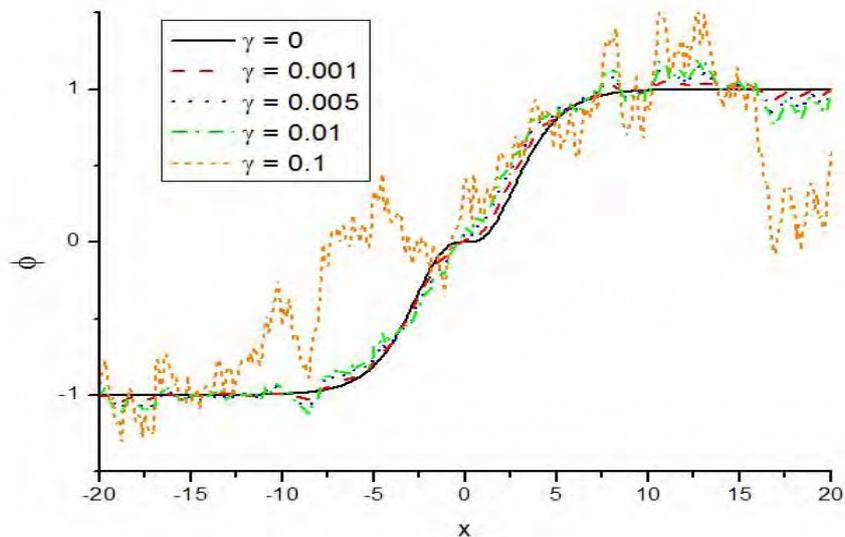


Figure 5.13: Solution $\phi(x)$ corresponding to $V_3(x)$ for various values of γ using a lattice of 16,384 points.

It is possible to see that for $\gamma = 0.001$ the shape of the kink near $x = 0$ deviates mildly from the plateau observed for the noise-free solution. For higher intensities, on the other hand, thermal fluctuations make the field insensitive to this symmetric minimum and eventually destroy this two-kink solution. For larger values of the noise intensity, the single kink starts to be destroyed.

We close this discussion mentioning that studies based on the GLL equation can be complemented with other methods to determine more precisely the critical value of γ . A particularly interesting approach is the use of the transfer operator method [47] in conjunction with the variational method - this approach was used in Ref. [33] for the double-well kink. The transfer operator method allows to write the partition function as a sum of the eigenvalues of this operator, in a way that one ends up with a problem similar to an eigenvalue problem in quantum mechanics. The use of the traditional variational method has shown its value in quantum mechanics and can be equally useful for finding the free-energy of the problem with $V_p(\phi)$. Another method is simply to solve numerically the eigenvalue problem for the transfer operator, as done in Ref. [48] for the double-well kink.

Chapter 6

Conclusions and future perspectives

In this work we have studied the Ginzburg-Landau-Langevin equation, sometimes called time-dependent Ginzburg-Landau equation, in a variety of contexts, focusing on how they arise and describe physical phenomena. We have also performed a perturbative expansion and numerical simulation of such equations to determine its behavior for one-dimensional systems.

In Chapter 2, we presented a brief introduction to Statistical Mechanics through the extremization of the Shannon information entropy. The partition function for the most common statistical ensembles, namely the micro-canonical, canonical and grand-canonical, were constructed after the thermodynamic entropy was identified with the maximum of the information entropy. Then we studied the Langevin equation: how it was first used to describe the Brownian motion and find the associated Fokker-Planck equation for the probability distribution of the Brownian particle velocities. After, we sketched how it could be used as a toy-model for a non-equilibrium system relaxing to the equilibrium and made a few considerations regarding the entropy of such systems.

In Chapter 3, we showed a few situations where the Ginzburg-Landau-Langevin equation are used. In the context of phase transitions, systems in which an order parameter changes its behavior when certain parameters reach critical values, we argued that the GLL equation can be used to model the actual evolution over time of the order parameter, which usually varies much slower in time than the microscopic variables. Also, it presents an alternative way to generate system configurations that obey certain probability distributions by looking at its long time limit. An active research field in which the GLL equation is preferred over Monte Carlo simulations is quantum field theory at non-zero chemical potential. Then we reviewed the path integral formulation of quantum

mechanics and quantum field theory to show Parisi and Wu's method of stochastic quantization where the dynamical variables obey a GLL equation in a higher-dimensional space. Finally we discussed defect structures in field theory. In $1+1$ dimensions 'kink' structures arise as non-perturbative and non-dispersive solutions to the equations of motion. For higher dimensional spaces such coherent structures, called domain walls, are not stable unless the potential is deformed to support vortexes or monopoles. In contact with a heat bath thermal fluctuations (phonons) interact with the defect structures and may disrupt them. Field configurations consisting of kinks and thermal phonons can be generated and studied via a GLL equation.

In Chapter 4, we investigated a perturbation scheme in which the physical field is expanded in powers of the noise intensity. In situations where the Ginzburg-Landau free energy (or Euclidean action in stochastic quantization) is a complicated nonlinear function or functional of the dynamical variables, or even nonlocal in space and time, and the noise, which may be colored, is weak the method of Noise Perturbation Theory may be used to write a noise-free equation of motion for the zeroth order solution and a set of *linear* stochastic differential equations for the higher order corrections. We then gave two applications of such method: stochastic cosmological inflation, a model that studies quantum effects over the early universe, and the statistical mechanics of coherent structures interacting with low intensity thermal phonons.

Finally, in Chapter 5, we presented results of numerical simulations of the Ginzburg-Landau-Langevin equation. The finite differences method was presented as a way to translate the continuous differential equations into discrete functions which in turn may be simulated by a computer. To evaluate the effect of the noise intensity in the Langevin equation we performed numerical computations of a one dimensional field with a self-interaction in the form of a double-well potential for various values of the intensity of the noise correlation function, γ . We concluded that $\gamma \gtrsim 0.4$ allows thermal fluctuations to drive the field away from the minimum energy (constant) solution, i.e., it becomes insensitive to the potential barrier. During this study the importance of finite size effects became clear. In one dimension, at the thermodynamic limit, the field should relax to zero for any $\gamma > 0$, however in small lattices we observed a non-zero equilibrium value. Simulations using larger lattices were performed and confirmed that the solution tends to relax to $\phi = 0$.

Next, we analysed the performance of the noise perturbation theory by applying it to different situations. As a general rule, the method works well for large lattices and low-intensity noises. At last, we simulated the $V_p(\phi)$ potential of section 3.3.2 for $p = 1$ and $p = 3$ for different values of γ and compared them with the zero temperature solution. Again we have seen that, for our small lattice, intensities above 0.3 destroy the one kink ($p = 1$) solutions, as the finite size effects are overwhelmed by thermal fluctuations. In the larger lattice the kink ceased to exist for $\gamma \geq 0.5$, in qualitative agreement with [33]. The two-kink solution of V_3 exhibited a plateau near $x = 0$ for $\gamma \approx 0$ which is rapidly destroyed by the fluctuations for slightly higher intensities, and intensities of the order 10^{-1} were sufficiently strong to completely disrupt the kinks.

As a conclusion to this work, we can say that the Ginzburg-Landau-Langevin equation appears in a wide variety of contexts, from classical to quantum mechanics, relativity and statistical mechanics. Through the stochastic noise it models environmental effects over physical observables, such as thermal phonons interacting with a stable defect structure, quantizes an Euclidean field theory, where the noise takes the quantum fluctuations into account, and allows the study of the vicinity of a phase transition.

Our results have shown that care must be taken when performing and analyzing numerical simulations: finite size effects can lead to non-zero values to order parameters in one dimension, pointing to a phase transition that does not exist - large lattices, to make finite size effects negligible must be used. Then we studied thermal effects on kink solutions, in one dimension, or domain walls, for deformed potentials that can be reduced to a $1D$ theory. Our expectation that the kink should be destroyed above a critical value of the intensity of the noise correlation function was easily seen in our simulations: the phonons dominate topological field configurations and their fluctuations effectively bring the different minima together. Further investigations have shown that the Noise Perturbation Theory applied to the Ginzburg-Landau-Langevin equation in one dimension provide a good approximation scheme for low-intensity noise. The method also represents a useful approximation for larger lattices and higher dimensions, as demonstrated in [12] where it is applied to a double-well potential in 3 dimensions.

As a future perspective, we envisage to extend our study to the color dielectric model for QCD described in Appendix C. The inclusion of

fermions makes the model particularly interesting to study finite temperature effects in the context of the physics of the quark gluon plasma. The destruction of the topological field configurations of the scalar field in the model due to temperature effects would provide a model for the deconfinement transition in QCD. Moreover, since introduction of quantum and finite temperature effects in the model will lead to a complicated action, see e.g. Ref. [49], the use of noise perturbation theory might be very useful to include quantum and thermal corrections in a systematic manner. On a more formal basis, our study can also be extended to the pure gauge sector of QCD where instanton solutions, kinks in the (Euclidean) time direction, are candidates to explain non-perturbative phenomena. Instantons lead to the formation of the gluon condensate [50], the topological susceptibility needed to cure the $U(1)$ paradox [51] and provide a beautiful mechanism for the spontaneous chiral symmetry breaking [52]. Although instantons do not lead to confinement, they do generate a potential for a heavy quark-antiquark pair that grows with distance at intermediate separations [53].

Appendix A

Stochastic Integration

Definition

In this appendix we follow closely [54] to define integrals of the form

$$\int_{t_0}^t G(t') d\omega(t') \quad (\text{A.1})$$

where

$$d\omega(t') = \xi(t') dt' \quad (\text{A.2})$$

and $\xi(t')$ is a standard Gaussian white noise, i.e., with zero mean and unity variance. Equations like eq. (A.1) cannot be treated as usual Riemann integrals as will be shown below.

Let us now take $G(t') = \omega(t')$ for a moment. We divide the interval $[t_0, t]$ in n subintervals $[t_i, t_{i+1}]$, $i = 0, \dots, n$, and define $\tau_i \in [t_i, t_{i+1}]$ as an intermediate point for each interval. Then, from the definition of integral,

$$\int_{t_0}^t \omega(t') d\omega(t') = \lim_{n \rightarrow \infty} S_n = \lim_{n \rightarrow \infty} \sum_{i=0}^n \omega(\tau_i) [\omega(t_{i+1}) - \omega(t_i)], \quad (\text{A.3})$$

where it is assumed that $|t_{i+1} - t_i| \rightarrow 0$ as $n \rightarrow \infty$. In the case of stochastic integrals the value of S_n depends on the particular choice of τ_i , as can be seen by calculating the average value

$$\langle S_n \rangle = \sum_{i=0}^n \langle \omega(\tau_i) [\omega(t_{i+1}) - \omega(t_i)] \rangle. \quad (\text{A.4})$$

From the definition of $\xi(t)$ we have that

$$\begin{aligned} \langle \omega(t)\omega(t') \rangle &= \int_{t_0}^t \int_{t_0}^{t'} \langle \xi(t_a)\xi(t_b) \rangle dt_a dt_b \\ &= \int_{t_0}^{\min(t,t')} dt_a = \min(t, t') - t_0, \end{aligned} \quad (\text{A.5})$$

and we may evaluate $\langle S_n \rangle$ to be

$$\begin{aligned}\langle S_n \rangle &= \sum_{i=0}^n [\min(\tau_i, t_{i+1}) - \min(\tau_i, t_i)] \\ &= \sum_{i=0}^n [\tau_i - t_i],\end{aligned}\tag{A.6}$$

since, by definition, $t_i \leq \tau_i \leq t_{i+1}$.

The *Ito stochastic integral* $I[G]$ is defined as the mean-square limit of the partial sums S_n with $\tau_i = t_i$,

$$\begin{aligned}I[G] &= \int_{t_0}^t G(t') d\omega(t') = \text{ms-} \lim_{n \rightarrow \infty} \left\{ \sum_{i=0}^n G(t_i) [\omega(t_{i+1}) - \omega(t_i)] \right\} \\ &\Leftrightarrow \lim_{n \rightarrow \infty} \langle (S_n - I[G])^2 \rangle = 0.\end{aligned}\tag{A.7}$$

Nonanticipating functions

In order for the above results to be valid the function $G(t)$ must belong to a class of functions called *nonanticipating functions*. This is a physically reasonable concept, otherwise causality would be violated. If $G(t)$ is the solution of some stochastic differential equation it should only depend on $\omega(t')$ for $t' < t$. Formally it means that, for any t and s with $t < s$, $G(t)$ is statistically independent of $\omega(s) - \omega(t)$. In other words, the function G at time t is independent of the behavior of the Wiener process in the future of t . Symbolically,

$$\langle G(t)[\omega(s) - \omega(t)] \rangle = \langle G(t) \rangle \langle \omega(s) - \omega(t) \rangle, \quad \text{for } t < s.\tag{A.8}$$

Ito's rules

Given the definitions of Ito stochastic integrals and nonanticipating functions we may demonstrate the so-called Ito's rules for stochastic calculus, schematically written as

$$\langle d\omega(t) \rangle = 0\tag{A.9}$$

$$\langle d\omega(t)d\omega(t) \rangle = dt\tag{A.10}$$

$$\langle d\omega(t)^N \rangle = 0, \quad \text{for } N > 2.\tag{A.11}$$

These rules are to be understood as the mean-square limit of stochastic integrals, e.g.

$$\begin{aligned} \langle d\omega(t) \rangle = 0 &\Leftrightarrow \text{ms-} \lim_{n \rightarrow \infty} \left\{ \sum_{i=0}^n G(t_i) [\omega(t_{i+1}) - \omega(t_i)] \right\} = 0 \\ &\Leftrightarrow \lim_{n \rightarrow \infty} \left\langle \left\{ \sum_{i=0}^n G(t_i) [\omega(t_{i+1}) - \omega(t_i)] - 0 \right\}^2 \right\rangle = 0. \end{aligned} \quad (\text{A.12})$$

We write $G_i \equiv G(t_i)$ and $\omega_i \equiv \omega(t_i)$ and split the above limit as

$$\begin{aligned} &\lim_{n \rightarrow \infty} \left\langle \left\{ \sum_{i=0}^n G_i [\omega_{i+1} - \omega_i] - 0 \right\}^2 \right\rangle \\ &= \lim_{n \rightarrow \infty} \left\langle \sum_{i=0}^n G_i^2 [\omega_{i+1} - \omega_i]^2 + \sum_{i>j=0}^n G_i G_j [\omega_{i+1} - \omega_i] [\omega_{j+1} - \omega_j] \right\rangle. \end{aligned} \quad (\text{A.13})$$

Now, assuming $G(t)$ to be a nonanticipating function,

$$\begin{aligned} &\lim_{n \rightarrow \infty} \left\langle \left\{ \sum_{i=0}^n G_i [\omega_{i+1} - \omega_i] - 0 \right\}^2 \right\rangle \\ &= \lim_{n \rightarrow \infty} \left\{ \sum_{i=0}^n \langle G_i^2 \rangle \langle [\omega_{i+1} - \omega_i]^2 \rangle + \sum_{i>j=0}^n \langle G_i G_j \rangle \langle [\omega_{i+1} - \omega_i] \rangle \langle [\omega_{j+1} - \omega_j] \rangle \right\} \\ &= \lim_{n \rightarrow \infty} \left\{ \sum_{i=0}^n \langle G_i^2 \rangle [t_{i+1} - t_i]^2 \right\}. \end{aligned} \quad (\text{A.14})$$

As long as $G(t)$ is a well-behaved function the above limit vanishes, thus proving eq. (A.9). The other rules may be proved in a similar manner.

Ito's lemma

The Langevin equation

$$\frac{dx}{dt} = \alpha(x, t) + \beta(x, t)\xi(t), \quad (\text{A.15})$$

can be written as an Ito stochastic differential equation (SDE),

$$dx = \alpha(x, t)dt + \beta(x, t)d\omega(t), \quad (\text{A.16})$$

which should be interpreted as

$$x(t) = x(t_0) + \int_{t_0}^t \alpha[x(t'), t']dt' + \int_{t_0}^t \beta[x(t'), t']d\omega(t'), \quad (\text{A.17})$$

for all t and t_0 . Consider now a function of $f(x, t)$. In ordinary calculus the differential equation describing f can be obtained from the chain rule. However, since x obeys a SDE we expect f to be a stochastic function itself. An infinitesimal increment in df reads

$$\begin{aligned}
df &= f(x + dx, t + dt) - f(x, t) \\
&= \frac{\partial f}{\partial x} dx + \frac{\partial^2 f}{\partial x^2} dx^2 + \frac{\partial f}{\partial t} dt + \mathcal{O}(dt^2, dx^3) \\
&= \frac{\partial f}{\partial x} \alpha dt + \frac{\partial f}{\partial x} \beta d\omega + 2 \frac{\partial^2 f}{\partial x^2} \alpha \beta dt d\omega \\
&\quad + \frac{\partial^2 f}{\partial x^2} \beta^2 d\omega^2 + \frac{\partial f}{\partial t} dt + \mathcal{O}(dt^2, d\omega^3). \tag{A.18}
\end{aligned}$$

The deterministic part of df can be obtained by averaging out the random terms,

$$\langle df \rangle = \left[\frac{\partial f}{\partial x} \alpha + \frac{\partial^2 f}{\partial x^2} \beta^2 + \frac{\partial f}{\partial t} \right] dt + \mathcal{O}(dt^2), \tag{A.19}$$

where we have used the Ito's rules. The stochastic part of df is given by

$$df - \langle df \rangle = \frac{\partial f}{\partial x} \beta d\omega. \tag{A.20}$$

Therefore, neglecting higher order terms in dt , we arrive at the Ito's lemma:

$$df = \left[\frac{\partial f}{\partial x} \alpha + \frac{\partial^2 f}{\partial x^2} \beta^2 + \frac{\partial f}{\partial t} \right] dt + \frac{\partial f}{\partial x} \beta d\omega. \tag{A.21}$$

Appendix B

Elliptic sine function

The equation of motion for the field $\phi(x, t)$ in the quartic double-well potential of section 4.4 is

$$\frac{\partial^2 \phi}{\partial t^2} = \frac{\partial^2 \phi}{\partial x^2} + m^2 \phi - \lambda \phi^3. \quad (\text{B.1})$$

Assuming $\phi(x, t) = uf(\kappa\gamma(x - vt) + \delta)$, where v is the kink velocity and $\gamma = (1 - v^2)^{-1/2}$, it can be written as

$$u\kappa^2 f'' + m^2 uf - \lambda u^3 f^3 = 0. \quad (\text{B.2})$$

Defining a constant k such that

$$\kappa^2 = \frac{m^2}{1 + k^2}, \quad (\text{B.3})$$

the equation for $f(y)$, $y = \kappa\gamma(x - vt) + \delta$, can be put in the form

$$\frac{d^2 f}{dy^2} + (1 + k^2) - 2k^2 f^3 = 0, \quad (\text{B.4})$$

with

$$\frac{2k^2}{1 + k^2} = \frac{\lambda u^2}{m^2}, \quad (\text{B.5})$$

which has the Jacobi Elliptic Sine function of modulus k

$$f = u \operatorname{sn}(y + \delta|k) \quad (\text{B.6})$$

as solution [34, 35].

The elliptic sine function is defined in terms of the elliptic integral of the first kind

$$y(\varphi|k) = \int_0^\varphi \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}} \quad (\text{B.7})$$

as

$$\operatorname{sn}(y|k) = \sin(\varphi(y|k)), \quad (\text{B.8})$$

where $\varphi(y|k)$ is the inverse function of $y(\varphi|k)$. It is a double periodic meromorphic function of period $4K(k^2)$ where

$$K(k^2) = \operatorname{sn}(\pi/2|k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}}, \quad (\text{B.9})$$

and we have that

$$\operatorname{sn}(y + 2nK(k^2) + 2n'iK(k^2)|k) = (-1)^n \operatorname{sn}(y|k) \quad (\text{B.10})$$

for $n, n' = 0, \pm 1, \pm 2, \dots$. From here on we take $n' = 0$ since an imaginary argument would introduce poles to the elliptic sine function [35]. The quarter period $K(k')$ is monotonically increasing with k and diverges at $k = 1$, as shown in fig. (B.1).

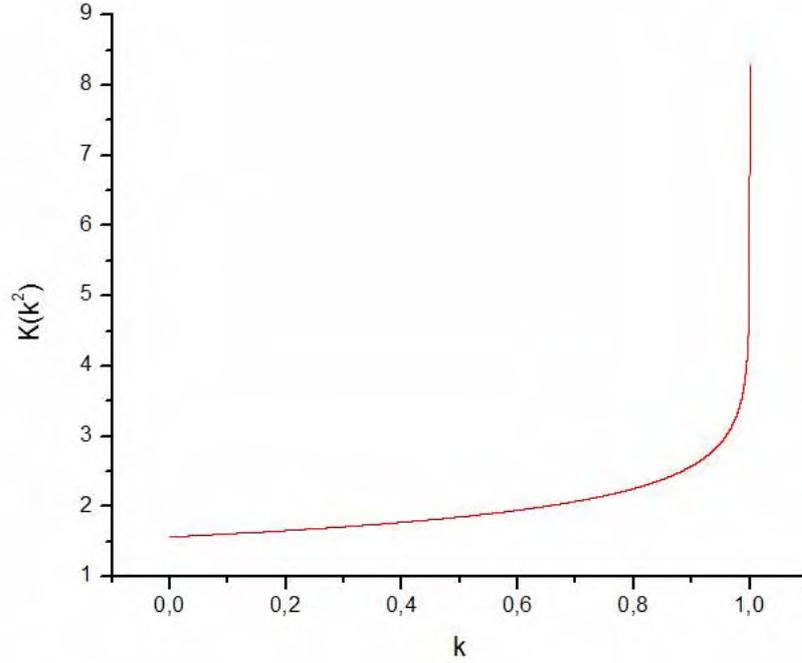


Figure B.1: Graph of the complete elliptic integral of modulus k .

A graph of $\operatorname{sn}(y|k)$ is shown in fig. (B.2) for various values of k .

For situations where the field is contained in a confined space, let us consider the static kink solutions for the field in a $1 - D$ box of length $2L$. In the limit $k \rightarrow 1$ the elliptic sine function reduces to

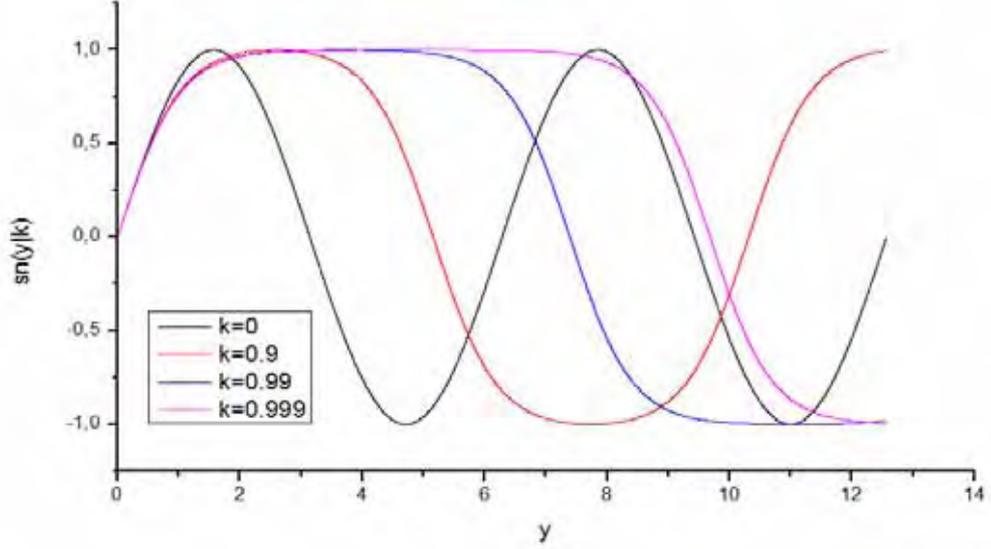


Figure B.2: Graph of the Jacobi elliptic sine of modulus k .

the hyperbolic tangent which interpolates between the field values that minimize the potential, $\phi = \pm m/\sqrt{\lambda}$, and so the boundaries of the box the field must satisfy $\text{sn}(y + 2L) = -\text{sn}(y)$, which gives the relation

$$nK(k^2) = L \quad (\text{B.11})$$

between the modulus, box length and the number of nodes $n \geq 0$, provided that

$$\delta = \frac{1}{2} [1 - (-1)^{n+1}] K(k^2). \quad (\text{B.12})$$

The width of the transition across a kink is given by

$$\Delta(k) = \frac{2}{\kappa} = 2\sqrt{\frac{1+k^2}{m^2}}. \quad (\text{B.13})$$

As $k \rightarrow 1$ the transition width sharpens to $\Delta = \sqrt{8/m^2}$. Thus, the maximum number n_S of kinks in the box is

$$n_S = \frac{2L}{\Delta} = L\sqrt{\frac{m^2}{2}}. \quad (\text{B.14})$$

We can determine the value of the modulus k in terms of the kink density n/n_S using the relation

$$\left(\frac{n}{n_S}\right)^2 = \frac{1}{K(k^2)(1+k^2)}. \quad (\text{B.15})$$

In the essentially non-linear region $k \sim 1$ the density of kinks approaches zero, i.e., it is dilute relative to the geometrical maximum density.

Appendix C

Derivation of eq. (3.130)

Lagrangian densities that support domain walls in $D+1$ dimensions, like the one in eq. (3.130),

$$\mathcal{L} = \partial_\mu \phi \partial^\mu \phi - \frac{1}{2r^{2D-2}} W_\phi^2(\phi) \quad (\text{C.1})$$

for $\mu = 0, \dots, D+1$, can be thought of as an effective Lagrangian coming from a more fundamental theory. Following [40] we consider a simplified Lagrangian for the color dielectric model [55] in the absence of fermions [56]

$$\mathcal{L}' = \partial_\mu \phi \partial^\mu \phi - f(\phi) F^{\mu\nu} F_{\mu\nu}. \quad (\text{C.2})$$

This model describes a non-minimal coupling between a real scalar field and the gauge field A_μ through the dielectric function $f(\phi)$. The gauge field strength tensor $F_{\mu\nu}$ is defined as usual, namely, $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. For spherically symmetric static configurations in the electric sector, i.e.,

$$E_i = F_{0i} = E_i(r), \quad (\text{C.3})$$

$$\sum_{i=1}^D E_i E_i = E_r^2, \quad (\text{C.4})$$

$$\partial_0 E_i = 0, \quad (\text{C.5})$$

$$B_i = \varepsilon_{ijk} F^{jk} = 0, \quad (\text{C.6})$$

where $i, j = 1, \dots, D$, the equation of motion for the matter field is

$$\partial_\mu \partial^\mu \phi - \frac{1}{2} f'(\phi) E_r^2 = 0, \quad (\text{C.7})$$

with $f'(\phi) = df/d\phi$. The equation of motion for the gauge field, in general, reads

$$\partial_\mu [f(\phi) F^{\mu\nu}] = 0, \quad (\text{C.8})$$

and for the above described configuration it reduces to

$$\partial_i [f(\phi)E^i] = \nabla \cdot [f(\phi)\vec{E}] = 0. \quad (\text{C.9})$$

Writing the above equation in spherical coordinates we have

$$\frac{1}{r^{D-1}} \frac{\partial}{\partial r} [r^{D-1} f(\phi) E_r] = 0 \quad (\text{C.10})$$

which has as solution

$$E_r = \frac{k}{r^{D-1} f(\phi)}, \quad (\text{C.11})$$

for some real constant k . Redefining $f(\phi)$ to absorb k we arrive at

$$\partial_\mu \partial^\mu \phi - \frac{1}{2r^{2D-2}} \frac{f'(\phi)}{f^2(\phi)} = 0 \quad (\text{C.12})$$

which can be derived from eq. (C.1) if we make the identification $f(\phi) = 1/V(\phi)$, for the potential V defined in eq. (3.130).

Appendix D

Landau's argument on phase transitions

A simple argument by Landau [57] explains why one-dimensional systems cannot exhibit phase transitions. By analysing how different configurations affect the Helmholtz free energy $F = E - TS$ it is possible to determine whether different phases can coexist in a given system. The existence of a phase transition depends on the competition of ordered states, which minimize the internal energy E , and unordered states, which increase the entropy S .

We begin by exploring the phase transition in a two-dimensional toy-model similar to an Ising system. We show that there is a certain temperature value T_c below which larger domains tend to form, while for $T > T_c$ domains are smaller. Then we move to the $1D$ case and see that for any temperature $T > 0$ the formation of small domains is favored.

Two dimensions

Let us consider a system composed of two distinct phases defined on N sites of a two-dimensional lattice with free boundary conditions*. Let us also assume that the energy is increased by an amount J when two neighboring sites are in different states. A domain is characterized by a group of neighboring sites in the same phase embedded in a larger group of sites in the other phase. This domain has a wall of length L and thus the energy difference from the ground-state is

$$\Delta E = LJ. \tag{D.1}$$

On the other hand, given L interfaces between phases there are at least 2^L states available, giving

$$\Delta S = k \ln \Omega \geq kL \ln 2 \tag{D.2}$$

*In the thermodynamic limit $N \rightarrow \infty$ the boundary effects are negligible.

as a lower bound for the entropy increase. The free energy increment then reads

$$\Delta F = \Delta E - T\Delta S = L[J - kT \ln 2]. \quad (\text{D.3})$$

That is, for a $2D$ system we have the following scenarios, with $T_c \equiv J/(k \ln 2)$:

- if $T < T_c$ an increase in the number of interfaces raises the free energy, thus making it unfavorable. Sites on the same phase will tend to be together, e.g., two separated sites will have a total of $L = 8$ interfaces, while two neighboring sites will have $L = 6$;
- if $T > T_c$ larger values of L will be favored, as they low the free energy. Domains will be smaller and scattered over the lattice;
- finally, if $T = T_c$ all domain sizes are possible since the free energy increment does not depend on L .

It is worth stressing that the above value for the critical temperature T_c is a mean field estimative for this Ising-like model.

One dimension

Let us consider now a one dimensional system also composed of two distinct phases defined in a lattice of N sites, and assume again that the interface energy is J . In such system the number of different states with m interfaces between the two phases is given by [58]

$$\Omega = \frac{N!}{m!(N-m)!}, \quad (\text{D.4})$$

and thus the free energy reads

$$F = F_0 + mJ - kT \ln \left(\frac{N!}{m!(N-m)!} \right). \quad (\text{D.5})$$

where F_0 is the ground state energy. It is easy to see that the free energy is lowered when, for example, $m = 1$ for *any* $T > 0$, in the thermodynamic limit $N \rightarrow \infty$. This motivates us to look for the value m^* of m that minimizes F . The phase space volume Ω has a maximum at $m = N/2$, and thus we assume that $m^* \sim N$. Using Stirling's approximation for the thermodynamic limit we have

$$F \approx m^*J - kTm^* \ln \left(\frac{N e}{m^*} \right). \quad (\text{D.6})$$

Differentiating F with respect to m^* and equating to zero gives

$$m^* = Ne^{-J/(kT)}. \quad (\text{D.7})$$

In other words, for any nonzero temperature the appearing of phase interfaces is favored - in contrast to the $2D$ case. Moreover, all configuration with the same number of interfaces have the same energy and thus are equally probably to happen. In an Ising system, for example, a state with m spins down and $N - m$ spins up is as likely to happen as the one with $N - m$ spins up and m down. Averaging over all (energetically) equivalent states always gives a zero net magnetization, except for $T = 0$.

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