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Multi-loop expansion in lattice Φ^4 -theory using stochastic quantization

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Orientador

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Dedication

Há poucos meses, pareceria loucura me imaginar vivendo uma devastadora catástrofe global, onde não se pode abraçar, beijar, ou compartilhar momentos especiais com pessoas queridas. Pareceria insanidade deixar de ver as notícias para não perder as esperanças, com o número de mortes pelo mundo ultrapassando o incontável. Pareceria pesadelo pensar que ficaria meses e meses trancafiado entre quatro paredes sem o calor dos abraços e apertos de mão de meus amigos. Mas a maior insanidade de todas, é que enquanto escrevia estas linhas, tudo isso acontecia simultaneamente.

2020 tem sido um ano marcado por muitas perdas, lágrimas e saudade, e será para sempre lembrado como aquele em que máscaras eram quase tão importantes quanto nossas vestes. Mas também será lembrado como o ano em que sentimos falta das coisas mais corriqueiras da vida. Aquelas que muitas vezes passam inteiramente despercebidas, como um simples sorriso nos rostos familiares do dia-a-dia. Por sorte, sempre fui rodeado por pessoas únicas que me proporcionaram inestimável companhia do início ao fim, e especialmente durante o período de tormentas na pandemia do coronavírus. A essas pessoas dedico o meu trabalho.

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Abstract

A variety of techniques were devised in the last century to consistently describe the quantum theory of fields and connect it to experiments in the context of particle physics and fundamental interactions. One of these techniques is the so-called stochastic quantization, which uses the Langevin equation to generate stochastic processes where a noise source plays the role of quantum fluctuations. In this work, we explore stochastic quantization on a lattice framework to approach quantum field theory through numerical simulations. As the only known fully non-perturbative regularization method, lattice simulations offer a promising route to handle the awkward divergencies arising from the ultraviolet spectrum of quantum theories. In this scenario, we carry out many multi-thread numerical simulations in 2, 3 and 4 dimensions to compute non-perturbative correlation functions of the Euclidean Φ^4 theory with and without symmetry breaking. We also approach stochastic quantization with multi-loop expansions in powers of $\hbar$ to show its order-by-order consistency. In this approach, the quantum corrections result from the solution of an infinite set of coupled Langevin equations. These equations were truncated and numerically solved with a code developed in this work up to large powers of $\hbar$. We demonstrate that the results agree in high precision with analytical predictions from standard perturbation theory for several values of the couplings constant within a given interval. Finally, we sketch a numerical renormalization procedure to obtain physical parameters in the continuum limit.

Key-words: Quantum field theory - Stochastic Quantization - Numerical Simulations.

Fields of knowledge: Quantum field theory - Statistical Mechanics - High-Performance Computing.

Resumo

Uma variedade de técnicas foi desenvolvida no século passado para descrever a teoria quântica de campos de forma consistente e conectá-la aos experimentos no contexto da física de partículas e interações fundamentais. Uma dessas técnicas é a chamada quantização estocástica, que usa a equação de Langevin para gerar processos estocásticos onde uma fonte de ruído faz o papel das flutuações quânticas. Neste trabalho, exploramos a quantização estocástica na rede para abordar a teoria quântica de campos através de simulações numéricas. Sendo o único método conhecido de regularização não-perturbativa, as simulações na rede oferecem uma rota promissora para lidar com as complexas divergências que surgem do espectro ultravioleta de teorias quânticas. Neste cenário, executamos várias simulações numéricas em paralelo em duas, três e quatro dimensões para calcular funções de correlação não-perturbativas da teoria escalar euclidiana Φ^4 com e sem quebra espontânea de simetria. Também abordamos a quantização estocástica com expansões em muitos loops em potências de $\hbar$ para mostrar sua consistência ordem a ordem. Nessa abordagem, as correções quânticas resultam da solução de um conjunto infinito de equações de Langevin acopladas. Essas equações foram truncadas e resolvidas numericamente com um código desenvolvido neste trabalho até altas potências de $\hbar$. Nós demonstramos que os resultados concordam em alta precisão com as previsões analíticas da teoria de perturbação padrão para alguns valores da constante de acoplamentos dentro de um dado intervalo. Por fim, esboçamos um procedimento de renormalização numérica para obter parâmetros físicos no limite do contínuo.

Palavras-chaves: Teoria quântica de campos - Quantização estocástica - Simulações na rede

Áreas do conhecimento: Teoria quântica de campos - Mecânica estatística - Computação de alta performance.

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Chapter 1

Introduction and Motivation

In the last decades, lattice methods have played an essential role in modern problems of High-Energy Physics (HEP). The efficient computation of physical quantities through robust lattice simulations have boosted our understanding of fundamental particles and their interactions. In this scenario, lattice QCD stands as one of the most prominent and rapidly evolving areas within HEP. It uses importance sampling algorithms to compute expectation values from the Euclidean path integral, using field configurations with a Boltzmann weight. Among the achievements of lattice simulations within the Standard Model are the precise determination of the quark masses, and the strong force contribution to the magnetic moment of the muon (for details, we refer to the reviews [[Sanfilippo, 2015](#), [Meyer and Wittig, 2019](#)], respectively).

Despite their remarkable success in Euclidean space, importance-sampling-based algorithms are known to fail in Minkowski-space problems, and for HEP under extreme conditions. In these cases, the path integral has a non-positive probability measure due to a complex factor in the exponent, rendering importance sampling meaningless. A situation where the method is said to suffer from a numerical sign problem or, more generically, a complex phase problem [[Goy et al., 2017](#)]. Therefore, from the theoretical side, the understanding of HEP theories under extreme conditions has been hindered by the lack of tools

to treat the sign problem. On the other hand, from the experimental side, new hadronic colliders, like FAIR and NICA, which aim to investigate the high chemical potential region of the QCD phase diagram, have triggered the efforts to find a solution to the sign problem. With Monte Carlo hindered by this problem, we need to look for alternative solutions that can shed some light on finite chemical potential systems in QFT.

In 1981, another approach, called stochastic quantization, was developed by Parisi and Wu as an attempt to circumvent the problem of Gribov ambiguity in non-Abelian gauge theories by avoiding gauge-fixing [Parisi et al., 1981]. In turn, stochastic quantization uses the Langevin equation, from non-equilibrium statistical mechanics, to generate stochastic processes whose thermal equilibrium gives the correct distribution as dictated by the Euclidean path integral. Since the '80s, many authors have explored applications of this technique in plenty of physical contexts, which go across Ginzburg-Landau systems [Attanasio, 2013], cosmological inflation [Kunze, 2006], where the inflaton field is modeled through the stochastic dynamics, fermionic fields [Ridky, 1995], gauge-invariant fields [Kapoor, 2018], semi-classical gravity [dos Reis et al., 2019], etc. Some authors have also argued that stochastic quantization might provide a route towards the solution to the sign problem, and thus lead to a better understanding of finite density QCD [Aarts, 2009].

In this work, we apply stochastic quantization to study the Φ^4 -theory as a toy model in the lattice framework through a novel simulation code. This code was developed from scratch as part of this investigation to comply with our needs in simulating the Langevin equation. We use this code to compute the exact n -point correlation functions by solving the full Langevin equation with quartic interaction. We also apply the so-called Noise Perturbation Theory to expand the field in powers of $\hbar$ within the Langevin equation and derive a set of coupled differential equations providing quantum corrections to the zeroth-order. We truncate and implement this set within our code to obtain its solution up to order $\hbar^{10}$. Thence, we compute numerical propagators in the perturbative framework and compare with available analytical expressions up to 2 loops, showing the accordance between the

two even for large coupling. Even though we stop at 2 loops, we argue that this method can be straightforwardly implemented to go far beyond the analytical perturbation theory. Therefore, this text is organized as follows: in chapter 2, we review stochastic processes, which form the underpinnings of stochastic quantization. In chapter 3, we use the concepts from chapter 2 to discuss the main aspects of stochastic quantization, and review its applications to non-relativistic quantum mechanics and quantum field theory. In chapter 4 we formulate stochastic quantization on the lattice and use our novel lattice code to reproduce some results obtained by others. Afterward, in chapter 5, we present our new results on high-order expansion in 2 and 4-dimensions. In chapter 6, we review a numerical renormalization scheme from previous works and apply it to our case-study, generating new data in 2, 3, and 4 dimensions. In chapter 7, we finally conclude and discuss future perspectives in the field.

Chapter 2

Review of Stochastic Processes

Natural phenomena driven by statistical fluctuations are among the most common happenings in daily life. For centuries, the physics of such phenomena has been studied by plenty of eminent scientists. With the outcome of statistical mechanics, it became possible to describe the stochastic behavior of a huge set of interacting objects. While Newtonian mechanics gives the precise motion of one or two particles interacting, statistical mechanics focus on average properties from myriads of particles. Take for instance the famous two-body problem, like two heavy-weight asteroids orbiting one another in the Kuiper belt. Although to carry out all calculations requires considerable effort, the equations of motion for this problem were shown to be solvable analytically. With a third asteroid in the surroundings, only under special symmetry conditions can they be treated exactly. However, as we continue to jam hundreds, billions, trillions of bodies together, single orbits and velocities start to become unimportant, for collective behavior begins to dominate over individual features. In this scenario, determinism gives space to stochastic fluctuations, and Newtonian mechanics gives space to statistical mechanics, reducing uncountable microscopic degrees of freedom to a small set of relevant parameters. Even though statistical mechanics and Newton's theory bear intimate relationships, pioneers like Ludwig Boltzmann never succeeded in the proof that the former comes from the latter. Instead, they resigned themselves to the use of it, in

the description of statistically fluctuating systems, since the laws describing a huge number of objects are surprisingly simpler than the ones for just several of them. As a consequence of that, statistical mechanics triggered an enormous breakthrough in the study of many-particle systems and their thermodynamic effects. Therefore, in the next pages, we focus on reviewing the most prominent physical and mathematical aspects of stochastic systems.

2.1 Brownian motion

Before rushing to the operational part, we go through a short digression to introduce the historical context. During an eminent experiment by the Scottish botanist Robert Brown in 1827, a grain of pollen was seen, through the lens of a microscope, performing a mysterious motion over the surface of the water. This quirky behavior raised the question of why pollen, and other light objects, had an odd tendency to jiggle while floating on water. Think of a toy boat sailing across the plane waters of a beach on a mild day, without wind, waves, or external impulses, and it seems unnatural to expect the boat to randomly sway sideways. So what is the big deal with an ordinary grain of pollen? The point is that toy boats are usually macroscopic objects, billions of times larger than tiny water molecules, and thus collisions between them do not affect the boat's trajectory significantly. However, pollen particles are typically only a few micrometers long, and therefore much more susceptible to collisions and changes in the direction of their motion. Due to the homogeneous bath of molecules in the medium, hits happen isotropically and they force the pollen to shake, producing an overall disordered motion. A phenomenon that is known as Brownian motion, and thenceforth the starting point of this review.

In mathematical terms, Brownian-moving particles have their stochastic trajectory determined by a very simple differential equation:

$$dW_t = \eta(t)dt \tag{2.1.1}$$

where t is time and η the noise source. In physical terms, the noise source η encodes the information about the haphazard collisions in a medium with several mols of particles¹, which makes it a sort of mathematical summary of the random pushes conveyed by the environment to the substrate embedded on it. To illustrate the origin of the noise source, consider a grain of pollen, like in Robert Brown's experiment, subject to collisions with medium particles in two spatial directions, as in Figure 2.1. The dynamics of this particle may have infinitely

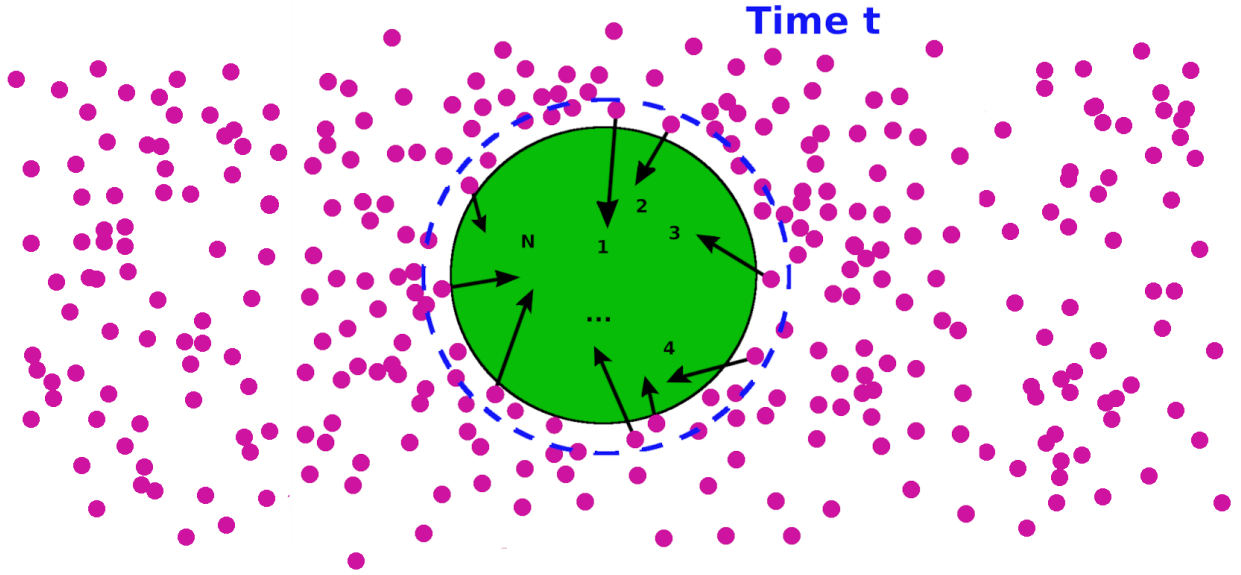


Figure 2.1: At a given instant of time t , we would have a configuration as shown in this figure. The N particles in magenta are colliding with the pollen (green) at time t .

many patterns depending on the choice of η to plug into Eq.(2.1.1). So what functional shape should a random source have? Very likely, no other but an ill-defined expression is suitable to describe $\eta(t)$. However, remember that the only important degree of freedom is the average effect of the noise upon the particle, and the probability distribution beneath this average is smooth and well-defined. Pictorially, $\eta(t)$ can be regarded as vector whose components are proportional to the sum of the forces provided by the medium particles in the x and y directions. Considering $\mathbf{F}^{(i)}$ to be the force vector aforementioned, the components of $\eta(t)$ can be written as an average of forces bestowed by each particle (in magenta) colliding with

¹Recall that a mol has roughly 10^{23} particles.

the pollen (in green) at time t :

$$\eta_x(t) \propto \frac{F_x^{(1)} + F_x^{(2)} + \dots + F_x^{(N)}}{N} \quad \eta_y(t) \propto \frac{F_y^{(1)} + F_y^{(2)} + \dots + F_y^{(N)}}{N} \quad (2.1.2)$$

According to a recurrent theorem in probability theory, known as the central limit theorem, if the number of particles N in the ensemble is huge (we consider 10^{23} to be so!) then the probability distribution underlying $\eta_x(t)$ and $\eta_y(t)$ is well approximated by a Gaussian distribution. In formal terms, we can state it in several different ways, among which we present the version by Lindeberg and Lévy:

Theorem 1. *Suppose $\{F_x^{(1)}, F_x^{(2)}, \dots, F_x^{(N)}\}$ is a set of N random numbers with mean μ and variance $\sigma^2 < \infty$. Then as N approaches infinity, the quantity $\sqrt{N}(\eta_x(t) - \mu)$ approaches a Gaussian distribution with mean zero and variance σ^2 .*

This pictorial view, alongside the central limit theorem, helps us to develop an intuition about why the bell-shaped distribution is a natural choice in the context of Brownian motion. An identical version of this theorem is valid when we switch x by y in the previous statement, and so it would be if we considered extra spatial directions. Notice that we did not need to specify with which probability the numbers $F_x^{(i)}$ are selected. Even if we tried, it would be useless spending time on a binge to determine with what force each particle shocks with the pollen. Luckily, Nature makes collective behavior prevail over individual behavior when N is large enough, and the probability dictating the sum of these forces becomes nearly Gaussian anyway. A stochastic process of this type is characterized as a Wiener process and it bears the following properties:

- $W_0 = 0$.
- W_t evolves with independent steps, *i.e.*, the incrementation step at time $t + dt$ does not depend on the step at time t .
- The steps of W_t are selected according to a Gaussian distribution with mean 0 and

variance dt .

- It has a non-neglectable square variation dW^2 , which is equivalent to time variation inside stochastic integrals: $dW^2 \sim dt$.

From now on, we focus on the more operational aspects of Wiener processes. These aspects attempt to convey a meaning to calculus in the context of stochastic processes, and they come in two main varieties, each of them is approached next.

2.2 Itô calculus

As far as stochastic processes are concerned, it turns out that the usual definitions of Riemannian calculus are not appropriate. Ultimately, we want to solve Eq.(2.1.1) for a given set of Gaussian numbers $\eta(t)$ and predict the average trajectory of the Brownian particle. Due to the stochastic nature of the noise source η , conventional derivation and integration concepts no longer apply. Therefore, they must be modified in order to encompass the needs of stochastic dynamics. Recall that in ordinary calculus, we define the Riemannian integral of a function $f(x)$ inside the interval $[a, b]$, given a partition $\{a = x_0 < x_1 < \dots < x_N = b\}$, as the limit of partial sums of rectangular areas:

$$\int_a^b f(x)dx \equiv \lim_{N \rightarrow \infty} \sum_{n=1}^N f(x_{n-1})(x_n - x_{n-1}) \quad (2.2.1)$$

Moreover, we could also extend this idea to a more general concept of integral, for instance, regarding the integration measure not as a variable, but as a smooth function of x . This extension leads to the definition of the Riemann-Stieltjes integral of $f(x)$ with respect to another function $\omega(x)$:

$$\int_{\omega(a)}^{\omega(b)} f(x)d\omega(x) \equiv \lim_{N \rightarrow \infty} \sum_{n=1}^N f(x_{n-1})[\omega(x_n) - \omega(x_{n-1})] \quad (2.2.2)$$

In the special case of $\omega(x) = x$, we recover the commonplace definition of Riemannian integral. The two sums in the right-hand sides of Eqs.(2.2.2) and (2.2.2) have the remarkable property of converging to a unique value for their correspondent left-hand sides regardless of the exact point whereby we draw the rectangles. In this sense, we could have replaced $f(x_{n-1})$ in the definitions above by the rightmost choice $f(x_n)$, the midpoint $f((x_n + x_{n-1})/2)$ or any other point within the interval $[x_n, x_{n-1}]$ and these integrals would still be unique. Giving a step further, suppose we want to compute an integral similar to Eq.(2.2.2), but with f and α depending not on x , but on the Brownian variable $X_t \equiv X(t)$. Naming this integral Y_t , this is how it looks like:

$$Y_t = \int_0^t f(X) d\alpha(X) \equiv \lim_{N \rightarrow \infty} \sum_{n=1}^N f(X_{n-1}) [\alpha(X_n) - \alpha(X_{n-1})] \quad (2.2.3)$$

Y_t is called Itô integral and at first sight it seems identical to Eq.(2.2.2). However, as a consequence of X being a stochastic process, the right-hand side of the Itô integral does not necessarily converge to a unique. Instead, depending on the point of reference, Eq.(2.2.3) may or may not equal the Riemman-Stieltjes integral. Indeed, it only does so when we choose the leftmost point in the interval, *i.e.* $f(x_{n-1})$. Notwithstanding this odd property, Itô integrals turn out to be extremely important in the mathematical description of stochastic processes, as we will see throughout this text, for they allow systematic operations with them. Moreover, instead of just analyzing how X_t evolves with time, we might be interested in studying the dynamics of functions of that variable. Consider, for instance, an arbitrary function of the Brownian motion, $f(X_t)$. Once we know from Eq.(2.1.1) the behavior of X_t for all times, without difficulties, we can find out the behavior of $f(X_t)$ by computing its variation through Taylor expansion:

$$\begin{aligned} df(X_t) &= f(X_t + dX_t) - f(X_t) \\ &= \cancel{f(X_t)} + f'(X_t)dX_t + \frac{1}{2}f''(X_t)(dX_t)^2 + \dots - \cancel{f(X_t)} \end{aligned}$$

$$= f'(X_t)dX_t + \frac{1}{2}f''(X_t)(dX_t)^2 + \mathcal{O}(3) \quad (2.2.4)$$

Truncating in second order and using Eq.(2.1.1):

$$df(X_t) = f'(X_t)dX_t + \frac{1}{2}f''(X_t)(dX_t)^2 \quad (2.2.5)$$

$$df(X_t) = f'(X_t)dX_t + \frac{1}{2}f''(X_t)dt \quad (2.2.6)$$

Eq.(2.2.6) is known as Itô's lemma and it implies that any function of the Brownian motion $f(X_t)$ also evolves as a stochastic process. Notice that it resembles the familiar chain rule in ordinary calculus, except for the extra term involving the second derivative of $f(X_t)$. Despite the difference, the appearance of this term is the hallmark of Itô calculus and it presents no conceptual flaws whatsoever. Nevertheless, sometimes it might be easier to treat equations if that extra term is absent, not to mention that it would look more familiar given our acquaintance with the chain rule of calculus. Therefore, it is convenient to resort to another very common way of defining stochastic integrals in physics and mathematics. We deal with this alternative in the next section.

2.3 Stratonovich calculus

Stratonovich calculus is a reformulation of Itô's approach that redefines its integral so that the chain rule, as we know it from ordinary calculus, is valid for stochastic processes as well. Since both of them provide consistent mathematical results, whether an Itô or Stratonovich approach should be used is completely dictated by the particular features of the problem. Integration, in the Stratonovich sense, is denoted with an empty circle $\circ$ and is defined as:

$$S_t = \int_0^t f(W) \circ dW \equiv \lim_{N \rightarrow \infty} \sum_{n=1}^N \frac{f(W_n) + f(W_{n-1})}{2} (W_n - W_{n-1}) \quad (2.3.1)$$

To make a connection between Itô and Stratonovich integrals, we start separating the sums above:

$$S_t \equiv \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N f(W_n)(W_n - W_{n-1}) + \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N f(W_{n-1})(W_n - W_{n-1}) \quad (2.3.2)$$

$$S_t = \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N f(W_n)(W_n - W_{n-1}) + \frac{1}{2} Y_t \quad (2.3.3)$$

where in the last line we recognized the second term as the definition of Itô's integral. Now we relate $f(W_n)$ to $f(W_{n-1})$ by Taylor expansion:

$$f(W_n) = f(W_{n-1} + dW) = f(W_{n-1}) + \frac{\partial f(W_{n-1})}{\partial W} dW \quad (2.3.4)$$

Noticing that $dW = W_n - W_{n-1}$ and replacing the expansion above up to order one:

$$S_t = \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N \left[f(W_{n-1}) + \frac{\partial f(W_{n-1})}{\partial W} dW \right] (W_n - W_{n-1}) + \frac{1}{2} Y_t \quad (2.3.5)$$

$$= \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N f(W_{n-1})(W_n - W_{n-1}) + \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N \frac{\partial f(W_{n-1})}{\partial W} (W_n - W_{n-1})^2 + \frac{1}{2} Y_t \quad (2.3.6)$$

$$= \frac{1}{2} \lim_{N \rightarrow \infty} \sum_{n=1}^N \frac{\partial f(W_{n-1})}{\partial W} (W_n - W_{n-1})^2 + Y_t \quad (2.3.7)$$

Since the first term in the right-hand side is just the definition of Itô's integral for the derivative of f , this relation can be written as:

$$S_t = \frac{1}{2} \int \frac{\partial f(W)}{\partial W} dW^2 + Y_t \quad (2.3.8)$$

Recall that Wiener processes have a non-neglectable square measure dW^2 , which can be replaced by dt inside the stochastic integral:

$$S_t = \frac{1}{2} \int \frac{\partial f(W)}{\partial W} dt + Y_t \quad (2.3.9)$$

This is the basic conversion recipe for swapping between Itô and Stratonovich prescriptions. All the content of this chapter forms the foundation for the following topics to be discussed next. In the coming chapter, we will insert stochastic theory in the context of classical mechanics, and finally, extrapolate the ideas to quantum problems.

Chapter 3

Review of Stochastic Quantization

In the last chapter, we reviewed the Brownian motion as the simplest of stochastic processes. To define the concept of stochastic integrals, we used the pure Brownian motion, without any other source of dynamics, and generalized Riemannian integrals to stochastic variables, as originally done by Itô and Stratonovich. In spite of its simplicity, there is a surprisingly large number of systems that can be modeled as Wiener processes, either inside or outside physics. However, considerable attention must be paid to other types of systems that require physics beyond Brownian motion to have their behavior precisely understood. In this chapter, we commence by reviewing the Ornstein-Uhlenbeck process, in the form of the so-called Langevin equation, as the first natural generalization to the Wiener process. This process will be a strong underpinning to prepare the ground to apply stochastic quantization in quantum mechanics, as done by other authors [[Houard and Irac-Astaud, 1992](#), [Namiki, 2008](#)]. In simple terms, stochastic quantization stands as a robust tool for deriving the quantized version of classical theories employing stochastic processes. It also provides a useful conceptual bridge between quantum and statistical physics, playing an important role in numerical simulations. This statement is true in both contexts of quantum mechanics and quantum field theory. We postpone the latter until the next chapter.

3.1 The Langevin equation

Imagine that in the same medium where Brownian motion is taking place, the pollen particle is also subject to a friction force, that tends to dissipate energy. Additionally, suppose we want to access the full dynamics of the particle and predict its trajectory and velocity within this medium. To do so, it requires no more than Newton's second law of classical mechanics:

$$F = m \frac{dv}{dt} \quad (3.1.1)$$

Now, we need to know beforehand which ingredients to plug into the force F . Since the particle is embedded in a fluid, there must be a drift force (F_d) associated with the friction bestowed by the surrounding environment acting against the particle's motion. Not unlike the familiar case of a pointlike object moving across the air, the drift force can be reasonably modeled as proportional to the first power of velocity: $F_d = -\lambda v$. Where λ is a medium-dependent constant that measures the strength of this resistance. The other force, which arises from the endless collisions between the pollen and the microscopic molecules of the medium, is stochastic. Hence, from the interpretation given by Eq.(2.1.2), this force can be very suitably regarded as pure Brownian motion. Putting everything together, we end up with a very simple equation of motion:

$$m \frac{dv(t)}{dt} = -\lambda v(t) + \eta(t) \quad (3.1.2)$$

A first-order stochastic differential equation, describing the velocity of a test particle with mass m at each instant of time, called the Langevin equation. It belongs to a class of stochastic processes named Ornstein-Uhlenbeck, which differs from a Wiener process by a drift term $-\lambda v(t)$, accounting for the resisting environment. Notice that in the case of no resistance ($\lambda = 0$) we recover the Brownian motion equation, with $dW_t \equiv m dv(t)$.

Hitherto we are not able to determine the solution to the Langevin equation since no functional form was specified to the noise. The only thing we know about it is what the central

limit theorem taught us, and it might contain a clue on where to seek the missing information about the noise. Intuitively, the absence of external fields (electric, magnetic, etc.) implies that the collisions on a homogeneous isotropic medium can not have any preferential direction. In other words, by averaging over many collisions for long enough the result should be nearly zero. This condition is indeed one of the criteria used to define the Wiener process in section 2.1. Furthermore, time-averages in statistical mechanics are equivalent to ensemble averages by the ergodic hypothesis, where ensemble means a collection of particles. Therefore, instead of “long enough”, we could think of several replicas of the system with which we average over the different noises in each of them. This is like having a large number of independent copies of the situation illustrated in Figure 2.1. This isotropy feature is translated into the compact notation of stochastic average as $\langle \eta(t) \rangle_\eta = 0$.

In order to guess the second noise property, let us assume the structure of all molecules colliding to be irrelevant, such that they can be approximated by point sources. This assumption constraints the collisions to happen locally, lasting for an infinitesimal time interval, implying that two collisions at different times, say t and t' , have no overlap and are thus completely uncorrelated. Therefore, it seems reasonable to have a proportionality between the correlation function of two noises and a Dirac delta function: $\langle \eta(t)\eta(t') \rangle_\eta \propto \delta(t - t')$, for it must be zero when $t \neq t'$ and infinite (entirely correlated) when $t = t'$. Therefore, we guess the second property should have the form:

$$\langle \eta(t)\eta(t') \rangle_\eta = \alpha\delta(t - t') \quad (3.1.3)$$

where α is a proportionality constant to be determined. Any kind of noise satisfying this property is called white noise, referring to the fact that it receives a contribution from all frequencies¹. To express α in terms of known physical parameters, we search for solutions to the Langevin equation. Using variation of parameters, the solution of Eq.(3.1.2) can be

¹Recall that a Dirac delta can be expressed in Fourier series as an infinite sum of sines and cosines with equal weight.

expressed as:

$$v(t) = v_0 e^{-\lambda t/m} + \frac{1}{m} \int_0^t dt_1 \eta(t_1) e^{\lambda(t_1-t)/m} \quad (3.1.4)$$

And the square velocity is:

$$\begin{aligned} v(t)^2 = & v_0^2 e^{-2\lambda t/m} + \frac{2v_0}{m} e^{-\lambda t/m} \int_0^t dt_2 \eta(t_2) e^{\lambda(t_2-t)/m} + \\ & + \frac{1}{m^2} \int_0^t \int_0^t dt_1 dt_2 \eta(t_1) \eta(t_2) e^{\lambda(t_1+t_2-2t)/m} \end{aligned} \quad (3.1.5)$$

Since the noise function η appearing on the right-hand side depends on the individual motion of each molecule in the medium, in practical terms, it is not possible to know the velocities of each molecule colliding with the test particle. This means it only makes sense to compute the above integrals within average brackets $\langle \cdot \rangle_\eta$. Using the first property to eliminate the average of the second term, the average square velocity is given by:

$$\langle v(t)^2 \rangle_\eta = \langle v_0^2 \rangle_\eta e^{-2\lambda t/m} + \frac{1}{m^2} \int_0^t \int_0^t dt_1 dt_2 \langle \eta(t_1) \eta(t_2) \rangle_\eta e^{\lambda(t_1+t_2-2t)/m} \quad (3.1.6)$$

From Eq.(3.1.3), the equation above becomes:

$$\langle v(t)^2 \rangle_\eta = \langle v_0^2 \rangle_\eta e^{-2\lambda t/m} + \frac{\alpha}{m^2} \int_0^t \int_0^t dt_1 dt_2 \delta(t_1 - t_2) e^{\lambda(t_1+t_2-2t)/m} \quad (3.1.7)$$

$$= \langle v_0^2 \rangle_\eta e^{-2\lambda t/m} + \frac{1}{m^2} \int_0^t dt_1 e^{2\lambda(t_1-t)/m} \quad (3.1.8)$$

$$= \langle v_0^2 \rangle_\eta e^{-2\lambda t/m} + \frac{\alpha}{2\lambda m} (1 - e^{-2\lambda t/m}) \quad (3.1.9)$$

Using this result, the average kinetic energy associated with the motion of the Brownian particle is given by:

$$\langle E(t) \rangle_\eta = \frac{1}{2} m \langle v(t)^2 \rangle_\eta = \frac{1}{2} m \langle v_0^2 \rangle_\eta e^{-2\lambda t/m} + \frac{\alpha}{4\lambda} (1 - e^{-2\lambda t/m}) \quad (3.1.10)$$

At this point, we introduce another fundamental theorem in statistical physics called the

equipartition theorem:

Theorem 2. *Each degree of freedom of any thermodynamic system in thermal equilibrium at temperature T has average energy equal to $k_B T/2$.*

Therefore, in thermal equilibrium, when $t \rightarrow \infty$, the equipartition theorem must hold:

$$\lim_{t \rightarrow \infty} \langle E(t) \rangle_\eta = \frac{1}{2} k_B T = \frac{\alpha}{4\lambda} \quad \therefore \quad \alpha = 2\lambda k_B T \quad (3.1.11)$$

that also gives, for v^2 :

$$\lim_{t \rightarrow \infty} \langle v(t)^2 \rangle_\eta = \frac{k_B T}{m} \quad (3.1.12)$$

and we are finally able to write the complete relations satisfied by the noise:

• **Property 1:**

$$\langle \eta(t) \rangle_\eta = 0 \quad (3.1.13)$$

• **Property 2:**

$$\langle \eta(t)\eta(t') \rangle_\eta = 2\lambda k_B T \delta(t - t') \quad (3.1.14)$$

Properties (3.1.13) and (3.1.14) fully specify the Gaussian shape of the noise $\eta(t)$ since we have the two required moments of the probability distribution. Figure 3.1 shows how the probability distribution of the noise indeed converges to a Gaussian profile for large samples. Even though we have presented the Ornstein-Uhlenbeck process for a special case (when the drift force has the form $-\lambda v$), the Langevin equation describing this process, and also properties 1 and 2, come from far more general principles. Instead of a resisting force proportional to the velocity, we could think of other potential functions and write a more comprehensive equation:

$$m \frac{dv(t)}{dt} = -\frac{\partial U(v, t)}{\partial v} + \eta(t) \quad (3.1.15)$$

where $U(v, t)$ is a generic potential function to which the particle is subject. To restore the special case of Eq.(3.1.2), we simply choose a quadratic potential $U(v, t) = \lambda v^2/2$. After

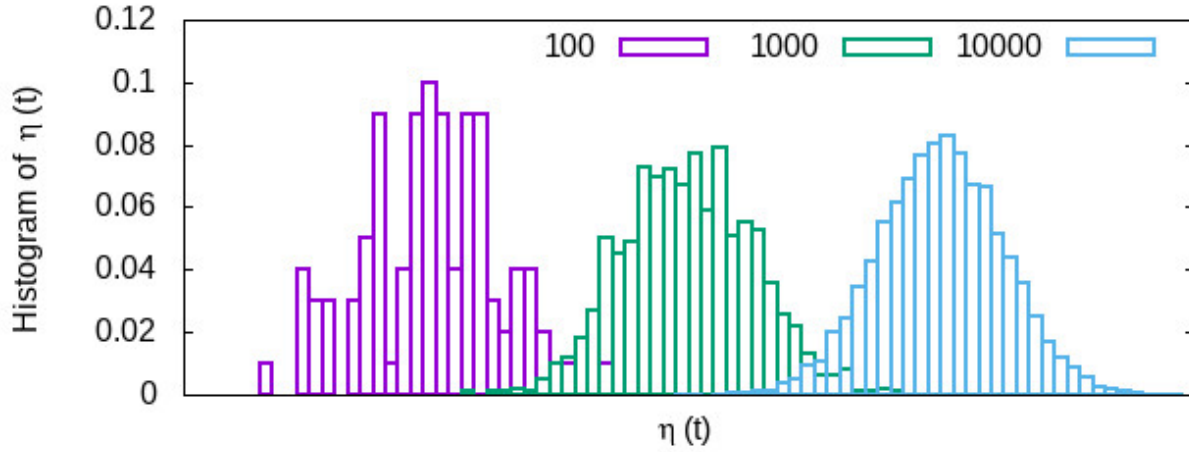


Figure 3.1: Noise probability distributions for samples of different sizes normalized by the amount of random numbers in each sample. The green and the blue histograms have been displaced horizontally for the sake of clarity. Notice how the distribution converges to a Gaussian profile as the sample size increases.

solving the Langevin equation with a given potential $U(v, t)$, our ultimate goal is to compute stochastic averages and draw as much information as we can about the system. How this equation connects statistical mechanics to quantum mechanics we shall see in the next section by looking at the probability distribution underlying $v(t)$ in the Langevin equation.

3.2 The Fokker-Planck equation

Alternatively to having a dynamical equation, like the Langevin equation, solving it and then computing expectation values, as we did in the previous section, we could rush directly to the last part if we had at our immediate disposal the probability distribution that governs the system. In the case of statistical mechanical systems, the latter is usually the preferred route since we often have absolutely no knowledge about the equation describing their dynamics before equilibrium in terms of stochastic processes. What we know is the probability content, after equilibrium, which is encoded in a mathematical object called the partition function. For instance, there is no apparent manner to describe the particles of a van der Waals gas as Brownian-moving entities and still, we can write an elegant partition function that carries

everything to be known about the equilibrium state of the gas. That is why in this section we follow [Namiki, 2008] to interpret the Langevin equation in terms of probability through the concept of partition function. In a more general context, a partition function $\mathcal{Z}$ for a 1-dimensional system at temperature T with potential energy $E(x)$ can be roughly expressed as:

$$\mathcal{Z} \sim \int dx e^{-E(x)/k_B T} \quad (3.2.1)$$

In the quantum realm, as opposed to classical mechanics, we lack the option of describing the complete dynamics of particles, for we never know their exact trajectories. If we did, this would imply a rude violation of Heisenberg's uncertainty principle. Yet, Nature allows us to have access to their full probabilistic content through the probability amplitudes, or wave functions. In the Feynman picture of quantum mechanics, we even have a sort of partition function, as in statistical mechanics, called the path integral. Without details on its derivation (for which we refer the reader to [Zee, 2010]), we present the Feynman partition function in Euclidean space for a system with action $S_E[x]$ as:

$$\mathcal{Z}_F = \int \mathcal{D}x e^{-S_E[x]/\hbar} \quad (3.2.2)$$

with the cursive $\mathcal{D}$ representing functional integration. Considering an arbitrary Ornstein-Uhlenbeck process, represented by the variable $v(t)$, a single stochastic trajectory of this process is given by one particular solution of the Langevin equation with external potential $U(v)$ and a noise ensemble² $\eta(t)$:

$$m \frac{dv(t)}{dt} = -\frac{\partial U(v(t))}{\partial v} + \eta(t) \quad (3.2.3)$$

$$dv(t) = -\frac{1}{m} \frac{\partial U(v(t))}{\partial v} dt + \frac{1}{m} dW(t) \quad (3.2.4)$$

²Since the Langevin equation is stochastic, different trajectories would come out with different sets of random numbers η .

where we have defined $dW(t) \equiv \eta(t)dt$, as in chapter 2. Now consider a test function f which depends on the variable $v(t)$ and let us compute the impact on f of performing an infinitesimal variation $v(t) \longrightarrow v(t) + dv$:

$$df(v(t)) = f(v(t) + dv) - f(v(t)) \quad (3.2.5)$$

By Taylor-expanding the right-hand side, we obtain:

$$df(v(t)) = \cancel{f(v(t))} + \frac{\partial f(v(t))}{\partial v} dv + \frac{1}{2} \frac{\partial^2 f(v(t))}{\partial v^2} dv^2 + \dots - \cancel{f(v(t))} \quad (3.2.6)$$

Using Eq.(3.2.4) and neglecting terms of order higher than dt :

$$df = -\frac{1}{m} \frac{\partial f}{\partial v} \frac{\partial U}{\partial v} dt + \frac{1}{m} \frac{\partial f}{\partial v} dW + \frac{1}{2m^2} \frac{\partial^2 f}{\partial v^2} dW^2 \quad (3.2.7)$$

In order to have an equilibrium state at $t \rightarrow \infty$, the variation of average values must vanish at such time: $\lim_{t \rightarrow \infty} \langle df \rangle_\eta = \lim_{t \rightarrow \infty} d \langle f \rangle_\eta = 0$. Since we will deal with equilibrium quantities from now on, we replace the notation $\lim_{t \rightarrow \infty} \langle \cdot \rangle_\eta$ by simply: $\langle \cdot \rangle$. Therefore, the right-hand side of the equation above must vanish on average too:

$$\left\langle -\frac{1}{m} \frac{\partial f}{\partial v} \frac{\partial U}{\partial v} dt + \frac{1}{m} \frac{\partial f}{\partial v} dW + \frac{1}{2m^2} \frac{\partial^2 f}{\partial v^2} dW^2 \right\rangle = 0 \quad (3.2.8)$$

From the variation of $v(t)$, combined with Eq.(3.2.4), we have:

$$v(t + dt) = v(t) + dv \quad (3.2.9)$$

$$v(t + dt) = v(t) - \frac{1}{m} \frac{\partial U(v(t))}{\partial v} dt + \frac{1}{m} dW(t) \quad (3.2.10)$$

Performing the time shift $t \longrightarrow t - dt$:

$$v(t) = v(t - dt) - \frac{1}{m} \frac{\partial U(v(t - dt))}{\partial v} dt + \frac{1}{m} dW(t - dt) \quad (3.2.11)$$

Because the value of v in the present time t is determined by the noise in the past time $t - dt$, there must be no correlations between $v(t)$ and $dW(t)$. Therefore, the second term in Eq.(3.2.8) vanishes. Besides that, from Eqs.(3.1.13) and (3.1.14), we can write the correlation of dW_t as: $\langle dW(t)dW(t') \rangle_\eta = 2\lambda k_B T dt$. These facts leave us with:

$$\left\langle -\frac{\partial f}{\partial v} \frac{\partial U}{\partial v} dt + \frac{\lambda k_B T}{m} \frac{\partial^2 f}{\partial v^2} dt \right\rangle = 0 \quad (3.2.12)$$

Applying the definition of average value from the probability distribution $\rho(v)$, the equation above can be written as:

$$\int dv \rho(v) \left[-\frac{\partial f}{\partial v} \frac{\partial U}{\partial v} + \frac{\lambda k_B T}{m} \frac{\partial^2 f}{\partial v^2} \right] = 0 \quad (3.2.13)$$

$$\int dv \left[-\frac{\partial f}{\partial v} \frac{\partial U}{\partial v} \rho(v) - \frac{\lambda k_B T}{m} \frac{\partial f}{\partial v} \frac{\partial \rho(v)}{\partial v} \right] = 0 \quad (3.2.14)$$

$$\int dv \frac{\partial f}{\partial v} \left[\frac{\partial U}{\partial v} \rho(v) + \frac{\lambda k_B T}{m} \frac{\partial \rho(v)}{\partial v} \right] = 0 \quad (3.2.15)$$

where in the second equality we have used integration by parts. From the equations above, it turns out that the probability distribution satisfies the following equation:

$$\frac{\partial U}{\partial v} \rho(v) + \frac{\lambda k_B T}{m} \frac{\partial \rho(v)}{\partial v} = 0 \quad (3.2.16)$$

This is the so-called Fokker-Planck equation for a system in contact with a thermal bath at temperature T and subject to an external potential $U(v)$. It plays a similar role as the Schrödinger equation, in the Schrödinger picture of quantum mechanics: that of describing how probabilities evolve. Moreover, it can be straightforwardly integrated, yielding the solution:

$$\rho(v) = \rho_0 e^{-mU(v)/\lambda k_B T} = \rho_0 e^{-E(v)/k_B T} \quad (3.2.17)$$

where $E(v)$ is the energy of the system. By requiring that the integral of $\rho(v)$ over v be equal to unity, as a normalization condition, we are able to determine ρ_0 and recast $\rho(v)$ as:

$$\rho(v(t)) = \frac{e^{-mU(v)/\lambda k_B T}}{\int du e^{-mU(u)/\lambda k_B T}} = \frac{1}{\mathcal{Z}} e^{-mU(v)/\lambda k_B T} \quad (3.2.18)$$

Thus, the solution of the Fokker-Planck equation is precisely equal to the Boltzmann weight of statistical mechanics for an arbitrary potential U . Therefore, given a stochastic variable undergoing a process respecting the Langevin dynamics, in the equilibrium limit the average of any function f of v is determined by integrating f over v with weights given by Eq.(3.2.18):

$$\langle f \rangle = \int dv f(v) \rho(v) = \frac{1}{\mathcal{Z}} \int dv f(v) e^{-E(v)/k_B T} \quad (3.2.19)$$

Applying it to the previous case of $U(v) = \lambda v^2/2$, the partition function $\mathcal{Z}$ is:

$$\mathcal{Z} = \int_{-\infty}^{\infty} dv e^{-mU(v)/\lambda k_B T} = \int_{-\infty}^{\infty} dv e^{-mv^2/2k_B T} = \sqrt{\frac{2\pi k_B T}{m}} \quad (3.2.20)$$

Let us take $f \equiv v^2$ as an example and compute its average, as in section 3.1:

$$\langle v^2 \rangle = \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} dv v^2 e^{-mv^2/2k_B T} = \sqrt{\frac{m}{2\pi k_B T}} \frac{1}{2} \sqrt{\pi} \left(\frac{2k_B T}{m} \right)^{3/2} = \frac{k_B T}{m} \quad (3.2.21)$$

Therefore, we see that the average value of v^2 as $\langle v^2 \rangle$ obtained from an equilibrium distribution equals the one coming from stochastic dynamics: $\lim_{t \rightarrow \infty} \langle v(t)^2 \rangle_\eta$, in Eq.(3.1.12). This result elegantly connects the stochastic averages that we had from the Langevin equation with the probabilistic content given by the partition function. It means that averaging along a stochastic trajectory for large t is equivalent to weight-average this function with the Boltzmann probability $e^{-E/k_B T}$ in equilibrium.

To go a bit further, if that probability distribution can be reproduced for an arbitrary potential function U , what could we do to have the same equivalence with Euclidean path integrals in quantum mechanics? The handwavy recipe to that is the following: replace the

thermodynamic measure $k_B T$ by the quantum measure $\hbar$ and redefine the potential function as the Euclidean action of the theory. That means $k_B T \rightarrow \hbar$ and $U \rightarrow S_E$. These replacements turn Eq.(3.2.19) into:

$$\langle f(v) \rangle_\eta = \frac{1}{\mathcal{Z}_F} \int \mathcal{D}v f(v) e^{-S_E[v]/\hbar} \quad (3.2.22)$$

where dv was replaced by $\mathcal{D}v$ to account for the functional nature of $S_E[v]$. The key idea of stochastic quantization is encoded in the relationship between Eq.(3.2.19) and the equation above. We formalize this idea in the following section, after a brief historical perspective of quantum mechanics.

3.3 Stochastic quantization in non-relativistic quantum mechanics

The first successful attempt to arrive at quantum mechanics from a classical theory was accomplished by Paul Dirac in 1926. The method, that consists in promoting classical variables to operators, was first presented in Dirac’s doctoral thesis as the “method of classical analogy”. Although this method, known today as canonical quantization, has been replaced by more modern approaches, it is still widely used for pedagogical purposes in quantum mechanics and quantum field theory textbooks. A few years later, a new idea was conceived by another brilliant mind. The concept of a path integral, shortly discussed in the previous section, was introduced by Richard Feynman and subsequently used as a powerful quantizing tool. His innovative idea to interpret quantization allowed physicists to build a theoretical bridge connecting quantum mechanics to statistical mechanics in an extremely intuitive fashion. Finally, in 1981, another fascinating technique to perform quantization, this time through stochastic processes, was developed by Parisi and Wu in [Parisi et al., 1981], the so-called stochastic quantization method.

We saw in the previous section that the Langevin equation obeys a probability law according to a decreasing exponential, with exponent U , that we readily recognized as the Boltzmann weight. In the same chapter, we also realized that we could obtain an analog of the Euclidean path integral if we replaced U by the action of a given classical theory and $k_B T$ by $\hbar$. Therefore, we need to recast the Langevin equation, with the derivative of a classical action playing the role of drift force. Since S_E is a functional object, for it is defined as an integral, we also replace partial differentiation by functional differentiation. Additionally, we postulate that the evolution of the Langevin equation is parametrized not by conventional time t but by a fictitious parameter called stochastic time³ τ such that the solution of the Langevin equation will be a stochastic function of τ and the actual time t . Therefore, the Langevin equation of stochastic quantization becomes:

$$\frac{\partial x(t, \tau)}{\partial \tau} = -\frac{\delta S_E[x]}{\delta x} + \eta(t, \tau) \quad (3.3.1)$$

where τ is the stochastic time used as a fictitious parameter to lead the system towards thermalization. Due to the drift term, this newly defined process should asymptotically converge to an equilibrium state. Since τ is merely fictitious, the solution to this equation only procures physical meaning when thermalization takes place, *i.e.* when $\tau \rightarrow \infty$, and the equation does not depend on τ anymore. Likewise the statistical mechanical case approached in the beginning of this chapter, in the quantum case the noise source $\eta(t, \tau)$ must obey two similar properties:

• **Property 1:**

$$\langle \eta(t, \tau) \rangle_\eta = 0 \quad (3.3.2)$$

• **Property 2:**

$$\langle \eta(t, \tau) \eta(t', \tau) \rangle_\eta = 2\hbar \delta(t - t') \delta(\tau - \tau') \quad (3.3.3)$$

where τ enters as an additional variable to the noise, introducing an extra Dirac delta function. In summary, given a classical action and a noise satisfying the properties above, the

³Even though we call it time, this new parameter has nothing to do with the real time whatsoever, denoted by t .

solution of the Langevin equation furnishes the quantized version of a classical system when $\tau \rightarrow \infty$. In this limit, the stochastic averages derived from it will correspond to the quantum expectation values. For instance, quantities of the type $\langle x(t_1, \tau)x(t_2, \tau)\dots x(t_N, \tau) \rangle_\eta$ equate the vacuum expectation value $\langle 0|\hat{X}(t_1)\hat{X}(t_2)\dots\hat{X}(t_N)|0\rangle$, in the operator formalism, for very large τ . This equivalence is a direct consequence of the fact that the Langevin equation obeys Boltzmann-like weights from the Fokker-Planck equation. Another remarkable fact about the Langevin equation is that any initial conditions for τ are acceptable, meaning that the system will always evolve to the same equilibrium regardless of the value of $x(t, 0)$.

Similar to the statistical mechanical case, where the noise source carried information about thermal fluctuations, in stochastic quantization it carries information about quantum fluctuations. This is an implication of property 2, whereby we deduce that $\eta(t, \tau)$ is proportional to $\sqrt{\hbar}$. Hence, to recover classical mechanics (no quantum fluctuations), we can forcibly turn the noise off. Besides that, due to the asymptotic equilibrium, the first derivative in the left-hand side of Eq.(3.3.1) must vanish for very large τ . Thus, applying both limits, the Langevin equation becomes:

$$\frac{\delta S_E[x]}{\delta x} = 0 \quad (3.3.4)$$

which is simply the Euler-Lagrange equation. This means that stochastic quantization, in the absence of noise, is equivalent to classical mechanics in the equilibrium limit.

To exemplify the usefulness of stochastic quantization in non-relativistic quantum mechanics, we apply the Langevin equation to quantize a classical harmonic oscillator, as done in [Namiki, 2008]. Thence we compute the quantum correlator $\langle 0|\hat{X}(t)\hat{X}(t')|0\rangle$ in the stochastic formalism and compare it to the path integral result. Consider the classical action of a harmonic oscillating system:

$$S[x] = \frac{1}{2} \int dt \left[m \left(\frac{\partial x}{\partial t} \right)^2 - m\omega_0^2 x^2 \right] \quad (3.3.5)$$

To make a direct connection with statistical mechanics, we need to perform a Wick rotation in the time variable and work with the Euclidean action. A Wick rotation rotates the time direction by 90° in the complex plane: $t \rightarrow -it$. By doing that, we end up with the Euclidean action:

$$S_E[x] = \frac{1}{2} \int dt \left[m \left(\frac{\partial x}{\partial t} \right)^2 + m\omega_0^2 x^2 \right] \quad (3.3.6)$$

Then, to compute $\langle 0 | \hat{X}(t) \hat{X}(t') | 0 \rangle$, in path integral, we need to solve:

$$\langle 0 | \hat{X}(t) \hat{X}(t') | 0 \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}x \, x(t) x(t') e^{-S_E[x]/\hbar} \quad (3.3.7)$$

Although dreadful, the calculation can be done analytically and the result is:

$$\langle 0 | \hat{X}(t) \hat{X}(t') | 0 \rangle = \frac{\hbar}{2m\omega_0} e^{-\omega_0 |t-t'|} \quad (3.3.8)$$

To turn around such costly hand-work, we can use stochastic quantization instead. Applying Eq.(3.3.1) to this system, by acting with the functional derivative on the action above, yields the following Langevin equation:

$$\frac{\partial x(t, \tau)}{\partial \tau} = m \frac{\partial^2 x(t, \tau)}{\partial t^2} - m\omega_0^2 x(t, \tau) + \eta(t, \tau) \quad (3.3.9)$$

where we now describe the position of the harmonic oscillator as a stochastically fluctuating function of t and τ . Similarly to the case of Brownian motion, step one is to solve Eq.(3.3.9), and step two computing stochastic averages. The first step can be accomplished by Fourier-transforming Eq.(3.3.9):

$$\frac{\partial \tilde{x}(\omega, \tau)}{\partial \tau} = -m(\omega^2 + \omega_0^2) \tilde{x}(\omega, \tau) + \tilde{\eta}(\omega, \tau) \quad (3.3.10)$$

and also Fourier-transforming the noise property in Eq.(3.3.3):

$$\langle \tilde{\eta}(\omega, \tau) \tilde{\eta}(\omega', \tau') \rangle_\eta = 2\hbar \delta(\omega + \omega') \delta(\tau - \tau') \quad (3.3.11)$$

Defining $\Omega^2(\omega) \equiv m(\omega^2 + \omega_0^2)$ to simplify notation, we use variation of parameters to write an explicit solution for Eq.(3.3.10) as:

$$\tilde{x}(\omega, \tau) = \tilde{x}(\omega, 0) e^{-\Omega^2(\omega)\tau} + \int_0^\tau d\tau_1 e^{\Omega^2(\omega)(\tau_1 - \tau)} \tilde{\eta}(\omega, \tau_1) \quad (3.3.12)$$

The analog of the quantum correlator $\langle 0 | \hat{X}(t_1) \hat{X}(t_2) | 0 \rangle$ in the stochastic formalism is given by the average $\langle x(t, \tau) x(t', \tau') \rangle_\eta$, which we first obtain in frequency space:

$$\begin{aligned} \langle \tilde{x}(\omega, \tau) \tilde{x}(\omega', \tau') \rangle_\eta &= \langle \tilde{x}(\omega, 0) \tilde{x}(\omega', 0) \rangle_\eta e^{-\Omega^2(\omega)\tau - \Omega^2(\omega')\tau'} + \\ &+ \tilde{x}(\omega, 0) e^{-\Omega^2(\omega)\tau} \int_0^{\tau'} d\tau_2 e^{\Omega^2(\omega')(\tau_2 - \tau')} \langle \tilde{\eta}(\omega', \tau_2) \rangle_\eta + \\ &+ \tilde{x}(\omega', 0) e^{-\Omega^2(\omega')\tau'} \int_0^\tau d\tau_1 e^{\Omega^2(\omega)(\tau_1 - \tau)} \langle \tilde{\eta}(\omega, \tau_1) \rangle_\eta + \\ &+ \int_0^\tau \int_0^{\tau'} d\tau_1 d\tau_2 e^{\Omega^2(\omega)(\tau_1 - \tau) + \Omega^2(\omega')(\tau_2 - \tau')} \langle \tilde{\eta}(\omega, \tau_1) \tilde{\eta}(\omega', \tau_2) \rangle_\eta \end{aligned} \quad (3.3.13)$$

Because of property 1: $\langle \tilde{\eta}(\omega, \tau_1) \rangle_\eta = \langle \tilde{\eta}(\omega', \tau_2) \rangle_\eta = 0$, and we are left with:

$$\begin{aligned} \langle \tilde{x}(\omega, \tau) \tilde{x}(\omega', \tau') \rangle_\eta &= \langle \tilde{x}(\omega, 0) \tilde{x}(\omega', 0) \rangle_\eta e^{-\Omega^2(\omega)\tau - \Omega^2(\omega')\tau'} + \\ &+ \int_0^\tau \int_0^{\tau'} d\tau_1 d\tau_2 e^{\Omega^2(\omega)(\tau_1 - \tau) + \Omega^2(\omega')(\tau_2 - \tau')} \langle \tilde{\eta}(\omega, \tau_1) \tilde{\eta}(\omega', \tau_2) \rangle_\eta \end{aligned} \quad (3.3.14)$$

Using the Fourier-transform of property 2 in the second term on the right-hand side to solve the double integral, considering the two possible cases (either $\tau \leq \tau'$ or $\tau > \tau'$), the solution becomes:

$$\langle \tilde{x}(\omega, \tau) \tilde{x}(\omega', \tau') \rangle_\eta = \langle \tilde{x}(\omega, 0) \tilde{x}(\omega', 0) \rangle_\eta e^{-\Omega^2(\omega)\tau - \Omega^2(\omega')\tau'} +$$

$$+ \frac{\hbar}{\Omega^2(\omega)} \delta(\omega + \omega') \left[e^{-\Omega^2(\omega)|\tau-\tau'|} - e^{-\Omega^2(\omega)(\tau+\tau')} \right] \quad (3.3.15)$$

Using the relation between the frequency-space correlation and the Green function from [Namiki, 2008]: $\langle \tilde{x}(\omega, \tau) \tilde{x}(\omega', \tau') \rangle_\eta = \delta(\omega + \omega') \tilde{G}(\omega, \tau - \tau')$, then integrating over ω' , the equation above can be rewritten in terms of the Green function in frequency space $\tilde{G}$ as:

$$\tilde{G}(\omega, \tau - \tau') = \tilde{G}(\omega, 0) e^{-\Omega^2(\omega)(\tau+\tau')} + \frac{\hbar}{\Omega^2(\omega)} \left[e^{-\Omega^2(\omega)|\tau-\tau'|} - e^{-\Omega^2(\omega)(\tau+\tau')} \right] \quad (3.3.16)$$

Making $\tau' = \tau$, we have:

$$\tilde{G}(\omega, 0) = \tilde{G}(\omega, 0) e^{-2\Omega^2(\omega)\tau} + \frac{\hbar}{\Omega^2(\omega)} \left[1 - e^{-2\Omega^2(\omega)\tau} \right] \quad \therefore \quad \tilde{G}(\omega, 0) = \frac{\hbar}{\Omega^2(\omega)} \quad (3.3.17)$$

Replacing it back into Eq.(3.3.16), we have a complete Green's function for the harmonic oscillator in frequency space:

$$\tilde{G}(\omega, \tau - \tau') = \frac{\hbar}{\Omega^2(\omega)} e^{-\Omega^2(\omega)|\tau-\tau'|} \quad (3.3.18)$$

Returning to position space through inverse Fourier transform:

$$G(t - t', \tau - \tau') = \frac{\hbar}{2\pi m} \int_{-\infty}^{+\infty} d\omega \frac{1}{\omega^2 + \omega_0^2} e^{i\omega(t-t') - \Omega^2(\omega)|\tau-\tau'|} \quad (3.3.19)$$

Identifying the existence of complex poles at $\omega = i\omega_0$ and $\omega = -i\omega_0$ in this integral, the equation above can be easily calculated through the residues theorem of complex analysis, which, after the asymptotic limit, results in:

$$\lim_{\tau=\tau' \rightarrow \infty} G(t - t', \tau - \tau') = G(t - t') = \frac{\hbar}{2m\omega_0} e^{-\omega_0|t-t'|} \quad (3.3.20)$$

The right-hand side of this equation is precisely the 2-point correlation function of a harmonic oscillating particle as we obtained through the path integral in Eq.(3.3.8). This result reflects

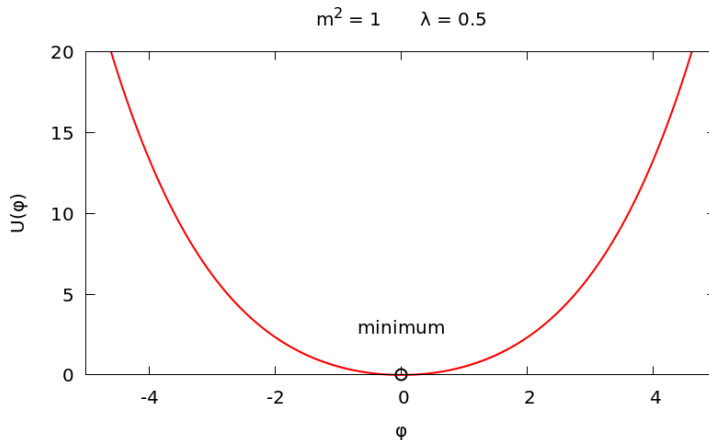
the equivalence between quantum mechanics and stochastic quantization in the asymptotic limit as claimed before. Although we presented this equivalence for a very specific case, the applicability of stochastic quantization does not come to a halt in the territory of quantum mechanics. Therefore, in the next section, we review stochastic quantization in quantum field theory.

3.4 Stochastic quantization in quantum field theory

To describe quantum field theory (QFT hereafter) in stochastic quantization, we simply need to adapt the formalism to a more fundamental object, other than quantum mechanical systems or grains of pollen. Throughout this work, we consider the Euclidean Φ^4 -theory to review and, later on, present our new results in QFT. In 1-dimensional space, the scalar field with symmetric phase (positive mass term) has an action given by:

$$S_E[\Phi] = \int dx \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{1}{2} m^2 \Phi^2 + \frac{\lambda}{4!} \Phi^4 \right) \quad (3.4.1)$$

The case of spontaneous symmetry breaking (when the mass term is negative) will be discussed in chapter 4. The shape of the interaction potential is given by Figure 3.2, and its expression is given by the equation beside it:



$$U(\Phi) = \frac{1}{2} m^2 \Phi^2 + \frac{\lambda}{4!} \Phi^4 \quad (3.4.2)$$

Figure 3.2: Potential function without spontaneous symmetry breaking. The empty black circle in the origin indicates the single classical vacuum for this potential. The square mass and coupling used in the plot are given in the upper part.

In order to insert the Φ^4 -theory in the stochastic formalism, we start by defining a new field to be a stochastic function of spacetime and τ : $\varphi(x, \tau)$, alongside its correspondent Langevin equation as:

$$\frac{\partial \varphi(x, \tau)}{\partial \tau} = - \left. \frac{\delta S_E[\Phi]}{\delta \Phi(x)} \right|_{\Phi \rightarrow \varphi} + \eta(x, \tau) \quad (3.4.3)$$

where the noise source $\eta(x, \tau)$ is required to satisfy analogous properties as well, similar to the case of the previous chapter:

• **Property 1:**

$$\langle \eta(x, \tau) \rangle_\eta = 0 \quad (3.4.4)$$

• **Property 2:**

$$\langle \eta(x, \tau) \eta(x', \tau) \rangle_\eta = 2\hbar \delta(x - x') \delta(\tau - \tau') \quad (3.4.5)$$

Notice the subtle difference between the physical field $\Phi = \Phi(x)$, and its stochastic counterpart $\varphi = \varphi(x, \tau)$. In the latter case there is an extra dependence on the fictitious time τ , since it is needed to describe the stochastic dynamics of φ . By acting with the functional derivative on Eq.(3.4.1) and doing $\Phi \rightarrow \varphi$, the correspondent Langevin equation can be easily obtained as:

$$\frac{\partial \varphi}{\partial \tau} = (\square - m^2)\varphi - \frac{\lambda}{6}\varphi^3 + \eta \quad (3.4.6)$$

For that equation and the following ones, we consider $\hbar \equiv 1$, unless we explicitly state the opposite. The dependencies on x and τ were omitted for simplicity. Once the Langevin equation is known, the remaining task is to find its solution by following the same procedure of section 3.3. Furthermore, we could work out the Langevin equation in momentum space by simply Fourier-transforming the field φ in the variable x :

$$\int dP e^{iPx} \frac{\partial \tilde{\varphi}(P, \tau)}{\partial \tau} = - \int dP e^{iPx} (P^2 + m^2) \tilde{\varphi}(P, \tau) +$$

$$-\frac{\lambda}{6} \int dP dq dk e^{i(P+q+k)x} \tilde{\varphi}(P, \tau) \tilde{\varphi}(q, \tau) \tilde{\varphi}(k, \tau) + \int dP e^{iPx} \tilde{\eta}(P, \tau) \quad (3.4.7)$$

Multiplying both sides by e^{-ipx} and integrating with respect to x introduces a Dirac delta $\delta(P - p)$ which kills the integral over P and simplifies the equation above to:

$$\frac{\partial \tilde{\varphi}(p, \tau)}{\partial \tau} = -(p^2 + m^2) \tilde{\varphi}(p, \tau) - \frac{\lambda}{6} \int dq dk \tilde{\varphi}(p - q - k, \tau) \tilde{\varphi}(q, \tau) \tilde{\varphi}(k, \tau) + \tilde{\eta}(p, \tau) \quad (3.4.8)$$

Since no approximations were done so far, the solution of Eqs.(3.4.6) and (3.4.8) can be used to obtain fully non-perturbative quantities exactly, either in position or momentum space. However, depending on the shape of the potential, this task might or might not be feasible. Unfortunately, the Φ^4 potential falls into the “not” case, so to turn around perturbation theory we need to resort to numerical techniques. These we postpone until section 4, for now we concentrate on n -point functions in quantum field theory.

3.5 Quantum n -point functions

The n -point correlation functions are the cornerstones to study physical processes in quantum field theory. Even though they are not observables themselves, they play an important role in obtaining observables from the so-called renormalization procedure, which will be the main topic of chapter 6. From the brief discussion on Feynman path integrals of section 3.2, the Euclidean n -point functions of a theory are computed in the operator formalism as the weighted sum given by a functional integration:

$$\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) \dots \hat{\Phi}(x_n) | 0 \rangle = \frac{1}{Z_F} \int \mathcal{D}\Phi \Phi(x_1) \Phi(x_2) \dots \Phi(x_n) e^{-S_E[\Phi]} \quad (3.5.1)$$

where $|0\rangle$ is the vacuum state of the theory. To compute the right-hand side of the equation above in stochastic quantization, we should start from the Langevin equation. Suppose we

managed to solve Eq.(3.4.6) for a given ensemble of noises $\eta(x, \tau)$ and a fixed initial condition for $\varphi(x, 0)$. The qualitative behavior of the solution would show up as a noisy profile tending to have an asymptotically flat average as τ grows. This flat part is precisely the equilibrium state that we seek to measure. However, since we have solved it only once, the measured value is embedded in statistical fluctuations. Therefore, we should solve it again, with another set of noises, and repeat the task many times. By collecting plenty of independent stochastic solutions of Eq.(3.4.6), say $\varphi_1, \varphi_2, \dots, \varphi_{N_r}$, where N_r is called the number of noise realizations, the arithmetic average of these values is a better estimation of the equilibrium state. In the limit of infinite solutions ($N_r \rightarrow \infty$), one would find a perfectly smooth curve, which recovers the path integral result as $\tau \rightarrow \infty$, with decreasingly small errors. Before that limit, we define the n -point correlation function in stochastic quantization for a finite τ as:

$$\langle \varphi(x_1, \tau) \varphi(x_2, \tau) \dots \varphi(x_n, \tau) \rangle_\eta = \lim_{N_r \rightarrow \infty} \frac{1}{N_r} \sum_{j=1}^{N_r} \varphi_j(x_1, \tau) \varphi_j(x_2, \tau) \dots \varphi_j(x_n, \tau) \quad (3.5.2)$$

According to the Fokker-Planck equation, in the large τ limit the φ 's must obey the Boltzmann distribution $e^{-S_E[\Phi]}$, thus the expectation values in Eq.(3.5.2) should agree with the path integral:

$$\lim_{\tau \rightarrow \infty} \langle \varphi(x_1, \tau) \varphi(x_2, \tau) \dots \varphi(x_n, \tau) \rangle_\eta = \frac{1}{\mathcal{Z}_F} \int \mathcal{D}\Phi \Phi(x_1) \Phi(x_2) \dots \Phi(x_n) e^{-S_E[\Phi]} \quad (3.5.3)$$

This is a direct consequence of the central limit theorem presented in chapter 2, which implies that an arithmetic average (left side) and a weighted average (right side) are identical in the infinite sample limit. This was seen in section 3.3 for the case of the 2-point function of a quantum harmonic oscillator, but it is valid in general for n -point functions in QFT. We conclude this section by summarizing how stochastic quantization is applied to calculate these quantities in real problems, which will be important for numerical simulations.

- Derive the correspondent Langevin equation for the target theory given its action, as shown in Eq.(3.4.3).

- Obtain numerous solutions with different noise sets for all x until τ is large enough for the system to be thermalized in each solution.
- Compute the arithmetic average of (products of) these solutions, as in Eq.(3.5.2), for large τ .

Chapter 4

Lattice Simulations in Φ^4 -theory

Lattice theories are among the most powerful techniques in non-perturbative QFT, for they dismiss the use of perturbative expansions and provide a natural path towards computer simulations. Hence, in this chapter, we use standard methods of lattice QFT from [Smit, 2002] to formulate stochastic quantization in discrete space. Thence, we introduce our new code to obtain numerical solutions of the Langevin equation in Φ^4 -theory and compute n -points function following the average procedure of [Berges and Stamatescu, 2005]. We commence by using the code to reproduce some of the known results of Φ^4 -theory and prepare the ground for our new results in the next chapter. To simulate the Langevin equation in the computer we need to discretize the field φ on a lattice, which consists of granulating it in a spacetime defined by lattice sites, instead of continuous variables.

4.1 The scalar field on a lattice

Everything so far has been done in continuous space, that is with the spacetime components $x \in \mathbb{R}$, but in lattice QFT the field is set to exist only in specific points placed a distance a , called lattice spacing, apart from its nearest neighbors. This construction conveys a crystalline structure to spacetime, making it look like a net of sewed strings, with the field

defined in the nodes. For a d -dimensional hypercubic lattice with N sites¹ in each spatial direction, its length is defined as $L \equiv aN$ and its volume as $V = L^d$. Moreover, we choose our lattices to be periodic, in which case the fields must satisfy periodic boundary conditions: $\varphi(x, \tau) = \varphi(x + L, \tau)$, $\forall \tau$. Figure 4.1 illustrates two types of lattice topologies for periodic conditions. This new framework requires replacing the original action by a discrete version

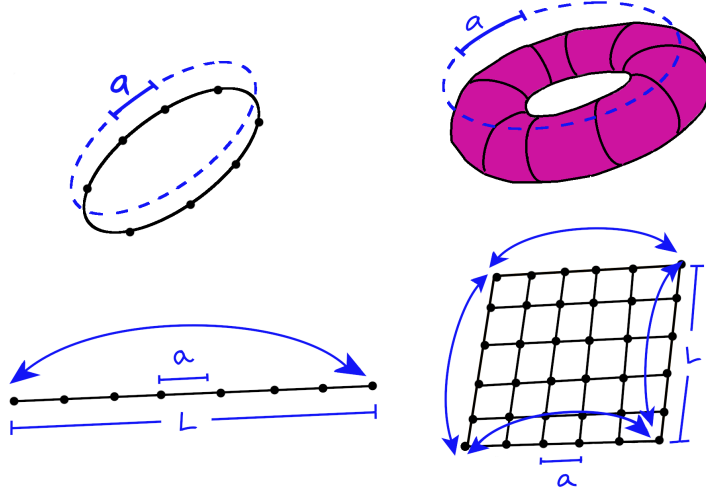


Figure 4.1: Lattice topologies for periodic boundary conditions in 1 dimension (left) and 2 dimensions (right). Due to the periodic boundary conditions, in one dimension the lattice assumes a ring-like shape, whereas in two it turns into a torus.

that encodes the same dynamics and restores its continuous counterpart in the appropriate limit. Usually, there are plenty of actions with this characteristic. In d dimensions, the simplest one resembling its continuous analog is the following:

$$S_E = a^d \sum_x \left[\sum_\mu \partial_\mu \Phi(x) \partial^\mu \Phi(x) + \frac{1}{2} m^2 \Phi^2(x) + \frac{\lambda}{4!} \Phi^4(x) \right] \quad (4.1.1)$$

where the continuous derivatives are redefined on the lattice as:

$$\partial_\mu \Phi(x) \longrightarrow \frac{1}{a} [\Phi(x + a\hat{\mu}) - \Phi(x)] \quad (4.1.2)$$

¹Not to be confused with the number of noise realizations N_r

and $\hat{\mu}$ is a unit vector pointing on a specific direction in spacetime. In the non-interacting case ($\lambda = 0$), this theory is completely solvable and the momentum space propagator can be obtained explicitly, as in [Montvay and Münster, 1997]:

$$\tilde{G}(k) = \left[\frac{4}{a^2} \sin^2 \left(\frac{k\pi}{N} \right) + m^2 \right]^{-1} \quad (4.1.3)$$

where k , with $-N/2 \leq k < N/2$, is the momentum quantum number. It can be verified that, due to periodic boundary conditions, the propagator satisfies: $\tilde{G}(k) = \tilde{G}(k + N)$. In the continuum limit ($a \rightarrow 0$ and $N \rightarrow \infty$), it can be proven that the equation above restores the free propagator of a scalar theory: $(k^2 + m^2)^{-1}$. Using the inverse Fourier transformation in discrete space, we obtain the position-space propagator for the free theory:

$$G^{(0)}(x_1, x_2) = \frac{1}{N} \sum_{k=0}^{N-1} \frac{e^{2i\pi(x_1-x_2)k/N}}{4 \sin^2(k\pi/N)/a^2 + m^2} \quad (4.1.4)$$

In the interacting case, obtaining an analytical expression requires perturbative corrections in lattice theory. These corrections arise from expansions in the path integral, giving birth to the so-called quantum loops. Leaving the details for the next chapter, we simply state that by expanding the interacting part within $S_E[\Phi]$ in the right-hand side of Eq.(3.5.1), namely the one where the coupling λ appears, one gets the desired corrections order by order. In the case of the 2-point function:

$$\langle 0 | \hat{\Phi}(x) \hat{\Phi}(x') | 0 \rangle = G^{(0)}(x, x') + G^{(1)}(x, x') + G^{(2)}(x, x') + \mathcal{O}(3) \quad (4.1.5)$$

where the superscript 0 refers to the free contribution and the other terms, which depend on the coupling, bear the interactions. However, in practical terms, we are unable to compute the full sum, for each term gets more and more complicated as the order increases. Therefore, given an order n , by truncating this infinite sum at some order, we define an approximate solution for the 2-point function, denoted by $G^{m\text{-loop}}(x, x')$, which takes into account terms

with proportionality from λ^0 up until λ^n . The explicit formulas of $G^{n-\text{loop}}(x, x')$ when $n = 1$ or 2 are provided through lattice perturbation theory in chapter 5 for the symmetric and broken phase cases.

4.2 Numerical simulations using LASER code

When the target theory features a complicated interaction term, hampering exact solutions to be obtained, numerical algorithms stand as magnificent resources. The most widely known among the lattice scientific community is called the MCMC, mentioned in the introduction, which consists in selecting relevant field configurations² and average over them with the Boltzmann weight e^{-S_E} (we make a few remarks concerning this topic in appendix A.2). On the other hand, through the stochastic quantization procedure, we can evolve a stochastic Partial Differential Equation (PDE) and obtain field configurations $\varphi(x, \tau)$ whose probability distributions $\rho[\varphi]$ are already given by the correct Boltzmann factor, and then compute their arithmetic average instead. A considerable part of the work for this master's thesis was to build a code from scratch that performed this task consistently. This code was entirely written in the C++ programming language and we call it LASER (an abbreviation of LAngevin SolvER). We use it in this chapter to reproduce quantities in the Φ^4 -theory that are previously known from perturbation theory. For simplicity, we take the 1-dimensional case and recast Eq.(3.4.6) in discrete form by turning continuous derivatives into discrete ones, with x and τ being replaced by lattice indices j and n :

$$\frac{\partial \varphi(x, \tau)}{\partial \tau} \longrightarrow \frac{1}{\Delta \tau} (\varphi_j^{n+1} - \varphi_j^n) \quad (4.2.1)$$

$$\frac{\partial^2 \varphi(x, \tau)}{\partial x^2} \longrightarrow \frac{1}{a^2} (\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n) \quad (4.2.2)$$

²From the minimum action principle, a relevant field configuration signifies one that minimizes the action.

Replacing them into Eq.(3.4.6) yields:

$$\varphi_j^{n+1} = \varphi_j^n + \Delta\tau \left[\frac{\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n}{a^2} - m^2\varphi_j^n - \frac{\lambda}{6}(\varphi_j^n)^3 + \eta_j^n \right] \quad (4.2.3)$$

where we have introduced the discrete version of the gaussian noise η_j^n in the place of $\eta(x, \tau)$. From the continuous properties 1 and 2, recalling a Dirac delta $\delta(y)$ has dimensions of $1/y$, the equivalent discrete properties are given by:

$$\langle \eta_j^n \rangle_\eta = 0 \quad \langle \eta_j^n \eta_k^m \rangle_\eta = \frac{2}{\Delta\tau a} \delta_{jk} \delta_{nm} \quad (4.2.4)$$

These properties are the touchstones of a gaussian white noise. They imply that the discrete noise must be of the form $\eta_j^n = \sqrt{2/\Delta\tau a} R_j^n$, where R_j^n is a random number to be selected with gaussian probability for given j and n , as we saw in Figure 3.1 of chapter 3. Replacing it into Eq.(4.2.3), we get:

$$\varphi_j^{n+1} = \varphi_j^n + \Delta\tau \left[\frac{\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n}{a^2} - m^2\varphi_j^n - \frac{\lambda}{6}(\varphi_j^n)^3 \right] + \sqrt{\frac{2\Delta\tau}{a}} R_j^n \quad (4.2.5)$$

Finding a suitable algorithm, Eq.(4.2.3) can be implemented and efficiently solved with high precision on codes (we briefly remark on algorithms in appendix A.1). For convenience, we eliminate the lattice spacing a from the equation above by naively fixing it as $a \equiv 1$, temporarily purging the Langevin equation of the lattice spacing. Chapter 6 will be entirely dedicated to exploring a more fundamental interpretation of this parameter in renormalization.

In 2 or more dimensions, we merely need to add more indices and extra derivatives relative to those indices. In Figures 4.2 below we show solutions of the Langevin equation for different initial conditions and for increasing noise realizations N_r . From the general definition in Eq.(3.5.2) one can readily obtain n -point correlation functions of the field as outputs of simulations by averaging over products of the field. In Figure 4.3, we compute a 2-point function of the type $\langle \varphi(x_1, \tau) \varphi(x_2, \tau) \rangle_\eta$ from $\tau = 0$ until τ sufficiently large to thermalize

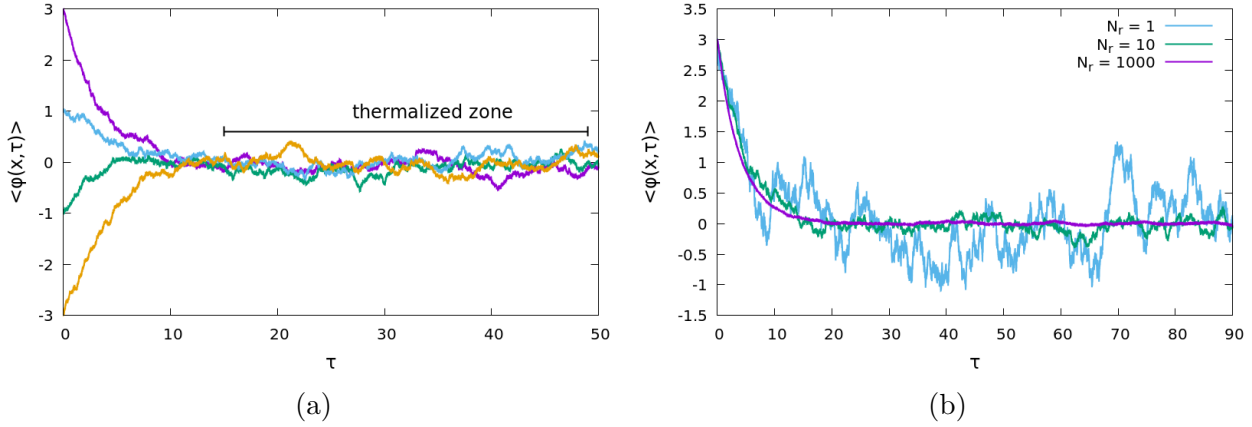


Figure 4.2: (a) Several solutions of the Langevin equation as a function of τ , using different initial conditions, reinforcing that the asymptotic solution is always the same and given by the thermalized zone. (b) Stochastic averages of the field φ with increasing number of noise realizations, where we notice drastic improvements as we go from 1 to 10, then from 10 to 1000 samples.

and converge to the QFT propagator $\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) | 0 \rangle$ in the free case for several lattice distances $x_1 - x_2$. Thereby, we analyze its accuracy by also plotting the expected analytical values given by Eq.(4.1.4). Similar results as a function of the stochastic time may be found in previous investigations of non-equilibrium scalar fields in [Berges and Stamatescu, 2005], and for semi-classical gravity fields in [dos Reis et al., 2019]. In Figure 4.4, we reproduce the free propagators of Φ^4 -theory computed for different lattice sizes using the average procedure illustrated in Figure 4.3. In the same plot, we compare the simulation outputs with the analytical values given by Eq.(4.1.4) for different number of sites, N . Notice that in all cases, the propagators as a function of the lattice distance $x_1 - x_2$ stand in accordance with the analytical values. Moreover, we could also estimate the QFT 4-point function $\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) \hat{\Phi}(x_3) \hat{\Phi}(x_4) | 0 \rangle$ using the large τ limit of the stochastic average of four fields, given by:

$$\chi_4(x_1, x_2, x_3, x_4) = \lim_{\tau \rightarrow \infty} \langle \varphi(x_1, \tau) \varphi(x_2, \tau) \varphi(x_3, \tau) \varphi(x_4, \tau) \rangle_\eta \quad (4.2.6)$$

and also the ones containing odd products of fields, like the 3-point function:

$$\chi_3(x_1, x_2, x_3) = \lim_{\tau \rightarrow \infty} \langle \varphi(x_1, \tau) \varphi(x_2, \tau) \varphi(x_3, \tau) \rangle_\eta \quad (4.2.7)$$

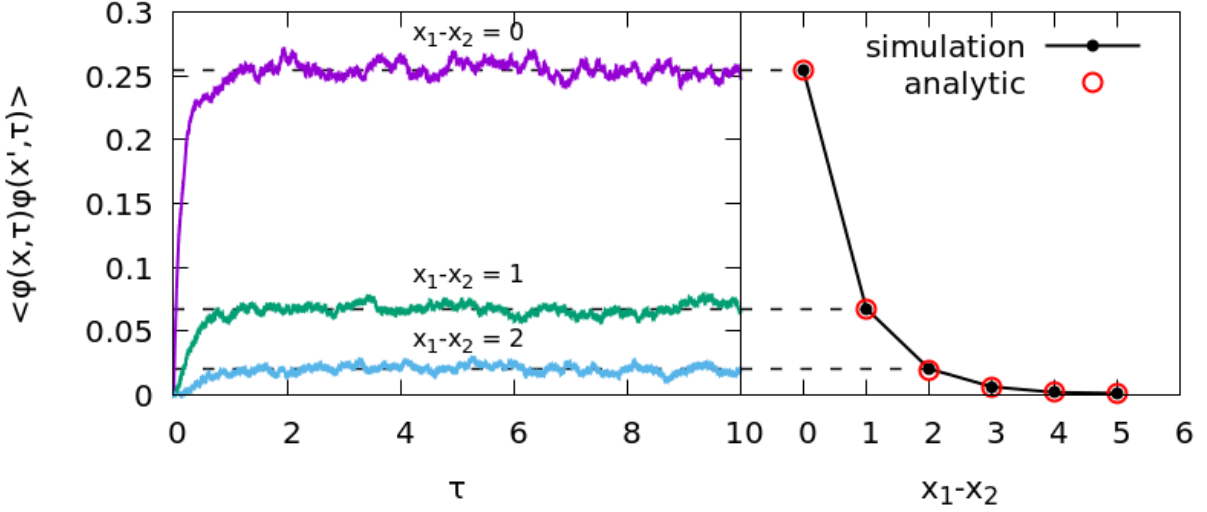


Figure 4.3: In the left-hand side, the fluctuating continuous lines show the convergence of stochastic averages of the free propagator on a 10×10 lattice computed for three distances as a function of τ . The dashed lines represent the mean value of the thermalized zone, using $N_r = 60$, leading to their physical value as a function of the distance $x_1 - x_2$ in the right-hand side. Empty red circles indicate the analytical result and their excellent match with the simulation.

However, we postpone the calculation of 4-point functions until chapter 6, where they play an essential role to perform the continuum limit of the lattice. Similar to the free case, we can execute simulations with non-zero coupling and solve the Langevin equation to its full extent for arbitrarily large λ . The results can then be compared with the perturbative expansion up to 2 loops as in Eq.(4.1.5), verifying the agreement between theory and simulations. In Figure 4.5, we show numerical and analytical propagators as functions of the distance for finite values of λ in a 10×10 lattice. For increasing values of the coupling, we barely notice deviations of the 2-loop analytical propagator from the simulation, showing that stochastic quantization remains consistent even for strong λ . As the last proof of the validity of stochastic quantization, consider that we are interested in reproducing the momentum-space 2-point function. To accomplish this task, we could proceed in two ways: either solve the Langevin equation directly in momentum space, namely Eq.(3.4.8), or solving it in position space and Fourier-transform the solution before computing averages. However, the former turns out to be extremely costly in terms of CPU time, for we need to solve an integro-differential equa-

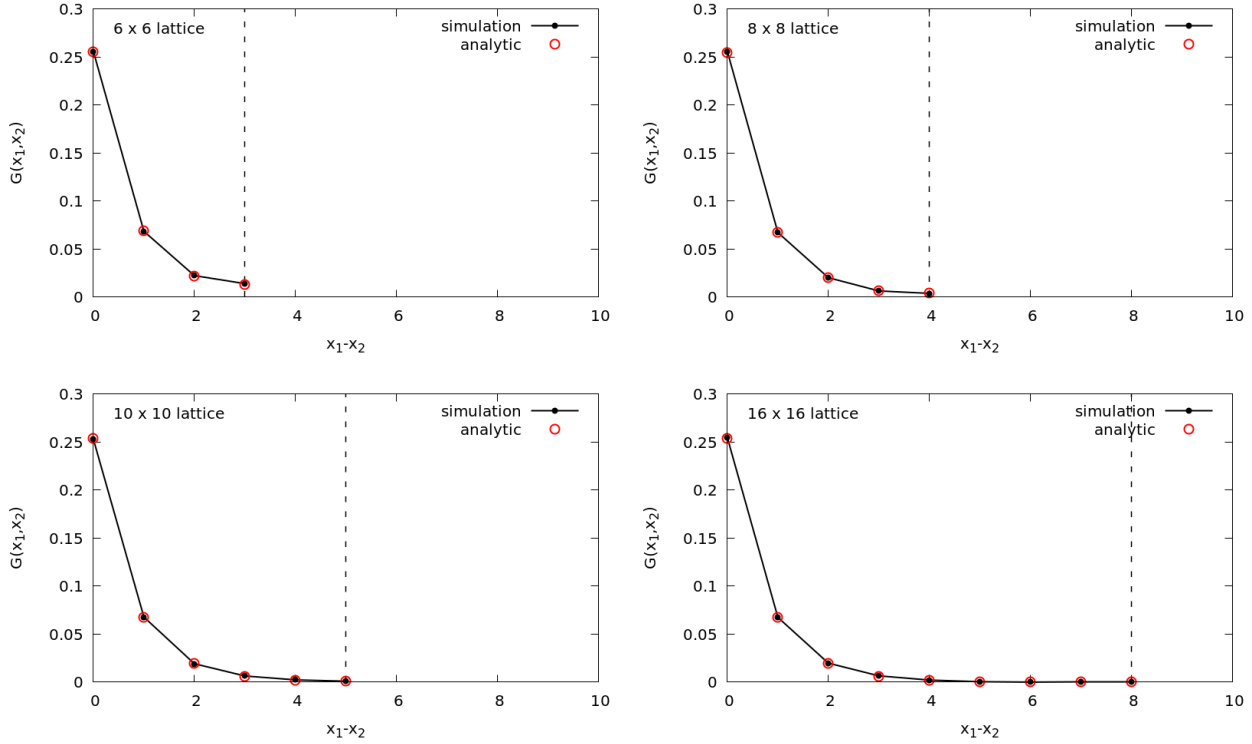


Figure 4.4: Numerical 2-point functions in the free case from stochastic quantization (black lines-and-points) for different lattice sizes compared to the exact analytical values (red empty circles). The dashed vertical lines are placed in the middle of each lattice, where it starts to be periodic.

tion. Therefore, we adopt the latter option and perform a Fourier transform with $\varphi(x, \tau)$ to obtain $\tilde{\varphi}(p, \tau)$ for several values of $p = 2\pi k/N$ by varying the quantum number k . In Figure 4.6, the results for the numerical propagators in momentum space are shown alongside the analytical perturbative calculations. Hitherto, plenty of successful examples have been added to the stochastic quantization repertoire for the symmetric case, *i.e.* when the theory has a single vacuum. Now, we deal with a case where the theory has more than one vacuum.

4.3 Spontaneous symmetry breaking

In the previous section, we saw that, because the theory had just one vacuum, the solution of the Langevin equation always converged to the same equilibrium, regardless of the initial conditions. In this sense, the theory was symmetric, since we could replace the vacuum Φ_0

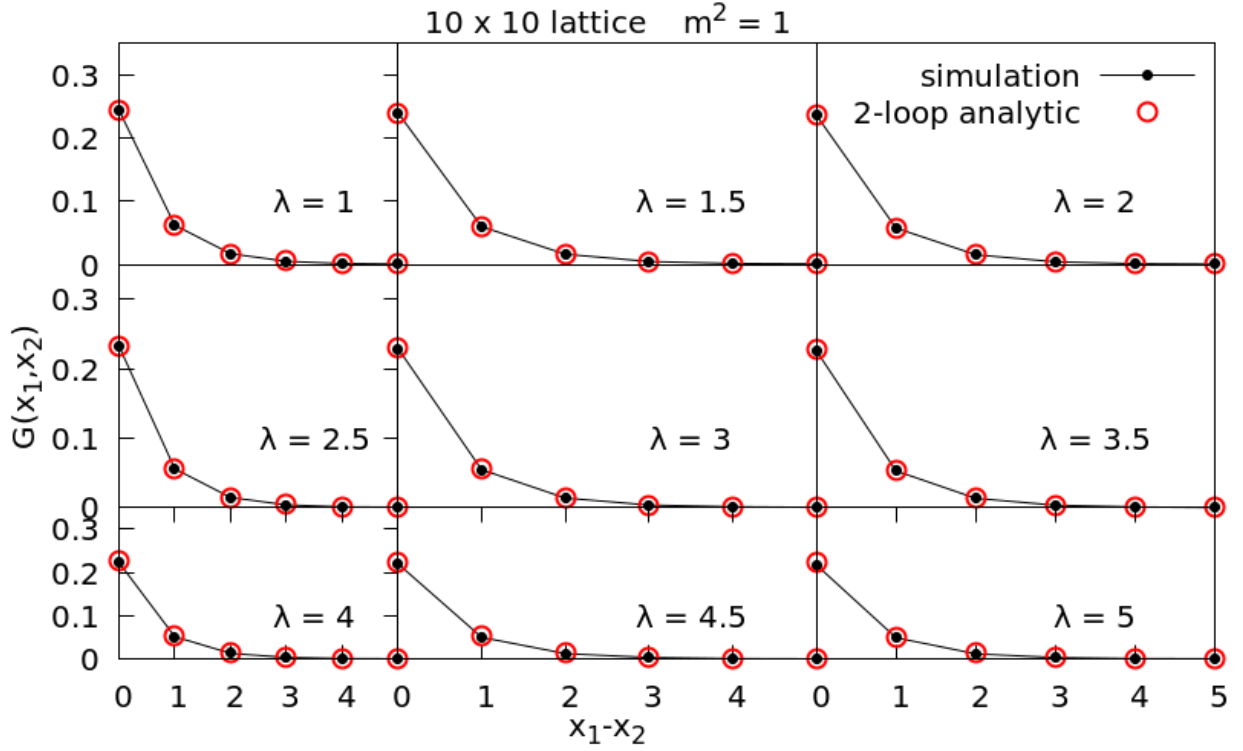


Figure 4.5: Numerical (black lines-and-points) and analytical (empty red circles) propagators for nine values of λ averaged with 100 noise realizations each. Notice that the 2-loop analytic propagator remains consistent with simulations.

by $-\Phi_0$, and nothing would change. On the other hand, if we invert the sign of the mass term in Eq.(4.1.1), such that the new action becomes:

$$S_E = a^d \sum_x \left[\sum_\mu \partial_\mu \Phi(x) \partial^\mu \Phi(x) - \frac{1}{2} m^2 \Phi^2(x) + \frac{\lambda}{4!} \Phi^4(x) \right] \quad (4.3.1)$$

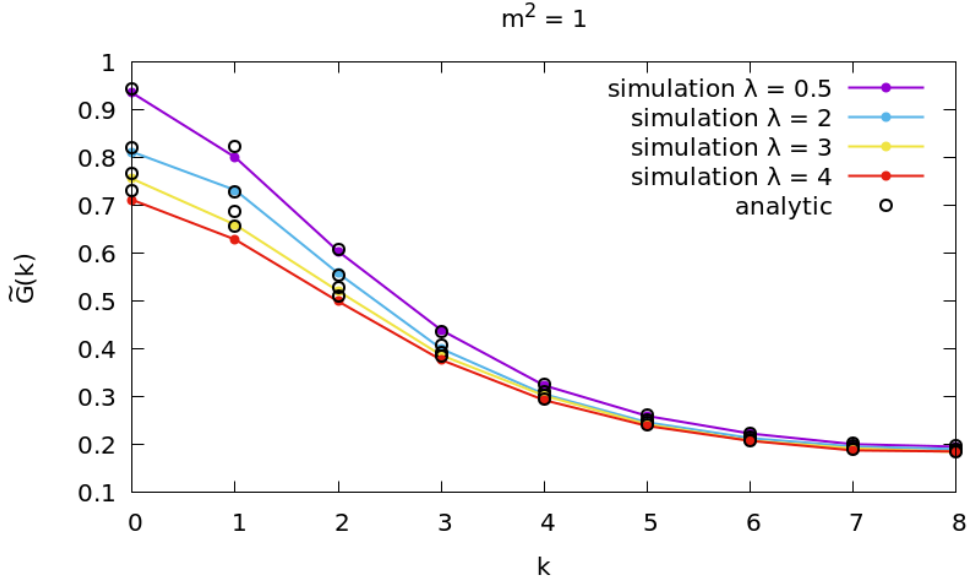


Figure 4.6: Numerical 2-point functions in momentum space (colourful lines-and-points) compared to the analytical perturbation theory (empty black circles) as a function of the quantum number k . The simulations were done on a 16×16 lattice.

the potential acquires a novel shape, as shown in Figure 4.7 below.

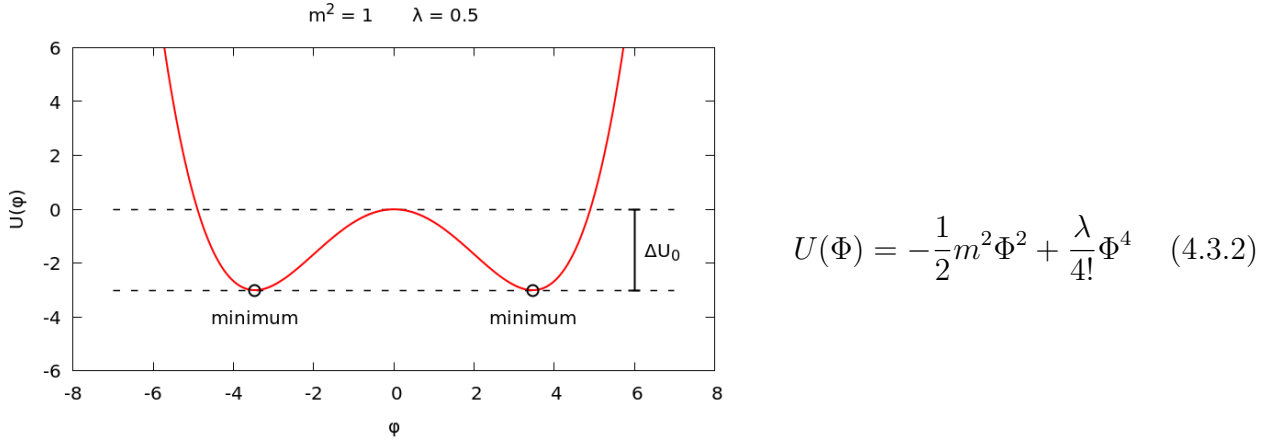


Figure 4.7: Potential function in the case of spontaneous symmetry breaking. The empty black circles indicate the two classical vacua for this potential. The square mass and coupling used in the plot are given in the upper part.

In this case, there are two available vacua on which the equilibrium can be placed, and the symmetry between Φ_0 and $-\Phi_0$ no longer exists. By either heading to the positive or to the negative vacuum, the field breaks the vacuum symmetry of the action, and this symmetry is said to be spontaneously broken, as discussed in [Smit, 2002]. This behavior

should manifest itself through the convergence of the Langevin equation to Φ_0 or $-\Phi_0$. Thus, equipped with the tools from the previous section, we can apply them to reproduce known results from spontaneous symmetry breaking in lattice Φ^4 -theory. The location of the two minima indicated in Figure 4.7 can be easily identified, applying simple rules of calculus to the potential in Eq.(4.3.2), as:

$$\Phi_0^\pm = \pm m \sqrt{\frac{6}{\lambda}} \quad (4.3.3)$$

Replacing the values used in the plot ($m^2 = 1$ and $\lambda = 0.5$), we find $\Phi_0^\pm = \pm \sqrt{12} \approx \pm 3.464$, which correspond to the two classical vacua of the theory. Thence we can determine the depth of the potential barrier of the vacua, given by $\Delta U_0 \equiv U(0) - U(\Phi_0^\pm)$:

$$\Delta U_0 = \frac{3m^4}{2\lambda} \quad (4.3.4)$$

In Figure 4.8 below, we demonstrate how the field bends towards one vacuum or the other depending on the initial condition by solving the Langevin equation with broken symmetry. Compare it with Figure 4.2, without symmetry breaking, where the vacuum at the origin was the only possibility. Even though the bosonic field can choose one vacuum or the other,

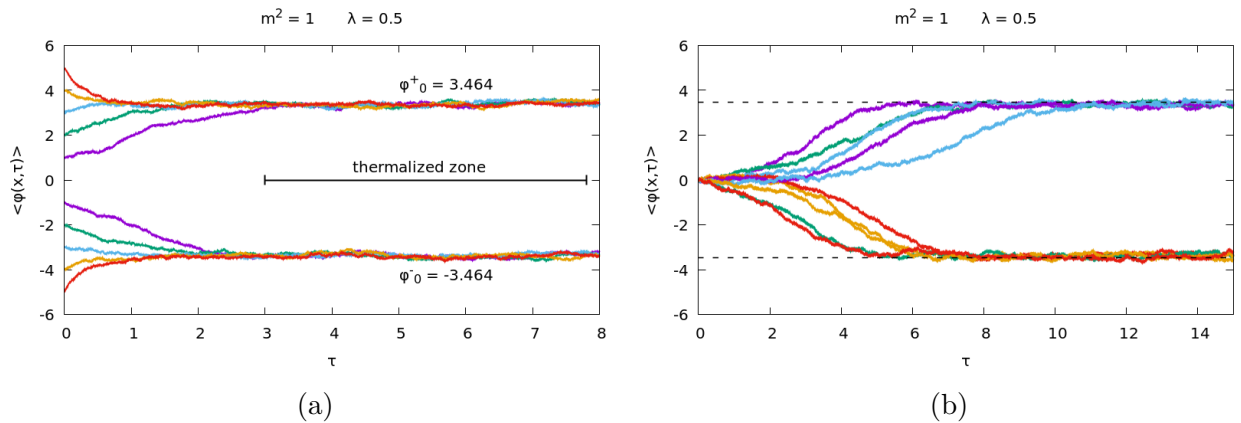


Figure 4.8: (a) Several solutions of the Langevin equation on a 8×8 lattice, with spontaneous breaking of symmetry using different initial conditions around each classical vacuum. (b) 10 more solutions, all with initial condition set to the origin (which corresponds to the local maximum of the potential). In this case, the solutions randomly select a vacuum to which they fall. The parameters used in the simulations are indicated above each plot.

dwelling the rest of its life there, if the coupling is strong enough, quantum fluctuations can induce transitions between the vacua. Since the potential barrier is inversely proportional to λ , from Eq.(4.3.4), the larger the coupling the less effort requires the particle to cross the energy obstacle. Therefore, there must be a critical value of λ for which the field would start to switch between Φ_0^+ and Φ_0^- from time to time. Furthermore, the transition rate (number of times the field crosses the potential barrier per unit of stochastic time) must be proportional to the coupling. Figure 4.9 shows three solutions with λ ten times bigger than in the other cases where we see the field crossing the potential barrier of the vacua and bouncing between them. In the broken symmetry case, since we can have either Φ_0^+ or Φ_0^- , in order to compute

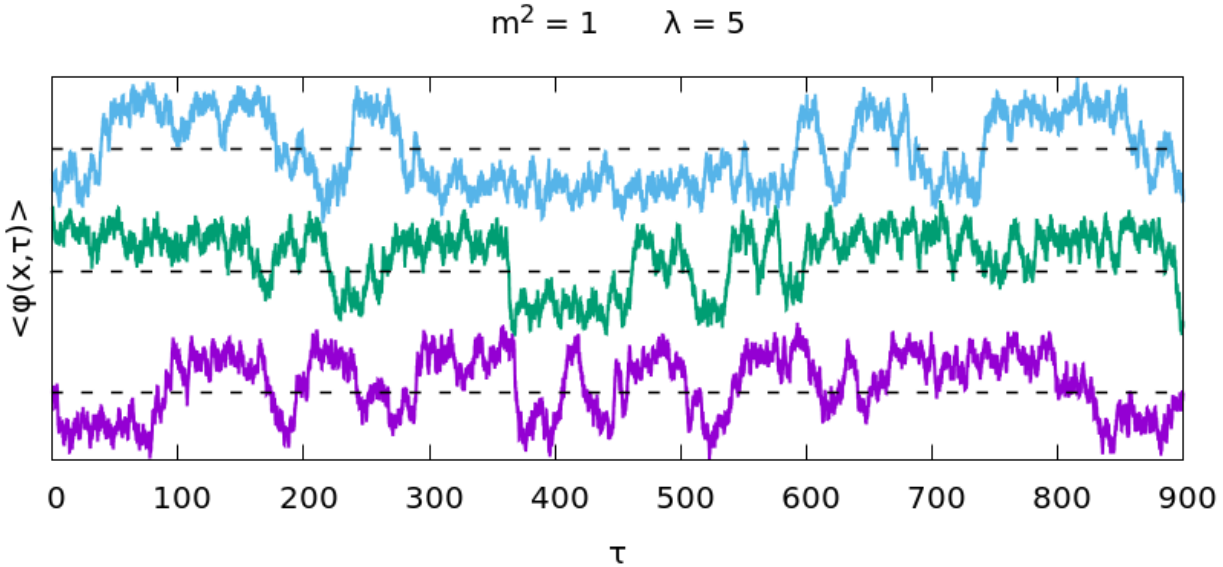


Figure 4.9: Three solutions with spontaneous symmetry breaking for large coupling ($\lambda = 5$), showing transition between the vacua. The two upper plots have been displaced vertically for clarity, with the dashed lines indicating the local maximum in each case.

the n -point functions, the vacuum contribution must be subtracted. Below, we show the new expression for the 2-point function with broken symmetry:

$$G(x_1, x_2) = \lim_{\tau \rightarrow \infty} \left[\langle \varphi(x_1, \tau) \varphi(x_2, \tau) \rangle_\eta - \langle \varphi(x_1, \tau) \rangle_\eta \langle \varphi(x_2, \tau) \rangle_\eta \right] \quad (4.3.5)$$

To this expression, we give the name of connected Green function. Notice that without

breaking of symmetry, the second term in the equation above is zero, since $\langle \varphi(x_1, \tau) \rangle_\eta = \langle \varphi(x_2, \tau') \rangle_\eta = 0$, and it reduces to the quantity previously calculated. Furthermore, with the vacuum expectation value being different from zero, in order to calculate the 2-point function, it turns out to be more convenient to shift the field and solve the Langevin equation around one of the classical vacua $\Phi_0^\pm$. To exemplify, let us choose the positive vacuum $\Phi_0 \equiv \Phi_0^+$ and define a shifted field as $\sigma \equiv \Phi - \Phi_0$. The action of the theory can thus be expressed in terms of σ as:

$$S_E[\sigma] = \sum_x \left[\frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2} m^2 (\sigma + \Phi_0)^2 + \frac{\lambda}{4!} (\sigma + \Phi_0)^4 \right] \quad (4.3.6)$$

$$= \sum_x \left[\frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2} m^2 (\sigma^2 + 2\sigma\Phi_0 + \Phi_0^2) + \frac{\lambda}{4!} (\sigma^4 + 4\sigma^3\Phi_0 + 6\sigma^2\Phi_0^2 + 4\sigma\Phi_0^3 + \Phi_0^4) \right] \quad (4.3.7)$$

Replacing the known expression for the classical vacuum $\Phi_0 = \sqrt{6m^2/\lambda}$ inside the equation above, we can simplify and reduce the equation above to:

$$S_E[\sigma] = \sum_x \left[\frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma + \frac{1}{2} m^2 \sigma^2 + \frac{\lambda}{4!} \sigma^4 + \sqrt{\frac{\lambda}{6}} m \sigma^3 - \frac{3m^4}{2\lambda} \right] \quad (4.3.8)$$

Since constant terms in the action do not contribute to the equations of motion, we can neglect the last term in the equation above. By making $\sigma \rightarrow \Phi$ again, we end up with:

$$S_E[\Phi] = \sum_x \left[\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{1}{2} m^2 \Phi^2 + \frac{\lambda}{4!} \Phi^4 + \sqrt{\frac{\lambda}{6}} m \Phi^3 \right] \quad (4.3.9)$$

This is the new action for the broken phase case. Notice that a new sort of interaction arises, which intermixes coupling and mass. This novel term, which is proportional to $\sqrt{\lambda}$, produces a phase with broken symmetry. Now, we can translate this system into a stochastic process through the Langevin equation:

$$\frac{\partial \varphi}{\partial \tau} = (\square - m^2) \varphi - \frac{\lambda}{6} \varphi^3 - \sqrt{\frac{3\lambda}{2}} m \varphi^2 + \eta \quad (4.3.10)$$

and in discrete form:

$$\varphi_j^{n+1} = \varphi_j^n + \Delta\tau \left[\frac{\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n}{a^2} - m^2\varphi_j^n - \frac{\lambda}{6}(\varphi_j^n)^3 - \sqrt{\frac{3\lambda}{2}}m(\varphi_j^n)^2 \right] + \sqrt{\frac{2\Delta\tau}{a}}R_j^n \quad (4.3.11)$$

Notice that in the free case (when $\lambda = 0$), both symmetric and non-symmetric cases have the same propagator, for they have the coupling-free content. Besides that, by switching the sign of φ in the equation above, the Langevin equation does not remain the same, as before, due to the term proportional to Φ^2 . The different behavior created by this term will also manifest itself in the analytical calculations presented in the next chapter when we approach stochastic quantization in perturbative expansion.

Chapter 5

Review of Noise Perturbation Theory and New Results

For most theories in the Standard Model of particle physics we can not find an exact solution, and perturbative expansion becomes the common approach to deal with them. In the path integral formalism, for example, we start from a given action and expand the part that depends on the coupling, leaving the free part unchanged, and compute perturbative approximations where each term is proportional to a power of this coupling. Each of these expanded terms corresponds to an intuitive picture, called a Feynman diagram, depicting a sort of interaction. In this chapter, we follow [\[Montvay and Münster, 1997\]](#) to review the main aspects of the perturbative method on the lattice, applied to the Φ^4 -theory case. comparing it with another type of perturbation in stochastic quantization. Afterwards, based on [\[Attanasio, 2013\]](#), we discuss how perturbation theory is implemented within stochastic quantization and present the new results with LASER, in 2 and 4 dimensions.

5.1 Feynman diagrams

Consider the 1-dimensional Euclidean action of a single scalar theory on the lattice with Φ^4 interaction term akin to chapter [4](#). The Feynman path integral for this theory can be written

as:

$$\mathcal{Z}_F = \int \mathcal{D}\varphi e^{-\sum_x \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{1}{2} m^2 \Phi^2 + \frac{\lambda}{4!} \Phi^4 \right)} \quad (5.1.1)$$

Even though we chose the 1-dimensional case, for simplicity, every step taken hereafter is identically mapped into higher dimensional cases with minor modifications. The 2-point function can be obtained from the path integral as:

$$\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) | 0 \rangle = \frac{1}{\mathcal{Z}_F} \int \mathcal{D}\Phi \Phi(x_1) \Phi(x_2) e^{-\sum_x \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{1}{2} m^2 \Phi^2 + \frac{\lambda}{4!} \Phi^4 \right)} \quad (5.1.2)$$

Expanding the term proportional to λ in the exponent:

$$\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) | 0 \rangle = \frac{1}{\mathcal{Z}_F} \sum_n \frac{1}{n!} \int \mathcal{D}\Phi \Phi(x_1) \Phi(x_2) \left[\frac{\lambda}{4!} \sum_x \Phi^4(x) \right]^n e^{-\sum_x \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{1}{2} m^2 \Phi^2 \right)} \quad (5.1.3)$$

Therefore, the 2-point function can be written as a sum of terms that depend on the summing index n with a factor λ^n :

$$\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) | 0 \rangle = \sum_n G^{(n)}(x_1, x_2) \quad (5.1.4)$$

which is precisely the formula we proposed in Eq.(4.1.5), with the definition:

$$G^{(n)}(x_1, x_2) \equiv \frac{\lambda^n}{\mathcal{Z}_F n! (4!)^n} \int \mathcal{D}\Phi \Phi(x_1) \Phi(x_2) \left[\sum_x \Phi^4(x) \right]^n e^{-\sum_x \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \frac{1}{2} m^2 \Phi^2 \right)} \quad (5.1.5)$$

Despite its scaring appearance, the right-hand side of this equation can be computed with a bunch of mathematical tricks involving functional derivatives. Due to the large number of steps, without any deep insights concerning stochastic theory, we choose not to show all of them explicitly. Instead, we refer the readership to this very detailed book on path integrals: [Das, 1993], where these tricks are presented in the continuum, whereby we adapt the steps to the lattice case. Each term generated by a given n produces some Feynman diagrams corresponding to interactions proportional to λ^n . The sum of all diagrams from $n = 0$ to

$n \rightarrow \infty$ result in the full interactive propagator. In Figure 5.1, we illustrate a few of these diagrams that come out from the loop expansion. First, to compute $G^{1\text{-loop}}(x_1, x_2)$ in the

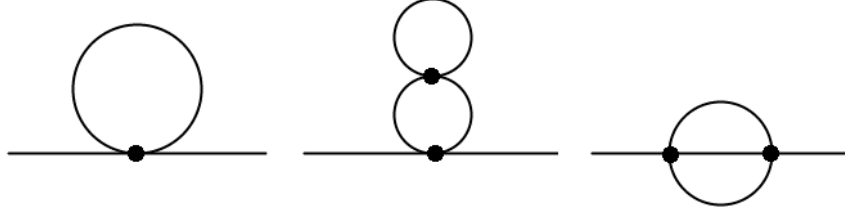


Figure 5.1: Relevant diagrams for perturbative Φ^4 -theory in the symmetric phase.

1-dimensional case, we need to solve the awful-looking Eq.(5.1.5) for $n = 1$ and add all contributions in the form of a so-called 1 Particle Irreducible (hereafter 1-PI) diagram, *i.e.*, a diagram that can not be broken into simpler diagrams. All the diagrams shown above are legitimate 1-PI diagrams, for they can not be separated into simpler pieces, whereas if we combined two of them with a propagator line it would not be 1-PI, since it would comprise two fundamental diagrams. At 1 loop, the solution to the right-hand side of Eq.(5.1.5) is given by:

$$G^{(1)}(x_1, x_2) = -\frac{\lambda}{2} \sum_x G^{(0)}(x_1, x) G^{(0)}(x, x) G^{(0)}(x, x_2) \quad (5.1.6)$$

which in momentum space looks like:

$$\tilde{G}^{(1)}(p) = -\frac{\lambda}{2} \tilde{G}^{(0)}(p) \left[\frac{1}{N} \sum_q \tilde{G}^{(0)}(q) \right] \tilde{G}^{(0)}(p) \equiv -\frac{\lambda}{2} \tilde{G}^{(0)}(p) J_1 \tilde{G}^{(0)}(p) \quad (5.1.7)$$

where N is the number of lattice sites¹, and we have introduced the function J_1 to aid in the following steps. Finally, we need to add up all combinations of 1-PI diagrams at 1-loop. Graphically, we have:

¹In the original expression it should be the lattice size $L = aN$, but since we made $a = 1$ for convenience, L can be replaced by N in this case.

$$\tilde{G}^{1-\text{loop}}(p) = \text{---} + \text{---} \overset{\text{red loop}}{\bullet} \text{---} + \text{---} \overset{\text{red loop}}{\bullet} \overset{\text{red loop}}{\bullet} \text{---} + \dots \quad (5.1.8)$$

$$= \tilde{G}^{(0)}(p) - \frac{\lambda}{2} \tilde{G}^{(0)}(p) \mathbf{J}_1 \tilde{G}^{(0)}(p) + \frac{\lambda^2}{4} \tilde{G}^{(0)}(p) \mathbf{J}_1 \tilde{G}^{(0)}(p) \mathbf{J}_1 \tilde{G}^{(0)}(p) + \dots \quad (5.1.9)$$

$$= \tilde{G}^{(0)}(p) [1 - \frac{\lambda}{2} \tilde{G}^{(0)}(p) \mathbf{J}_1 + \frac{\lambda^2}{4} \tilde{G}^{(0)}(p)^2 \mathbf{J}_1^2 + \dots] \quad (5.1.10)$$

where, in the first equality, the ellipsis (...) contains three bubbles, four bubbles and so on. Furthermore, we stressed through the red-coloured bubbles that the interpretation of the function J_1 is that of a quantum loop. Identifying above the alternate geometric series:

$$\tilde{G}^{1-\text{loop}}(p) = \tilde{G}^{(0)}(p) \sum_{n=0}^{\infty} (-1)^n \left[\frac{\lambda}{2} \tilde{G}^{(0)}(p) J_1 \right]^n \quad (5.1.11)$$

$$= \tilde{G}^{(0)}(p) \left[\frac{1}{1 + \lambda \tilde{G}^{(0)}(p) J_1 / 2} \right] \quad (5.1.12)$$

In the last equality, we used the formula for the sum of the alternate geometric series. Replacing the free propagator from Eq.(4.1.3), with $a \equiv 1$, we obtain:

$$\tilde{G}^{1-\text{loop}}(p) = \frac{1}{m^2 + 4 \sin^2(p/2)} \frac{1}{\left[1 + \frac{\lambda}{2} \frac{J_1}{m^2 + 4 \sin^2(p/2)} \right]} \quad (5.1.13)$$

$$= \frac{1}{m^2 + 4 \sin^2(p/2) + \frac{\lambda}{2} J_1} \quad (5.1.14)$$

the 1-loop propagator in position space is then straightforwardly obtained from an inverse Fourier transform:

$$G^{1-\text{loop}}(x_1, x_2) = \frac{1}{N} \sum_p \frac{e^{ip(x_1 - x_2)}}{m^2 + 4 \sin^2\left(\frac{p}{2}\right) + \frac{\lambda}{2} J_1} \quad (5.1.15)$$

Recall that $p = 2\pi k/N$, where k is the momentum quantum number. Therefore, the sum over p is equivalent to a sum over k from $-N/2$ to $N/2 - 1$. To compute the next order in

quantum correction, we introduce the momentum space functions below:

$$J_n = \frac{1}{N} \sum_p \left[\tilde{G}^{(0)}(p) \right]^n \quad (5.1.16)$$

$$I_2(p) = \frac{1}{N} \sum_q \tilde{G}^{(0)}(q) \tilde{G}^{(0)}(p-q) \quad (5.1.17)$$

$$I_3(p) = \frac{1}{N^2} \sum_q \sum_k \tilde{G}^{(0)}(q) \tilde{G}^{(0)}(k) \tilde{G}^{(0)}(p-q-k) \quad (5.1.18)$$

which result directly from solving Eq.(5.1.5) with $n = 2$, where J_n is a generalization of J_1 . Repeating the same 1-PI procedure with 2 loops, we can finally jot down the next-order approximation for the momentum-space propagator:

$$G^{2\text{-loop}}(x_1, x_2) = \frac{1}{N} \sum_p \frac{e^{ip(x_1-x_2)}}{m^2 + 4 \sin^2 \left(\frac{p}{2} \right) + \frac{\lambda}{2} J_1 - \frac{\lambda^2}{4} J_1 J_2 - \frac{\lambda^2}{6} I_3(p)} \quad (5.1.19)$$

Finally, we illustrate in Figure 5.2 the first three relevant diagrams in Φ^4 -theory with broken symmetry. The 1-loop propagator in this case is given by:

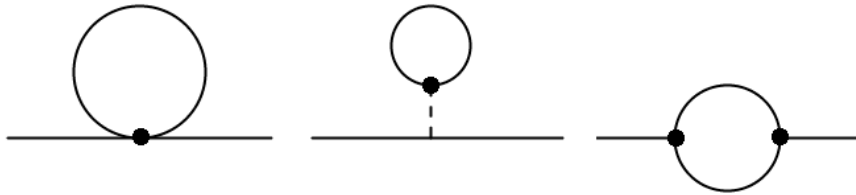


Figure 5.2: Relevant diagrams for perturbative Φ^4 -theory in the broken phase.

$$G^{1\text{-loop}}(x_1, x_2) = \frac{1}{N} \sum_p \frac{e^{ip(x_1-x_2)}}{m^2 + 4 \sin^2 \left(\frac{p}{2} \right) - \lambda J_1 - \frac{3}{2} \lambda m^2 I_2(p)} \quad (5.1.20)$$

Notice that in the last one, the 1-loop propagator has an additional term, akin to Eq.(4.3.10) in the previous chapter, that is proportional to the mass.

What if we wanted to make sure that, like analytical perturbation theory, stochastic quantization also makes sense order by order? There should be some resource to perform perturbative

expansions through the Langevin equation and compute solutions truncated at a given loop order. This tool is called noise perturbation theory, which is an equivalent of the standard perturbation theory method for the stochastic case. This technique will play an important role in the upcoming numerical simulations. We commence by presenting its analytical foundations, as in [Attanasio, 2013].

5.2 Multi-loop expansion in the stochastic formalism

Even though stochastic quantization has provided the full non-perturbative solution to the target theory up to noise errors, in the last section we addressed the question of whether it would make sense within a perturbative frame as well. To answer this question, in this section we expand the stochastic field φ inside the Langevin equation in powers of $\hbar$, arrange terms of equal power, and solve perturbative equations up to some order. This means that alternatively to adding corrections to the Green functions, we introduce them directly within the fields. A method called Noise Perturbation Theory (hereafter NPT). In this fashion, consider a Taylor expansion of φ in powers of $\hbar$ as:

$$\varphi = \varphi_0 + \varphi_1 \hbar + \varphi_2 \hbar^2 + \mathcal{O}(\hbar^3) \quad (5.2.1)$$

where we have put the $\hbar$ factor back for the sake of clarity and absorbed the factorials $1/k!$ into the definitions of the perturbative fields φ_k . Setting $\hbar \equiv 1$ again, we can replace Eq.(5.2.1) onto the Langevin equation:

$$\frac{\partial}{\partial \tau}[\varphi_0 + \varphi_1 + \varphi_2 + \dots] = (\square - m^2)[\varphi_0 + \varphi_1 + \varphi_2 + \dots] - \frac{\lambda}{6}[\varphi_0 + \varphi_1 + \varphi_2 + \dots]^3 + \eta \quad (5.2.2)$$

and collect terms with equal power of $\hbar$. The result is a series of coupled differential equations up to a given truncation order.

$$\frac{\partial \varphi_0}{\partial \tau} = (\square - m^2)\varphi_0 - \frac{\lambda}{6}\varphi_0^3 \quad (5.2.3)$$

$$\frac{\partial \varphi_1}{\partial \tau} = (\square - m^2)\varphi_1 - \frac{\lambda}{2}\varphi_0^2\varphi_1 + \eta \quad (5.2.4)$$

$$\frac{\partial \varphi_2}{\partial \tau} = (\square - m^2)\varphi_2 - \frac{\lambda}{2}(\varphi_0^2\varphi_2 + \varphi_0\varphi_1^2) \quad (5.2.5)$$

$$\frac{\partial \varphi_3}{\partial \tau} = (\square - m^2)\varphi_3 - \frac{\lambda}{6}(\varphi_1^3 + 6\varphi_0\varphi_2\varphi_1 + 3\varphi_0^2\varphi_3) \quad (5.2.6)$$

$$\frac{\partial \varphi_4}{\partial \tau} = (\square - m^2)\varphi_4 - \frac{\lambda}{2}(\varphi_2\varphi_1^2 + 2\varphi_0\varphi_3\varphi_1 + \varphi_0\varphi_2^2 + \varphi_0^2\varphi_4) \quad (5.2.7)$$

$$\frac{\partial \varphi_5}{\partial \tau} = (\square - m^2)\varphi_5 - \frac{\lambda}{2}(\varphi_1^2\varphi_3 + \varphi_1\varphi_2^2 + 2\varphi_0\varphi_1\varphi_4 + 2\varphi_0\varphi_2\varphi_3 + \varphi_0\varphi_5) \quad (5.2.8)$$

Due to the cubic power in the Langevin equation, this task becomes awkward very quickly for increasing orders, and we obtain them through an automatic routine implemented in the Wolfram Language. We could continue the process of expanding φ up to higher orders and collecting a larger set of coupled equations in a systematic way. However, these equations are implemented and solved in LASER only up to order 10, since the execution tends to slow down for higher orders as a consequence of the huge number of computations and memory use. Thence, we move on to the essential part of defining perturbative n -point functions in the stochastic sense.

5.3 Perturbative n -point functions

Besides replacing the expansion of φ in the Langevin equation to obtain the dynamics of each perturbative field, we could also derive 2-point functions in this approach. By plugging Eq.(5.2.1) into the definition of the momentum-space 2-point function, we obtain:

$$\tilde{G}(p) = \lim_{\tau \rightarrow \infty} \sum_x e^{ipx} \langle \varphi(x, \tau) \varphi(0, \tau) \rangle_\eta \quad (5.3.1)$$

$$= \lim_{\tau \rightarrow \infty} \sum_x e^{ipx} \langle [\varphi_0(x, \tau) + \varphi_1(x, \tau) + \varphi_2(x, \tau) + \dots][\varphi_0(0, \tau) + \varphi_1(0, \tau) + \varphi_2(0, \tau) + \dots] \rangle_\eta \quad (5.3.2)$$

Multiplying the crossed terms and separating the averages:

$$\begin{aligned} \tilde{G}(p) = \lim_{\tau \rightarrow \infty} \sum_x e^{ipx} [& \langle \varphi_0(x, \tau) \varphi_0(0, \tau) \rangle_\eta + \\ & \langle \varphi_1(x, \tau) \varphi_0(0, \tau) \rangle_\eta + \langle \varphi_0(x, \tau) \varphi_1(0, \tau) \rangle_\eta + \\ & \langle \varphi_2(x, \tau) \varphi_0(0, \tau) \rangle_\eta + \langle \varphi_1(x, \tau) \varphi_1(0, \tau) \rangle_\eta + \langle \varphi_0(x, \tau) \varphi_2(0, \tau) \rangle_\eta + \dots] \end{aligned} \quad (5.3.3)$$

Recognizing the pattern, we can truncate the sum above and write general formula for the propagator $\tilde{G}^{(\xi)}(p)$ up to order ξ :

$$\tilde{G}^{(\xi)}(p) = \lim_{\tau \rightarrow \infty} \sum_{n=0}^{\xi} \sum_{k=0}^n \sum_x e^{ipx} \langle \varphi_k(x, \tau) \varphi_{n-k}(0, \tau) \rangle_\eta \quad (5.3.4)$$

Similarly, the momentum-space 4-point function in the perturbative framework can be expressed as:

$$\chi_4^{(\xi)}(0) = \lim_{\tau \rightarrow \infty} \sum_{n+m+k+l \leq \xi} \sum_{x,y,z} \langle \varphi_n(x, \tau) \varphi_m(y, \tau) \varphi_k(z, \tau) \varphi_l(0, \tau) \rangle_\eta \quad (5.3.5)$$

In this case, since we have a product of four fields within the average brackets, this equation can not be simplified, and the condition for terms that account at order ξ is not straightforward to implement in simulations. We need to sum only over the fields whose non-negative integer indices $\{n, m, k, l\}$ satisfy the condition $n + m + k + l \leq \xi$, finding all possible 4-tuples (n, m, l, k) whose components add up to a number less or equal to the order². For low values of ξ , this could be done even by hand, however, we want to have means of calculating quantum corrections to the 4-point function up to high orders. And since χ_4 is proportional to

²In order to accomplish this in our code, we implemented the so-called Diphtantine analysis.

$\hbar^2$, $\xi = 2$ is the lowest value that will give a meaningful contribution to the quantum 4-point function, recalling that $\xi = 0$ would be the classical solution, proportional to $\hbar^0$. As the lowest order, $\xi = 2$ gives the free solution (*i.e.* $\lambda = 0$), by consistency, $\xi = 4$ would be the 1-loop correction, $\xi = 6$ the 2-loop correction and so on. This makes our lives much harder since the larger ξ the more terms has the sum of indices, which renders the sum in Eq.(5.3.5) even longer, and thus more CPU costly. In the following section, we provide the results of these computations numerically for dimensions 2 and 4.

5.4 New results with LASER

NPT has been applied before in other physical contexts, like in Ginzburg-Landau systems [Attanasio, 2013], stochastic inflation [Kunze, 2006, Martin and Musso, 2006a, Martin and Musso, 2006b], and so on. To start applying NPT in numerical simulations, we commence by the 2-dimensional Φ^4 -theory in the symmetric phase. Recall that using the Green functions $\tilde{G}^{(\xi)}(p)$ as perturbative corrections, in section 5.1 we did resummations through the 1-PI procedure to compute the final 1 and 2-loop lattice propagators analytically. Not surprisingly, this method can be identically applied to the multi-loop expansion presented in section 5.2 to obtain the numerical lattice propagators in NPT. Each term of the expanded propagator in Eq.(5.3.3) represents a diagram and thus can be resummed as such³. In Figure 5.3, the plot shows a comparison between simulation outputs and the analytical $\tilde{G}^{1\text{-loop}}(p)$ and $\tilde{G}^{2\text{-loop}}(p)$ for an array of couplings using the perturbative propagator at zero momentum. Notice that in both cases, the simulations would seem perfectly equal to the analytical results, was it not for a small difference making the latter appear displaced upwards by a tiny fraction relatively to the former. This slight disagreement comes from limitations in the integration method itself (on which we make a few remarks in Appendix A.1). This technique can be systematically applied to higher-loop numerical propagators,

³This numerical procedure is done after the accomplishment of all simulations by an external Python script which receives the stochastic averages from the expanded Langevin equation as inputs and applies the 1-PI resummation

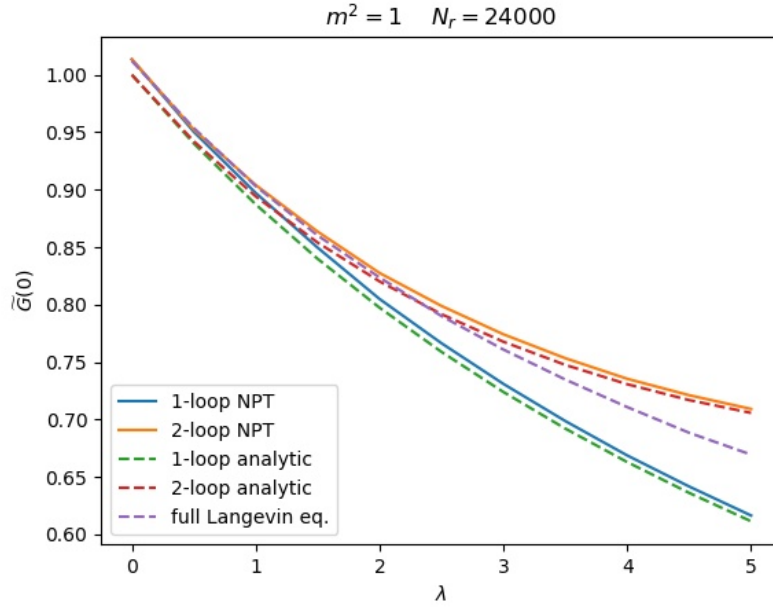


Figure 5.3: Comparison between the zero-momentum propagators on a 8×8 lattice from perturbative stochastic simulations (continuous lines) and analytical perturbation theory (dashed lines) up to 2 loops as a function of the coupling constant λ . The dashed purple line represents the full solution of the Langevin equation. On the top, the mass squared and the number of noise realizations used are shown.

even though their analytical counterparts become increasingly difficult.

Besides the 2-dimensional case, we also derive new results by simulating Φ^4 -theory on a 4-dimensional lattice in NPT. Definitely, simulating a 4-dimensional lattice on the computer is an extremely tough challenge, for the amount of computations per run rapidly increases with the number of sites in each direction. The Langevin equation in this case depends on five variables: the four Euclidean coordinates plus the stochastic time. With the 24 cores we had at our disposal to perform the calculations in parallel, NPT in 4 dimensions could only be finished at slow pace. Therefore, these simulations were limited to very small lattice sizes (no bigger than $N = 4$ in each direction), and the number of noise realizations did not reach that one from the 2-dimensional case. The results are shown in Figure 5.4

Now, we turn to analyze how precisely each order reproduces the exact solution (solving the full Langevin equation) and what is the influence of the coupling order by order. Hence, in the next section, we introduce the concept of error in each order relatively to the exact

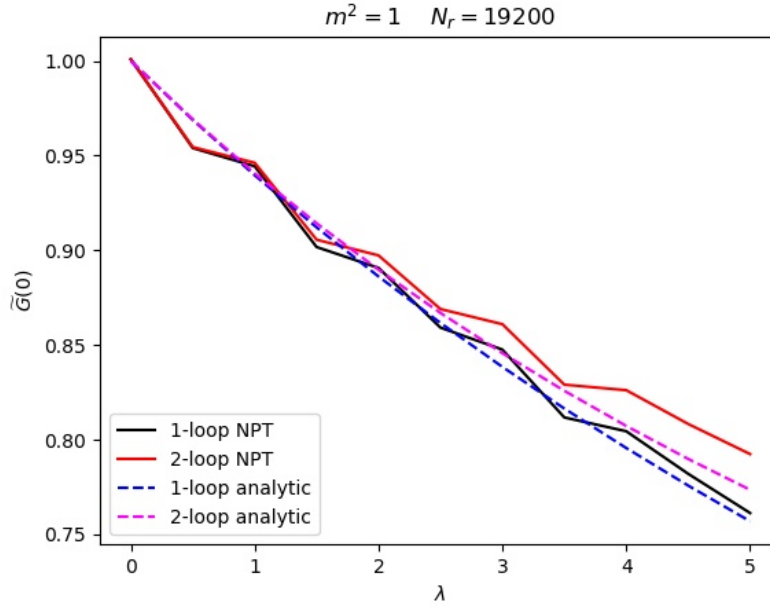


Figure 5.4: Comparison between the zero-momentum propagators on a $4 \times 4 \times 4 \times 4$ lattice from perturbative stochastic simulations (continuous lines) and analytical perturbation theory (dashed lines) up to 2 loops as a function of the coupling constant λ . On the top, the mass squared and the number of noise realizations used are shown.

numerical solution.

5.5 Error analysis in loop expansion

When the coupling constant becomes gradually larger, ordinary perturbation theory starts to flaw for low orders. And since higher orders are often very painfully difficult to achieve, as far as perturbation theory is concerned, we are forced to resign to mediocre results. On the other hand, NPT has aided in developing a systematic way to compute higher corrections at the expense of solving larger sets of coupled differential equation. Now, we are compelled to study how the accuracy of this approach is affected by the coupling. To exemplify, we pick up the position-space propagator of the Φ^4 -theory in the symmetric phase and define a

parameter of error as the fractional difference between the exact one and that from NPT:

$$E_\xi(x_1, x_2) = \left| \frac{G^{(\xi)}(x_1, x_2) - G(x_1, x_2)}{G(x_1, x_2)} \right| \quad (5.5.1)$$

Notice that, since $G \propto \hbar^2$, $\xi = 2$ represents the free case (just like $\xi = 4$ represented the free case for the 4-point function) and $\xi > 2$ furnishes quantum corrections. In Figure 5.5, we plot Eq.(5.5.1), using only even⁴ values of ξ , as a function of the lattice distance for several strengths of the coupling. In these plots, most orders remain below the 5% error line for increasing λ . Since $\mathcal{O}(2)$ gives the free propagator, it is not affected by strengthening the coupling, whilst $\mathcal{O}(4)$, $\mathcal{O}(6)$, $\mathcal{O}(8)$ (1, 2 and 3-loop corrections, respectively), should comprehend the effects of changing λ . Towards the right-most part of the plot, uncertainties grow for higher lattice distances because the values of the propagator become fainter due to the exponential decrease.

Furthermore, we also define the average error⁵ $\langle E_\xi(x_1, x_2) \rangle$ over the lattice distances and plot it as a function of λ for the same values used in Figure 5.5. Using the machinery developed so far, either NPT or through the exact Langevin equation, in the next chapter we turn attention to a fundamental problem ubiquitously attached to lattice theories. Everything until this point was strictly made on a discrete space, *i.e.* a lattice, but as far as we know the real world is not made of lattices comprising countable sites. Actually, the world is seen as smoothly filled by the continuous fabric of spacetime, a stage where physical processes take place and to whom we attribute continuous measurable quantities. Therefore, the final step is to find a path whereby we take the limit of the lattice recovering a continuous Euclidean space. We review and discuss such path in the upcoming chapter, where we also present our new results with LASER.

⁴In Φ^4 -theory with symmetric phase all odd orders in noise perturbation theory are null

⁵Do not confuse with the stochastic average $\langle \cdot \rangle_\eta$.

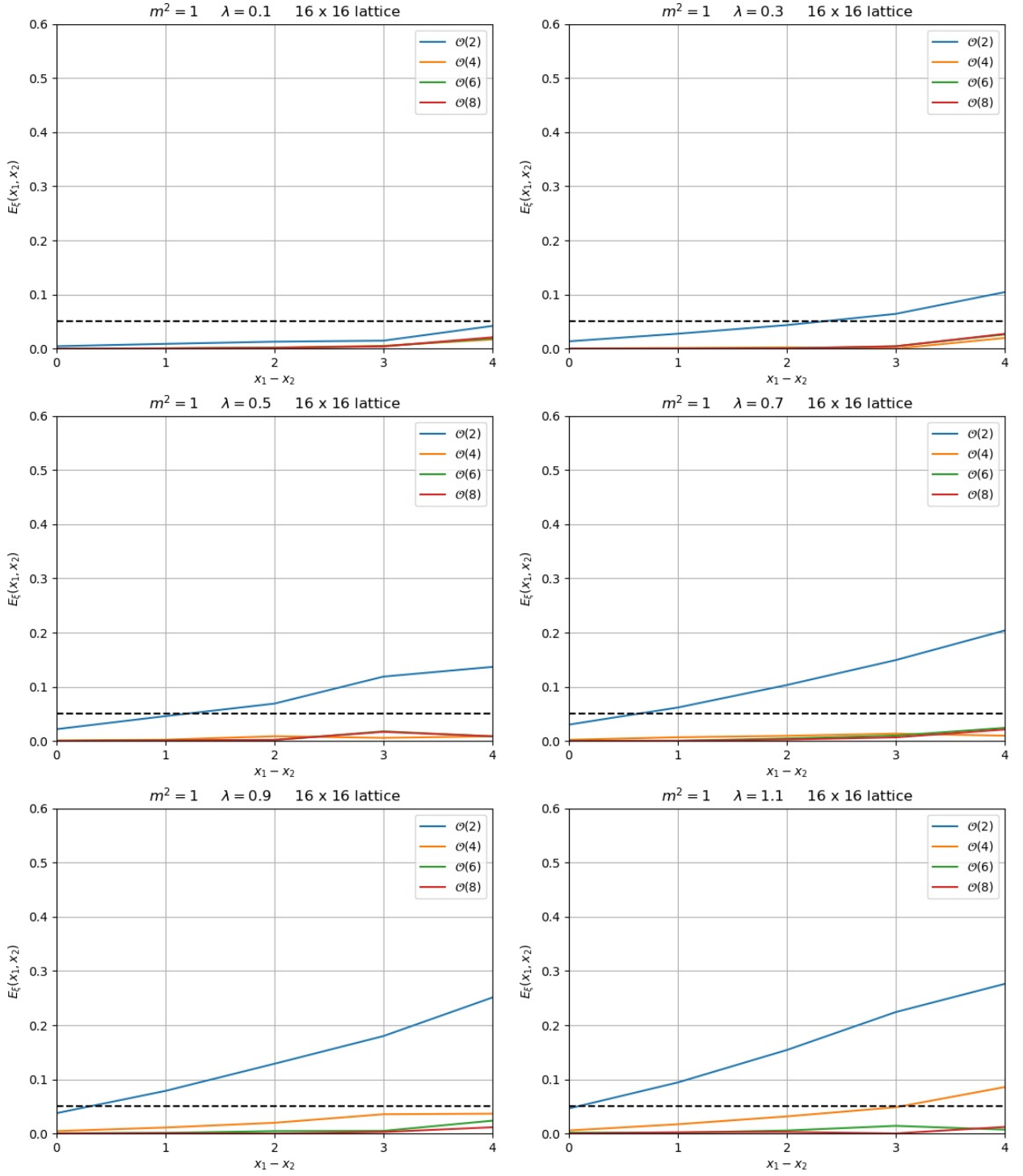


Figure 5.5: Fractional error plots for position-space propagators as a function of distance on a 16×16 lattice using $N_r = 10000$ and $m^2 = 1$. The dashed line in each plot represents the 5% error line taken as reference.

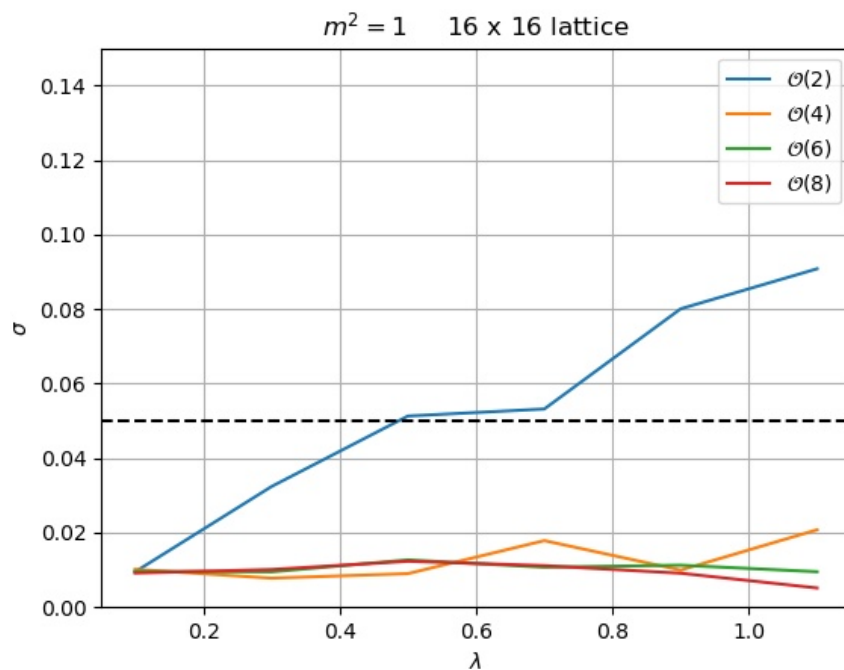


Figure 5.6: Average error as a function of the coupling constant up to $\mathcal{O}(8)$, using $N_r = 10000$ and $m^2 = 1$ in each simulation. The dashed line represents the 5% error taken as reference.

Chapter 6

Review of Lattice Renormalization and New Results

6.1 Why renormalization?

Renormalization exists to purge quantum theories of divergencies that appear from the computation of Feynman diagrams. These divergencies happen because some loop integrals in perturbation theory give infinite values. Truth be told, infinite quantities do not seem natural results in any theory, but we argue that the ones coming out from QFT are totally expected from the analytical point of view. These divergencies appear in two basic types: infrared (IR) and ultraviolet (UV). The UV divergencies, for example, bloom out of the high momentum part of the QFT spectrum, putting into evidence our utter ignorance when it comes to describing interactions in the smallest scales. This fact elucidates that our method of describing Nature is far from complete. If we had a thoroughly consistent theory of fundamental interactions, high momentum integrals would perfectly reproduce the physics of events from the macro world to the Planck scale, and no divergencies should exist. Nevertheless, lacking such a broadly comprehensive theory, physicists needed to devise an enlightened recipe to wipe out all the hidden degrees of freedom to which we have no access. The successful understanding

of such divergencies and the development of a consistent method to treat them make one of the most notable breakthroughs in the physics of the 21st century. Despite divergencies being almost ubiquitous to continuous QFT, lattice theories, lacking any sort of infinity, suffer none of it. In these theories, because the minimum interaction distance is strictly constrained by the lattice spacing (a), the maximum transferred momentum has a natural threshold and does not generate infinities. In Figure 6.1, we depict high momentum and low momentum interactions as waves across a 2-dimensional lattice. Although bestowed with such a remark-

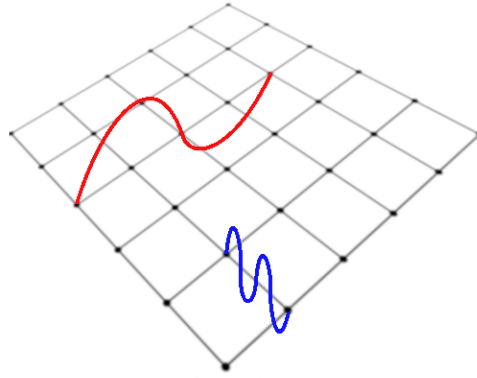


Figure 6.1: Long range interactions (red wavelength) generate low momentum transfer, while short range ones (blue wavelength) generate high momentum transfer. Notice that because the blue is the highest momentum transferred in this lattice, there are no UV divergencies.

able feature, lattice theories do not directly provide alone the real world observables, since spacetime is a continuous entity. That is why at some point any output from lattice theories must be considered in the continuum limit, where fundamental parameters like mass and coupling constant are physically measurable. We need thus a renormalization scheme to take the continuous limit of the lattice, avoiding the scales that we have no theory for, and preventing the fundamental parameters from blowing up.

Renormalization strategies have been discussed in Φ^4 -theory with broken phase [Cassol-Seewald et al., 2012a], in the context of the Ginzburg-Landau-Langevin (GLL) type of equation in [Cassol-Seewald et al., 2012b], to a model for the chiral phase transition in QCD [Krein, 2012] using GLL, etc. In this chapter, we review a renormalization method from [Wolff, 2009, Weisz and Wolff, 2011, Dalla Brida et al., 2017] to use in our case and

obtain new results in 2, 3, and 4 dimensions. Since the understanding of our renormalization outputs are yet ongoing, and due to challenges of CPU time imposed by 4-dimensional lattice simulations, the data that we generate in this chapter are still in their preliminary stage, needing future refinement and analysis. In spite of that, we report some fundamental differences regarding the three aforementioned works, concerning the possible triviality of Φ^4 -theory in 4 dimensions, *i.e.* that the renormalized coupling vanishes in the continuum limit, which remains a debated issue in the literature [Luescher and Weisz, 1987, Hogervorst and Wolff, 2012, Siefert and Wolff, 2014].

6.2 From lattice to continuum

In the universe of a lattice, where space only exists in some specific sites, there are two main scales to be considered when performing continuum limits. One of these is parametrized by the lattice spacing (a), measuring how close two adjacent lattice sites stand from each other, and it is associated with the ultraviolet domain. The second parameter is the actual lattice size (L), which bears the infrared scale of space. A proper continuum limit consists of varying these parameters, increasing L ($L \rightarrow \infty$), and decreasing a ($a \rightarrow 0$) until there are no voids left and discrete space turns into continuous Euclidean space. In Figure 6.2, we depict this process for a 2-dimensional lattice. In order to illustrate how to accomplish this process, we

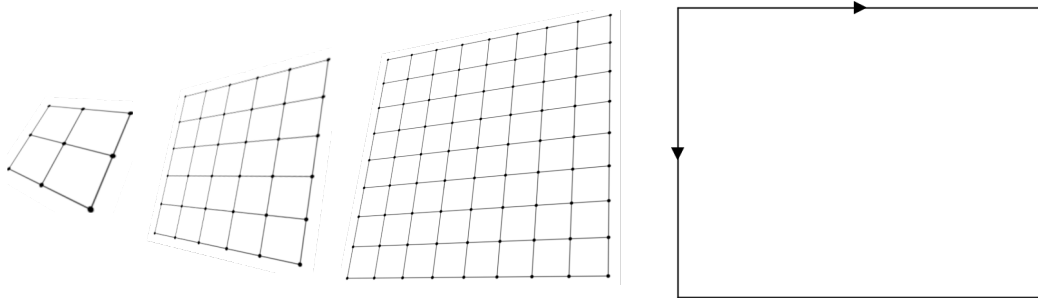


Figure 6.2: 2-dimensional representation of the infinite volume limite, where the lattice length and the number of sites must gradually increase, while the lattice spacing must decrease until we turn a lattice into a continuous Euclidean space.

shall consider the familiar example of the 1-dimensional harmonic oscillator with a unitary

mass in quantum mechanics that we have solved in section 3.3. Due to its simplicity, this system lacks any divergencies and thus makes up a perfect starting point. Recall that the Langevin equation associated with this system is given by Eq.(3.3.9) and it can be discretized as:

$$x_j^{n+1} = x_j^n + \Delta\tau \left[\frac{x_{j+1}^n - 2x_j^n + x_{j-1}^n}{a^2} - kx_j^n \right] + \sqrt{\frac{2\Delta\tau}{a}} R_j^n \quad (6.2.1)$$

then we can rewrite Eq.(6.2.1) in terms of rescaled quantities with the transformations:

$$\hat{k} \equiv a^2 k \quad \Delta\hat{\tau} \equiv \frac{\Delta\tau}{a^2} \quad \hat{R}_j^n \equiv \sqrt{a} R_j^n \quad (6.2.2)$$

By doing so, we end up with the new (rescaled) discretized Langevin equation:

$$x_j^{n+1} = x_j^n + \Delta\hat{\tau} \left[x_{j+1}^n - 2x_j^n + x_{j-1}^n - \hat{k}x_j^n \right] + \sqrt{2\Delta\hat{\tau}} \hat{R}_j^n \quad (6.2.3)$$

which does not depend explicitly on the lattice spacing. Notice that this rescaling procedure is equivalent to defining $a \equiv 1$ as we did in section 4.2, but now we replace that naive definition with a more solid interpretation. As opposed to section 4.2, a has not truly disappeared, instead, the a -dependency is now carried by the rescaled quantities ($\hat{k}$, $\Delta\hat{\tau}$, and $\hat{R}_j^n$). This fact has a straightforward implication: a change in the lattice scales (a and L) is equivalent to a change in the input quantities according to the recipe in Eq.(6.2.2). Therefore, by properly tuning these quantities, one might reproduce lattices closer and closer to the continuum limit. However, the parameter of which we have actual control in simulations is the number of sites N . Since it is related to the others by $L = aN$, the three numbers are not independent. One has to choose two of them to vary, and the third will be automatically determined. To show the continuum limit starting from a lattice, we use our example and compute its autocorrelation function $G(0)$ for increasing N and diminishing a . Table 6.1 below shows the parameters set used to perform the continuum limit. The deeper we move along the diagonal of this table the closer is the continuous estimation for the quantity $G(0)$.

$k = 1.0 \quad \Delta\tau = 0.001 \quad N_r = 7200$					
N	$G_{L=10}(0)$	$G_{L=20}(0)$	$G_{L=30}(0)$	$G_{L=40}(0)$	$G_{L=60}(0)$
10	0.447(3)				
20	0.487(3)	0.448(2)			
30	0.498(3)	0.475(2)	0.448(2)		
40	0.504(2)	0.488(2)	0.469(1)	0.448(1)	
50	0.510(3)	0.494(2)	0.480(2)	0.465(1)	
60	0.517(3)	0.498(3)	0.487(1)	0.476(1)	0.448(1)
70	0.525(3)	0.501(3)	0.492(2)	0.483(1)	0.460(1)
80	0.534(3)	0.505(2)	0.495(1)	0.487(1)	0.470(1)
90	0.543(3)	0.507(2)	0.498(1)	0.491(1)	0.476(1)
100	0.554(3)	0.510(2)	0.500(2)	0.494(1)	0.481(1)
110	0.569(2)	0.513(2)	0.503(2)	0.496(1)	0.485(1)
120	0.583(3)	0.517(2)	0.504(2)	0.498(1)	0.487(1)

Table 6.1: Autocorrelations for different lattice sizes L (columns) and different lattice sites N (lines). For each L , there is a best estimation for the continuous propagator highlighted in blue, found by varying N , and also $a = L/N$. The numbers in parenthesis are the noise uncertainties and refer to the last decimal digit.

In fact, from the highlighted values in the table above, $G(0)$ seems to be approaching 0.5, which is precisely the continuous value of autocorrelation as given by Eq.(3.3.20) with the parameters used:

$$G(0) = \frac{1}{2m\omega_0} e^{-\omega_0(0)} = \frac{1}{2 \times 1.0 \times 1.0} = 0.5 \quad (6.2.4)$$

where $\omega_0 = \sqrt{k}$. In Figure 6.3, we show the paths towards the continuum limits varying the lattice scale parameters. Likewise, we need to apply this procedure to the case of quantum field theory. As a first attempt, we can rescale the Langevin equation for the Φ^4 -theory as we did to the harmonic oscillator and run simulations with $N \rightarrow \infty$ and $a \rightarrow 0$, where the rescaled parameters carry the a -dependence. Figure 6.4 below shows where it leads to. QFT has intrinsically divergent quantities, and when we try to reach the continuum limit, they manifest through the Green functions. Through the blue fit in Figure 6.4, we show that $\tilde{G}(0)$ bears a divergence of the logarithmic type. This makes the continuum limit of fields a much more laborious task, otherwise, this chapter would end up here. As argued before, in the lattice they do not exist because the maximum transferred momentum $p = 2\pi k/L$ during

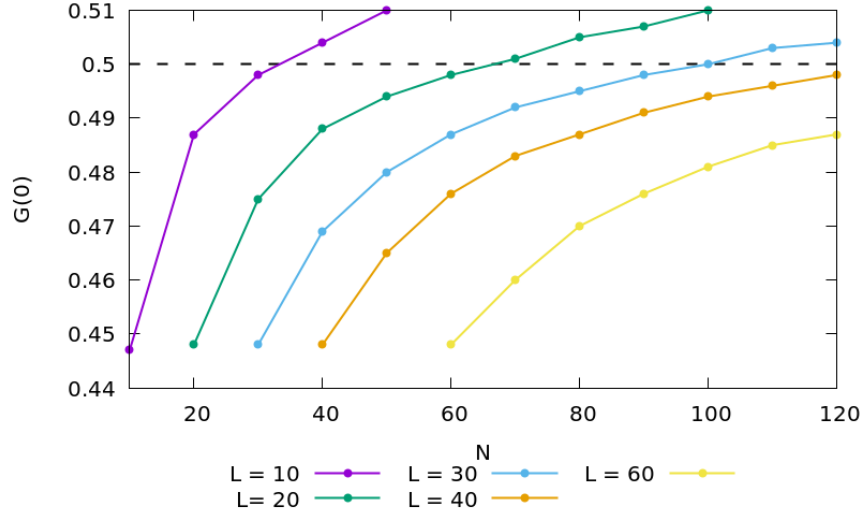


Figure 6.3: Autocorrelations as a function of the number of lattice sites for different sizes L . The dashed line marks the exact value of $G(0)$, in the continuum limit, from analytical calculations.

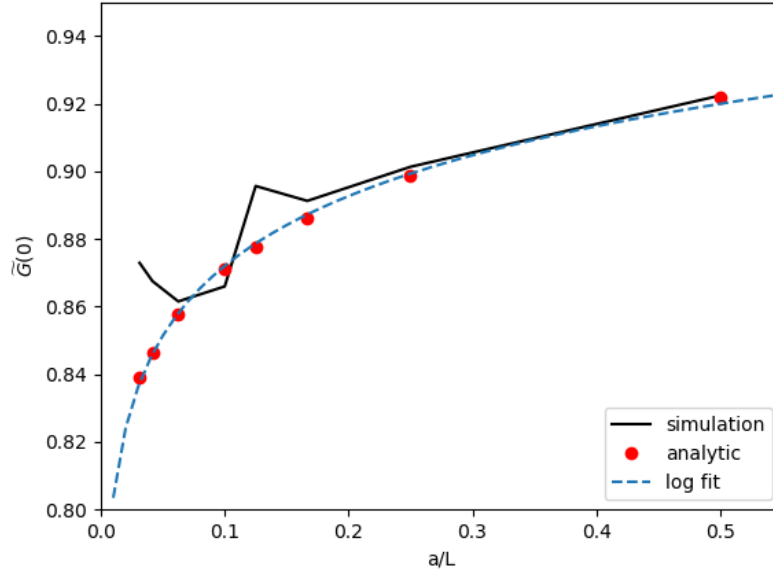


Figure 6.4: Momentum-space autocorrelation on a 2-dimensional lattice in the continuum limit as a function of the scale $a/L = 1/N$. The blue fit is a log function showing the type of divergence within $\tilde{G}(0)$.

any interaction was bounded by the highest ($k = N/2 - 1$) and lowest quantum numbers

($k = -N/2$):

$$|p| < \frac{2\pi}{L} \left(\frac{N}{2} \right) = \frac{\pi}{a} \quad \therefore \quad -\frac{\pi}{a} \leq p < \frac{\pi}{a} \quad (6.2.5)$$

But since a rushes towards infinity, the maximum and the minimum values of p are doomed to blow up. Hence, when sums are replaced by integrals of the type $\int_{-\infty}^{\infty} dp$, the latter will cover the infinite momentum range and cause n -point functions to diverge. It would mean the death of quantum field theory, was it not for a universal method to turn around such apparent inconvenience. This successful method, called renormalization, sweeps out every undesirable infinity haunting QFT. Since Φ^4 -theory has two fundamental parameters, mass, and coupling, there are essentially two sorts of renormalization to be performed. We discuss in detail each of them in the following sections.

6.3 Mass renormalization

The first parameter to be analyzed is the mass. Every mass that we have jotted down so far, denoted by m , either within n -point functions or in the label of a plot, is called bare mass. The name refers to the fact that this mass is the raw parameter as it appears in the action, and it is not the one actually measured on experiments in the laboratory. Notice that the bare mass of the free theory is identical to the square root of the inverse of the propagator at zero momentum:

$$\tilde{G}(p) = \frac{1}{4 \sin^2(p/2) + m^2} \therefore \tilde{G}(0) = \frac{1}{m^2} \therefore m = \sqrt{\frac{1}{\tilde{G}(0)}} \quad (6.3.1)$$

Since the mass bears such an intimate relationship with the 2-point function, this closeness may be somehow preserved in the continuum limit. One of the goals in renormalization is to obtain the real physical mass from the theory by expelling divergencies from the bare mass along the way. To commence, we need to get rid of a as done before, but this time we adopt the rescaling procedure discussed in section 6.2. Once we defined $\hbar \equiv 1$, it follows that the

action S_E , and each term thereof, must be dimensionless, and we can use this fact to rescale the field and parameters in terms of the lattice spacing to get rid of it. Let us see from Table 6.3 how every quantity in the action is written in terms of spatial units by staring at the Φ^4 -theory action. Thence we define the following dimensionless quantities which we mark

action:	$[S_E] = 1$		
1 st term:	$a^d \partial_\mu \Phi \partial^\mu \Phi / 2$	$[x]^d [\Phi]^2 [x]^{-2} = 1$	$[\Phi] = [x]^{1-d/2}$
2 nd term:	$a^d m^2 \Phi^2 / 2$	$[x]^d [m]^2 [\Phi]^2 = 1$	$[m] = [x]^{-1}$
3 rd term:	$a^d \lambda \Phi^4 / 4!$	$[x]^d [\lambda] [\Phi]^4 = 1$	$[\lambda] = [x]^{d-4}$

Table 6.3: Column 2: terms from the action. Column 3: imposes that every term has equal units to the action itself. Column 4: units of the field and physical parameters implied by column 3.

with a hat:

$$\hat{\varphi} \equiv \varphi a^{d/2-1} \quad \hat{m} \equiv m a \quad \hat{\lambda} \equiv \lambda a^{4-d} \quad \hat{\tau} \equiv \tau a^{-2} \quad \hat{\eta} \equiv \eta a^{1+d/2} \quad (6.3.2)$$

where d is the dimension of spacetime. The dimensions of the noise and stochastic time can be inferred very easily from the Langevin equation. For the remainder of this section, even though we omit the hats above rescaled parameters, for simplicity, we only work with the dimensionless quantities. Following the theory of lattice renormalization from [Montvay and Münster, 1997], and the numerical procedure from [Wolff, 2009, Weisz and Wolff, 2011, Dalla Brida et al., 2017], we define a finite and rescaled 2-point function called renormalized propagator as:

$$\tilde{G}_R(p) \equiv Z_R^{-1} \tilde{G}(p) = \left[4 \sin^2 \left(\frac{p}{2} \right) + m_R^2 + \mathcal{O}(p^4) \right]^{-1} \quad (6.3.3)$$

where m_R is the renormalized mass and Z_R is the field strength renormalization factor, that wipes out the divergencies from $\tilde{G}(p)$ by mutual cancellation. Then, we can avail of the previous equation to make a connection with Eq.(6.3.1) and define a renormalized mass from its corresponding propagator, this time in its finite version. Recalling that $p = 2\pi k/N$ and expressing the inverse propagators at zero momentum ($p = 0$, with $k = 0$) and at the minimum non-zero momentum ($p_* = 2\pi/N$, with $k = 1$), we have, respectively:

$$\tilde{G}_R^{-1}(0) = m_R^2 \quad (6.3.4)$$

$$\tilde{G}_R^{-1}(p_*) = m_R^2 + 4 \sin^2\left(\frac{p_*}{2}\right) + \mathcal{O}(p_*^4) \quad (6.3.5)$$

Presumably, their ratio shall be finite, since the renormalized propagators are also separately finite. Therefore, neglecting the $\mathcal{O}(p_*^4)$ terms:

$$\frac{\tilde{G}_R^{-1}(p_*)}{\tilde{G}_R^{-1}(0)} = \frac{Z_R \tilde{G}^{-1}(p_*)}{Z_R \tilde{G}^{-1}(0)} \approx \frac{m_R^2 + 4 \sin^2(p_*/2)}{m_R^2} \quad (6.3.6)$$

Notice that, although we have used an approximation in neglecting $\mathcal{O}(p_*^4)$ terms, in the continuum limit they become asymptotically close to zero since $p_* \rightarrow 0$. Therefore, in the end this approximation leads to an exact result anyway. From the previous equation, we write:

$$\frac{\tilde{G}(0)}{\tilde{G}(p_*)} \approx 1 + 4 \frac{\sin^2(p_*/2)}{m_R^2} \quad (6.3.7)$$

In the infinite volume limit, such equality becomes exact, and the renormalized mass can be computed as:

$$m_R = \lim_{L \rightarrow \infty} 2 \sin\left(\frac{p_*}{2}\right) \sqrt{\frac{\tilde{G}(p_*)}{\tilde{G}(0) - \tilde{G}(p_*)}} \quad (6.3.8)$$

On top of that, we must have some sort of control parameter that sets a rule on how we shall vary the scales of the theory until the large L limit is reached. Remembering that $L = aN$, where a is the lattice spacing and N is the number of sites, by increasing the length of space and decreasing the lattice spacing, it is obvious that the number of sites must increase.

Additionally, from Eqs.(6.3.2), changes in the fabric of the lattice comes accompanied by rescalings in the parameters of the theory, which in turn modify the lattice propagators inside Eq.(6.3.8). Hence, there must be something constraining the way L , N , a , $\hat{m}$, and $\hat{\lambda}$ are modified. That is why we introduce the control parameter of the renormalization scheme:

$$z \equiv mL = \frac{\hat{m}}{a}aN = \hat{m}N \equiv \text{constant} \quad (6.3.9)$$

The z parameter must be kept fixed in every step towards renormalization. Since each value of z defines a different renormalization scheme, once we have chosen a value for it, we have also constrained the variation of one parameter relative to another, since m must be such that:

$$\hat{m} = \frac{z}{N} \quad (6.3.10)$$

To summarize, the mass renormalization scheme is characterized by a constant z and must comply with all these lattice modifications at once and, hopefully, m_R will approach some finite value, which we shall call the renormalized mass of the theory. Hitherto, we are 50% ready for the thorough renormalization of Φ^4 -theory, and we proceed to the renormalization of the next parameter.

6.4 Coupling renormalization

Depending on the dimension of space, this section may or may not be unnecessary. Let us explain it: for a similar reason that the renormalized mass bears a relationship with the 2-point function, the renormalized coupling bears one with the 4. Luckily, the 4-point function does not always diverge, only in the case that is useful to the real world: in 4 dimensions. In a nutshell, the continuous 4-point function in d dimensions can be roughly calculated as:

$$\chi_4(p) \sim \int d^d k \frac{1}{m^2 + k^2} \frac{1}{m^2 + (k - p)^2} \quad (6.4.1)$$

Therefore, if the numerator has a smaller power of momentum than the denominator, χ_4 is finite, namely, for $d = 1, 2$, or 3 . However, if the powers are equal up and down (when $d = 4$), χ_4 presents a divergence of the logarithmic type. Since it is not the scope of this work to study in detail all kinds of divergences, for more on this topic, we refer the reader to chapter 10 of [Peskin, 2018]. Supposing we adopt 4 dimensions, besides the mass, it is also necessary to renormalize the coupling constant. In terms of the mass and the zero-momentum 4-point function (also known as susceptibility), the renormalized coupling can be defined as:

$$\lambda_R = -\frac{1}{V} \frac{\chi_4}{\tilde{G}^2(0)} (m_R)^d \quad (6.4.2)$$

where V is the lattice volume, which eliminates the IR divergencies due to the lattice growing, turning λ_R into an intensive parameter, in the thermodynamic sense. Moreover, χ_4 is obtained as before, through the connected expectation value of four fields:

$$\chi_4 = a^{3d} \lim_{\tau \rightarrow \infty} \sum_{x,y,z} \langle \varphi(0, \tau) \varphi(x, \tau) \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta^c \quad (6.4.3)$$

In this calculation, we have restored the lattice spacing to make explicit its dependence on a . Expanding the connected correlation function into non-connected parts, we have:

$$a^{3d} \sum_{x,y,z} \langle \varphi(0, \tau) \varphi(x, \tau) \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta^c = \quad (6.4.4)$$

$$a^{3d} \sum_{x,y,z} \langle \varphi(0, \tau) \varphi(x, \tau) \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta - a^{3d} \langle \varphi(0, \tau) \varphi(x, \tau) \rangle_\eta \langle \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta -$$

$$a^{3d} \langle \varphi(0, \tau) \varphi(y, \tau) \rangle_\eta \langle \varphi(x, \tau) \varphi(z, \tau) \rangle_\eta - a^{3d} \langle \varphi(0, \tau) \varphi(z, \tau) \rangle_\eta \langle \varphi(x, \tau) \varphi(y, \tau) \rangle_\eta = \quad (6.4.5)$$

$$a^{3d} \sum_{x,y,z} \langle \varphi(0, \tau) \varphi(x, \tau) \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta -$$

$$3 \left[a^d \sum_x \langle \varphi(0, \tau) \varphi(x, \tau) \rangle_\eta \right] \left[a^{2d} \sum_{y,z} \langle \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta \right] \quad (6.4.6)$$

Using the Fourier transform of the 2-point function:

$$\lim_{\tau \rightarrow \infty} \langle \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta = G(y - z) = \frac{1}{L^d} \sum_p e^{ip(y-z)} \tilde{G}(p) \quad (6.4.7)$$

Thence, we have:

$$a^{2d} \sum_{y,z} \lim_{\tau \rightarrow \infty} \langle \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta = a^{2d} \sum_{y,z} \left[\frac{1}{L^d} \sum_p e^{ip(y-z)} \tilde{G}(p) \right] \quad (6.4.8)$$

$$= \frac{1}{L^d} \sum_p \left(a^d \sum_y e^{ipy} \right) \left(a^d \sum_z e^{-ipz} \right) \tilde{G}(p) \quad (6.4.9)$$

$$= \frac{1}{L^d} \sum_p L^d \delta(p) \left(a^d \sum_z e^{-ipz} \right) \tilde{G}(p) \quad (6.4.10)$$

$$= a^d \sum_z \tilde{G}(0) = L^d \tilde{G}(0) \quad (6.4.11)$$

Replacing it into Eq.(6.4.6) and noticing that $\lim_{\tau \rightarrow \infty} \sum_x \langle \varphi(0, \tau) \varphi(x, \tau) \rangle_\eta = \tilde{G}(0)$:

$$\chi_4 = a^{3d} \lim_{\tau \rightarrow \infty} \sum_{x,y,z} \langle \varphi(0, \tau) \varphi(x, \tau) \varphi(y, \tau) \varphi(z, \tau) \rangle_\eta - 3L^d \tilde{G}(0)^2 \quad (6.4.12)$$

Graphically, it is quite easy to see why the equation above represents the connected 4-point function by looking at the negative term. Given four points in space (x_1, x_2, x_3, x_4) , the quantity in parenthesis accounts for all combinations of four lines that connect, in some way, to one another. While the factor of three represents the three possible diagrams that fail to satisfy this criterion. In Figure 6.5, these diagrams are depicted. We could perfectly



Figure 6.5: Three disconnected diagrams arising from the 4-point function that must be discounted.

implement on the simulations an algorithm to compute the right-hand side of Eq.(6.4.12) by brute force. Nonetheless, no matter how clever we are, this computation is intrinsically awkward to do, for it features three nested sums at once. Therefore, for the sake of sparing CPU time, we propose an equivalent, and yet much more profitable, expression for χ_4 , which can be derived by noticing that the triple sum and the average brackets commute:

$$\begin{aligned}
\chi_4 &= \lim_{\tau \rightarrow \infty} \left\langle \varphi(0, \tau) \cdot \sum_x \varphi(x, \tau) \cdot \sum_y \varphi(y, \tau) \cdot \sum_z \varphi(z, \tau) \right\rangle_\eta - 3L^d \tilde{G}(0)^2 \\
&= \lim_{\tau \rightarrow \infty} \langle \varphi(0, \tau) \cdot \tilde{\varphi}(0, \tau) \cdot \tilde{\varphi}(0, \tau) \cdot \tilde{\varphi}(0, \tau) \rangle_\eta - 3L^d \tilde{G}(0)^2 \\
&= \lim_{\tau \rightarrow \infty} \langle \varphi(0, \tau) \cdot \tilde{\varphi}(0, \tau)^3 \rangle_\eta - 3L^d \tilde{G}(0)^2
\end{aligned} \tag{6.4.13}$$

where $\tilde{\varphi}(0, \tau)$ is the zero momentum Fourier transform of $\varphi(x, \tau)$. In this hybrid formula, we just need to solve the Langevin equation for $\varphi(x, \tau)$, compute the zero momentum Fourier transform $\tilde{\varphi}(0, \tau)$, and average over the quantity within brackets in Eq.(6.4.13), which is way simpler than the three nested Fourier transforms as in Eq.(6.4.12). After perusing at the foundations of the method, we turn to our results in numerical simulations.

6.5 Numerical renormalization

The remaining work is to implement the calculation of renormalized parameters through the stochastic quantization formalism. In terms of simulations, the task we accomplished with LASER can be resumed by the following steps:

- For a constant size L , fix a value for the number of lattice sites N .
- From the knowledge of $a = L/N$, rescale the whole Langevin equation by redefining its input parameters according to the recipe in Eq.(6.3.2).
- Solve the equation and use the solution to obtain 2 and 4-point functions in momentum space for very large τ .

- Compute the renormalized parameters m_R and λ_R from Eqs.(6.3.8) and (6.4.2).

By repeating this procedure for an array of values for N , such that $N \rightarrow \infty$, we obtain renormalized parameters gradually closer to those in the continuum limit, thus renormalizing the theory numerically. Therefore, in Figures 6.6, 6.7 and 6.8, we present our new results so far. They correspond, respectively, to renormalizations in 2, 3 and 4 dimensions, where we set $z = 2$ for all of them.

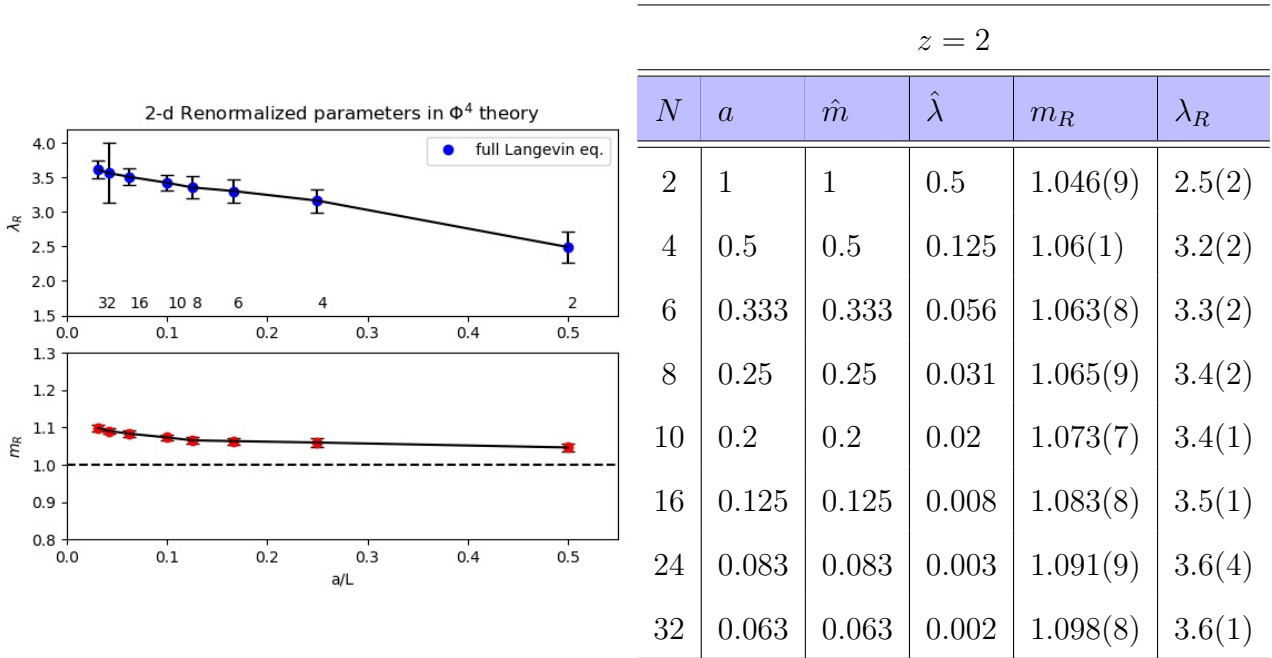


Figure 6.6: Renormalization in 2 dimensions with error bars. Top: renormalized coupling from full Langevin equation. Numbers above the x -axis are the values of N . Bottom: renormalized mass, with the dashed line showing the bare mass whereby we started the process. Both quantities are plotted as a function of the scale $a/L = 1/N$. The table on the right gives the input parameters of the simulation and the renormalized outputs.

Both renormalized parameters are then obtained by extrapolating the left tail of the m_R and λ_R curves until they touch their corresponding y -axis: $a/L \rightarrow 0$. Notice that, since $L = aN$, this limit corresponds to $1/N \rightarrow 0$ or $N \rightarrow \infty$, as illustrated in Figure 6.2. In Appendix A.4, we derive the formulas that we used to estimate the numerical errors of m_R and λ_R from the errors of the 2 and 4-point functions, which can be directly measured in simulations. The first challenge imposed by this method is to simulate lattices of growing size since the number

of CPU computations also increases with N . The magnitude of this growth is given by the dimension of space. The second challenge is to compute propagators with low mass, which enormously increases errors. In Figure 6.7, we also show the renormalization procedure in 3 dimensions.

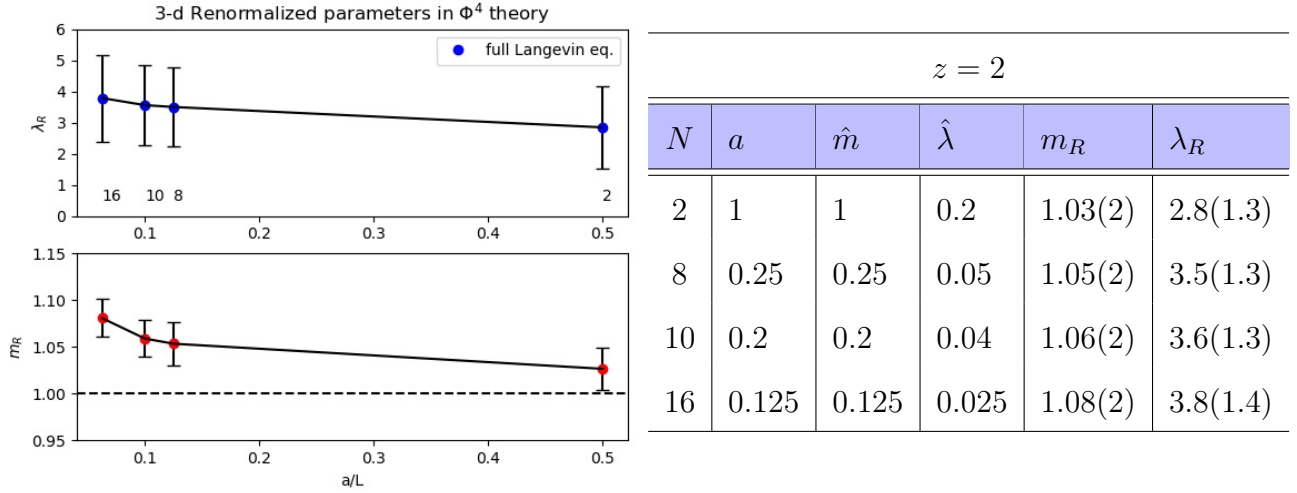


Figure 6.7: Renormalization in 3 dimensions with error bars. Top: renormalized coupling from full Langevin equation. Numbers above the x -axis are the values of N . Bottom: renormalized mass, with the dashed line showing the the bare mass whereby we started the process. Both quantities are plotted as a function of the scale $a/L = 1/N$. The table on the right gives the input parameters of the simulation and the renormalized outputs.

In Figure 6.8, we demonstrate the same renormalization procedure for the non-trivial 4 dimensional lattice. Notice that, because of the scaling laws in Eq.(6.3.2), the couplings in the 2 and 4-dimensional cases behave differently with the number of sites N . In the 2-dimensional case the parameter λ scales with the power -2 of the lattice spacing, which makes it diminish and tend to zero for growing N , whereas, in the 4-dimensional case, the coupling does not scale at all. This difference in scaling based on the a -dependence is precisely the watershed between the so-called super-renormalizable theories from the renormalizable theories. The former, such as the Φ^4 -theory in 2 dimensions, has only a finite number of divergent Feynman diagrams, and the latter, such as the same theory in 4 dimensions, needs to be renormalized for every order in perturbation theory, which, for all orders, contains an infinite number of divergent diagrams.

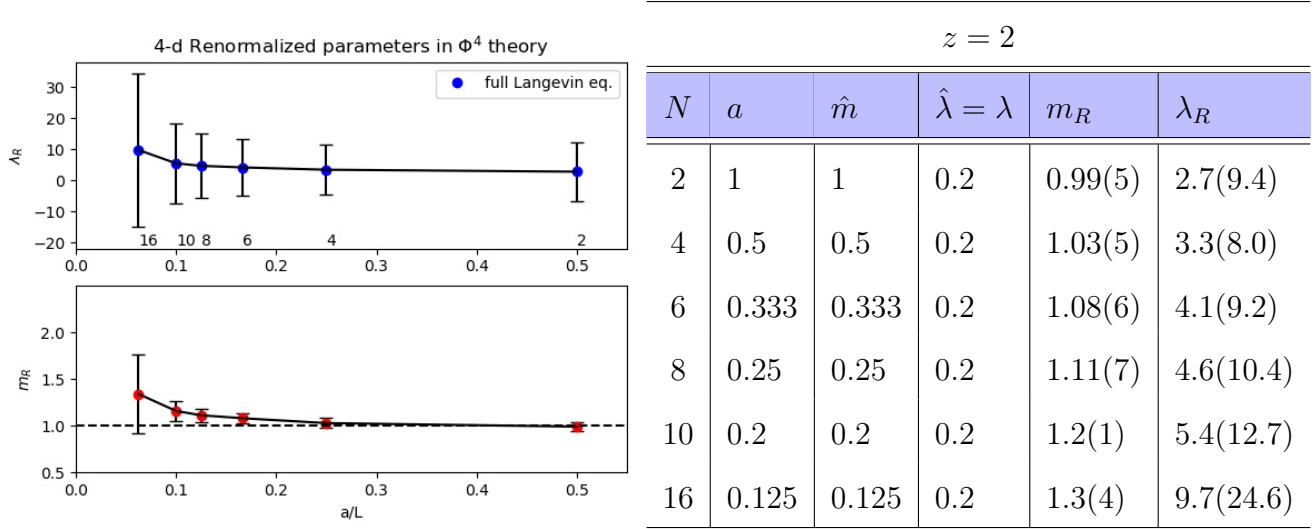


Figure 6.8: Renormalization in 4 dimensions with error bars. Top: renormalized coupling from full Langevin equation. Numbers above the x -axis are the values of N . Bottom: renormalized mass, with the dashed line showing the the bare mass whereby we started the process. Both quantities are plotted as a function of the scale $a/L = 1/N$. The table on the right gives the input parameters of the simulation and the renormalized outputs.

Chapter 7

Conclusions and perspectives

Throughout this text, we saw that stochastic quantization proved to be an invaluable tool to handle quantum mechanical and quantum field theory problems from stochastic processes. In chapter 2, we briefly reviewed the main aspects of stochastic processes, going across the definitions of Gaussian white noise, Itô, and Stratonovich integrals. We commenced by reviewing the Brownian motion as the simplest stochastic system, classifying it as a process of the Wiener type, and then generalized it to the so-called Ornstein-Uhlenbeck process to prepare the ground for stochastic quantization. The core of the formalism relies on the reinterpretation of quantum fluctuations as a source of noise that, through the Langevin equation, drives the dynamics of a stochastic variable on a fictitious parameter τ , called stochastic time. In chapter 3, we followed [Namiki, 2008] to exemplify this behavior through a stochastic variable that, described by the Langevin equation, and under the joint influence of a drift force and the noise, gradually evolved into the equilibrium state of a quantum harmonic oscillator. Thence, we showed that by computing the stochastic average $\langle x(t, \tau)x(t', \tau) \rangle_\eta$ analytically in the limit of $\tau \rightarrow \infty$, we could reproduce the propagator of this system from the equilibrium state of the stochastic process. The existence of this state was guaranteed by the solution of the Fokker-Planck equation, which converges to the Boltzmann factor in the asymptotic limit. This formidable fact conveyed a natural

interpretation of the Euclidean path integral as an ordinary statistical mechanical partition function. Afterward, we also demonstrated how to apply the same method to the scalar Φ^4 -theory in QFT and prescribed a general rule to draw n -point functions from stochastic quantization. In chapter 4, we used the tools from [Montvay and Münster, 1997, Smit, 2002] to formulate the Φ^4 -theory and its Langevin equation on the lattice to solve the latter in parallel numerical simulations with the novel lattice code, called LASER, that we developed for this work. With this code, we reproduced Green functions of the Φ^4 -theory in 2 dimensions with symmetric, and non-symmetric phases and the results were shown to be in excellent accordance with the analytical expressions, in the free case and the interactive case from perturbation theory. In chapter 5, we reviewed the theory of Feynman diagrams, where we gave a 1-dimensional example of how to compute quantum corrections in Φ^4 -theory up to 1 and 2 loops through the 1-PI resummation procedure. The resultant formulas had been used to test our simulations in the previous chapter for several values of the coupling constant. Similar to other authors [Attanasio, 2013, Martin and Musso, 2006a], we also approached stochastic quantization with perturbative expansions through Noise Perturbation Theory (NPT), which consisted in writing the stochastic field as a sum of terms proportional to powers of $\hbar$. Finally, we presented our new results on NPT in 2 and 4 dimensions with a numerical error analysis order by order relative to the full solution of the Langevin equation. Although the perturbative 2-point functions were truncated up to 2 loops, in the future, we intend to extend our implementation of the 1-PI resummation for higher loops, applying the Runge-Kutta algorithm to decrease the global errors. In chapter 6, we followed a numerical renormalization procedure from [Wolff, 2009, Weisz and Wolff, 2011, Dalla Brida et al., 2017] to obtain the fundamental parameters, namely the mass and the coupling, close to the continuum limit of our lattice. These parameters were renormalized in 2, 3, and 4 dimensions by performing simulations with an increasing number of sites and decreasing lattice spacing, where the smallest cutoff scales were $a/L = 0.03125$, in 2 dimensions, and $a/L = 0.0625$, in 3 and 4. We found that

in 2 and 3 dimensions the renormalized parameters seem to approach $m_R \approx 1.098 \pm 0.008$, $\lambda_R \approx 3.6 \pm 0.1$ and $m_R \approx 1.08 \pm 0.02$, $\lambda_R \approx 3.8 \pm 1.4$, respectively. However, in the 4-dimensional case, we found that the uncertainties were extremely large and impede us from drawing safe conclusions regarding the values of the parameters. Furthermore, we notice a deviation relative to the results presented by the references, where the 4-dimensional Φ^4 -theory is claimed to be trivial, which means $\lambda_R \rightarrow 0$ even though a coupling appears explicitly in the bare action. Such disagreement must be further clarified, but to do so, we need to enhance the quality of our data with more number of realizations. This task will also require the improvement in the efficiency of our code to allow simulations down to lower values of the scale cutoff. For future works, we also intend to renormalize the theory in NPT to compare with the results from the full Langevin equation.

Apart from the aforementioned perspectives, we also look forward to investigating further issues in stochastic quantization that did not fit in the scope of the present work. For instance, even though we chose to resign ourselves to approaching the scalar case in symmetric and broken phases, the vast range of possibilities where stochastic quantization can be applied is, by no means, restricted to such choice. In fact, there are plenty of other systems that can be adapted to the stochastic language and modeled through a Langevin equation. As we mentioned in the beginning, it is possible to find suitable stochastic processes befitting the characteristics of fermionic fields $\psi, \bar{\psi}$ [Ridky, 1995], gauge fields A_μ [Kapoor, 2018], and even semi-classical gravity fields [dos Reis et al., 2019]. Other authors have also applied stochastic quantization to deal with deconfining transitions in pure SU(2) theories [Fraga et al., 2007]. Aware of such versatility, we started this work with the idea of commencing a journey through the interplay between stochastic processes and quantum field theory, intending to explore lattice problems from an alternative perspective. In the frontline of those problems, we stress, for instance, the sign problem (also known as the complex-phase problem), which arises in lattice simulations where the traditional

MCMC method is applied. This problem affects calculations for, among others, strongly interactive fermionic systems, such as in QCD with finite chemical potential, and QFT in Minkowski space. In our case study with the Φ^4 -theory, the probability weights were always positive semi-definite quantities, *i.e.* the action was always a real functional of a scalar field, but when a system of fermions is strongly interactive, the action becomes a complex number, causing the Boltzmann weight to turn from $e^{-S_E[\psi, \bar{\psi}]}$, where S_E is real, to $e^{i|S_E[\psi, \bar{\psi}]|}$. This rotation along the complex plane renders Monte Carlo integration meaningless, since the notion of importance sampling vanishes, for the definition of normalized probability no longer holds if the weight is complex. On the other hand, we have stochastic quantization, which, although equivalent to Monte Carlo in practical terms, does not rely directly on the concept of probability. Instead, we generate stochastic processes that already come out with the desired weights using the Langevin equation, leaving thus the probabilistic content to the Fokker-Planck equation. Moreover, from a formal point of view, nothing prohibits the action in the Langevin equation to be a complex number [Hüffel and Rumpf, 1984, Fukuda and Higurashi, 1988], and circumvent the drawback that troubles Monte Carlo. We could define what is called a complex Langevin equation as:

$$\frac{\partial \varphi}{\partial \tau} = i \frac{\delta S_E[\varphi]}{\delta \varphi} + \eta \quad (7.0.1)$$

and prove through the Fokker-Planck equation that it satisfies a probability law of the form $e^{iS_E[\varphi]}$. Even though this approach itself has a couple of problems, like the outcome of the so-called runaway solutions, that apparently lead to unphysical results, there have been recent efforts in the literature to overcome them (see [Attanasio and Jäger, 2019, Drut, 2018, Berges and Sexty, 2008, Krein et al., 2014]). Therefore, we believe that it offers a promising route to tackle some of the hampering challenges imposed by up-to-date lattice demands. For an interesting discussion on the topic of the sign problem and stochastic quantization in the context of a Bose gas, we refer the reader to [Aarts, 2009]. We thus argue that the full horizon of applicability of this method has not been entirely exploited, leaving plenty of opportunities

opened by stochastic quantization, of which scalar Φ^4 is just one example. In the era of large hadron colliders and bold gravitational wave detectors, attentions are being turned to missing pieces of QFT thermodynamics, which hold keys to understand some mysteries in particle physics and fundamental interactions. In order to shed light on the high chemical potential region of the QCD phase diagram, an essential element to unveil the physics within the dense cores of neutron stars, and to comprehend the early stages of the Universe, we need to jump over the gap left behind by the sign problem. Therefore, we finalize this work with a claim that stochastic quantization, as an alternative to the traditional methods, can have a sound impact to handle this and other important questions that urgently demand an answer.

Appendices

Appendix A

A.1 Numerical algorithms

In order to integrate the Langevin equation, we needed to select a suitable algorithm to render the best results. Inside LASER, we have implemented two algorithms. The first is the traditional Euler integrator, which consists of discretizing the differential equation according to Eq.(4.2.5). This method produces local errors proportional to $\mathcal{O}(\Delta\tau^2)$, where $\Delta\tau$ is the stochastic time step, and global errors proportional to $\mathcal{O}(\Delta\tau)$. For most applications, the Euler method turned out to be sufficient. However, in some cases another method might be required. To handle these more complex cases, we have also implemented the second order Runge-Kutta method according to [Batrouni et al., 1985]. In this approach, the Langevin equation, for a given Euclidean action S_E , is modified to:

$$\varphi_j^{n+1} = \varphi_j^n - \frac{\Delta\tau}{2} \left[\frac{\delta S_E[\varphi_j^n]}{\delta \varphi_j^n} + \frac{\delta S_E[\sigma_j^{n+1}]}{\delta \sigma_j^{n+1}} \right] + \sqrt{2\Delta\tau} R_j^n \quad (\text{A.1.1})$$

where a was set to 1, and the auxiliary field σ_j^{n+1} is obtained from the lower-order Euler integrator with a sign change in the noise term:

$$\sigma_j^{n+1} = \varphi_j^n - \Delta\tau \frac{\delta S_E[\varphi_j^n]}{\delta \varphi_j^n} - \sqrt{2\Delta\tau} R_j^n \quad (\text{A.1.2})$$

By doing these changes and solving Eqs.(A.1.1) and (A.1.2) instead, the local errors decrease to $\mathcal{O}(\Delta\tau^3)$ and the global ones to $\mathcal{O}(\Delta\tau^2)$. Nevertheless, since we essentially need to perform twice as many integrations, we gain some extra computations to do on the go, which can critically slow down the code for huge lattices. Therefore, the Runge-Kutta approach should only be used when the Euler method fails.

A.2 Remarks on the Monte Carlo approach

In stochastic quantization, we have seen that in order to compute n -point functions, we had to evolve a stochastic field into an asymptotic limit and calculate the arithmetic average as given below:

$$\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) \dots \hat{\Phi}(x_n) | 0 \rangle = \lim_{\tau \rightarrow \infty} \langle \varphi(x_1, \tau) \varphi(x_2, \tau) \dots \varphi(x_n, \tau) \rangle_\eta \quad (\text{A.2.1})$$

where the right-hand side represents the arithmetic average of a set of fields generated with different noise sets, and the left-hand side is given by the Feynman path integral:

$$\langle 0 | \hat{\Phi}(x_1) \hat{\Phi}(x_2) \dots \hat{\Phi}(x_n) | 0 \rangle = \frac{1}{Z} \int \mathcal{D}\Phi \Phi(x_1) \Phi(x_2) \dots \Phi(x_n) e^{-S_E[\Phi]} \quad (\text{A.2.2})$$

On the other hand, among the lattice scientific community, Eq.(A.2.1) is not often the approached method. Instead, the routines devised to solve QFT numerically, such as in lattice QCD, are programmed to apply the so-called Markov chain Monte Carlo method (MCMC). In the MCMC approach, the algorithm generates plenty of field configurations $\Phi(x)$ according to the Boltzmann weight $e^{-S_E[\Phi]}$ and then calculates their weighted average. Even though these methods use different types of averages, the central limit theorem, introduced in chapter 2, guarantees that for sufficiently large samples, these two averages become arbitrarily close to each other. Moreover, when the sample sizes are infinite, the two become perfectly equal, thus making stochastic quantization equivalent to MCMC in the thermalization limit. To

summarize what has been said, in Table A.1 below we expose the main differences between MCMC and stochastic quantization:

	MCMC	stochastic quantization
Type of average	weighted	arithmetic
Generates	field configurations	stochastic processes
Solves	Feynman path integral	Langevin equation

Table A.1: Comparison between the main aspects of MCMC and stochastic quantization

A.3 Importance of reliable random number generation

One of the main points when simulating a huge set of pseudo-random numbers with computers is the choice of a suitable algorithm. The chosen random number generator has a strong impact on the quality of all numerical results, regardless of whether we use MCMC or stochastic quantization. In order to reproduce the random behavior of some natural processes, like Brownian motions, Ornstein-Uhlenbeck, etc., one needs to select a random number generator with finely-tuned characteristics, for a bad choice could be truly catastrophic. We have been seen since chapter 4 that stochastic quantization agrees with analytical predictions at a quite high level of precision. In all chapters of this work we calculated 2 and 4-point functions in different situations, with different parameters, and for different lattice spacings. For that sake, we used a couple of libraries from the GSL package, among which a function (in the programming sense) called `gsl_rng_gaussian()` is defined, and the agreements were notorious. What would happen if we rebuilt this thesis, replacing the actual calculations by new using the standard C++ uniform number generator (namely, the `rand()` function) in addition to the gaussian transformation function `gasdev()` from [Press et al., 2002]? To answer that question, we have to pay attention to an extremely important characteristic of

pseudo-number generators, which turns out to be the hallmark of a good or a bad generator. This characteristic is called the period of the generator. Every number generated by the computer is not truly random, they are obtained from totally predictable algorithms which, fed by a seed, strive to imitate randomness. Therefore, any algorithm has a maximum extension of output numbers before it begins to repeat itself. The length of this dead-end is one of the main characteristics of the algorithm and it sets a threshold of how many numbers can be safely computed. A bit of research and we find that **rand()** has a poor period of $2^{32} \approx 4.295 \times 10^9$. Resorting to the calculations done in chapter 6, for instance, in 2 dimensions we used lattices up to $N = 32$. Furthermore, to have a well-defined thermalized behavior, we ran simulations with 200000 steps in stochastic time and $N_r = 19200$ noise realizations to have good precision. Since at every point of the lattice we need a value of noise, which essentially comes from **rand()**, the total amount of numbers generated for this simulations was:

$$\mathcal{N} = 32 \times 32 \times 200000 \times 192000 \approx 3.932 \times 10^{12} \quad (\text{A.3.1})$$

Almost a thousand times more than we should! Since these crumbs surpassing the period are repeated numbers from the sequence, they would correlate with their previously generated twins, and overestimate the value of the 2-point function. As opposed to that, the GSL function used in this work was fed with a seed based on the so-called RANLUX algorithm, published by Martin Lüscher at [Lüscher, 1994]. This algorithm is a tremendously successful improvement of the known Marsaglia-Zaman algorithm. Why is it nearly impossible to repeat a sequence of numbers with RANLUX? First of all, because to merely initialize the algorithm, in its most efficient form, it requires not 1 but 24 seeds. Second, because each of these seeds can assume integer values from 0 to 2^{24} , which turns the repetition of seeds an extremely unlikely event. Third, because its period is equal to 10^{171} numbers! Therefore, in order to repeat a number with this generator, it would require much more than the age of the Universe!

A.4 Error estimation for m_R and λ_R

In chapter 6 we presented data with numerical uncertainties, but we did not actually show where they came from. The renormalized parameters are not obtained directly from the stochastic processes that we generated with the Langevin equation. Instead, they were computed from the 2 and 4-point functions, which are the actual outputs of the code. Therefore, at first we only have access to the uncertainties on the values of the n -point functions. The uncertainties on m_R and λ_R must then be derived from the latter ones. From the mass renormalization formula in Eq.(6.3.8), there are two sources of error: $\tilde{G}(0) \equiv \tilde{G}$ and $\tilde{G}(p_*) \equiv \tilde{G}_*$. Thence, we estimate the final error on m_R through the error propagation formula:

$$\sigma_{m_R} = \sqrt{\left(\frac{\partial m_R}{\partial \tilde{G}}\right)^2 \sigma_{\tilde{G}}^2 + \left(\frac{\partial m_R}{\partial \tilde{G}_*}\right)^2 \sigma_{\tilde{G}_*}^2} \quad (\text{A.4.1})$$

where the derivatives of the renormalized mass are given by:

$$\frac{\partial m_R}{\partial \tilde{G}} = -\frac{1}{2} p_*(\tilde{G}_*)^{1/2} (\tilde{G} - \tilde{G}_*)^{3/2} \quad (\text{A.4.2})$$

$$\frac{\partial m_R}{\partial \tilde{G}_*} = \frac{1}{2} p_*(\tilde{G}_*)^{-1/2} (\tilde{G} - \tilde{G}_*)^{-1/2} + \frac{1}{2} p_*(\tilde{G}_*)^{1/2} (\tilde{G} - \tilde{G}_*)^{-3/2} \quad (\text{A.4.3})$$

rewriting these equations in terms of the renormalized mass, they simplify to:

$$\frac{\partial m_R}{\partial \tilde{G}} = -\frac{m_R}{2(\tilde{G} - \tilde{G}_*)} \quad (\text{A.4.4})$$

$$\frac{\partial m_R}{\partial \tilde{G}_*} = \frac{m_R}{2} \frac{\tilde{G}}{\tilde{G}_*(\tilde{G} - \tilde{G}_*)} \quad (\text{A.4.5})$$

and therefore, replacing these equations back inside Eq.(A.4.1), the uncertainty on m_R can be computed through:

$$\sigma_{m_R} = \frac{m_R}{2(\tilde{G} - \tilde{G}_*)} \sqrt{\sigma_{\tilde{G}}^2 + \left(\frac{\tilde{G}}{\tilde{G}_*}\right)^2 \sigma_{\tilde{G}_*}^2} \quad (\text{A.4.6})$$

Notice that the modulus for moving the factor $(\tilde{G}-\tilde{G}_*)^2$ out of the square root are unnecessary since $\tilde{G} > \tilde{G}_*$. From the coupling renormalization formula in Eq.(6.4.2), there are three sources of numerical error, namely, the quantities: $\tilde{G}$, $\tilde{G}_*$ and χ_4 . Therefore, we can estimate the global error over the renormalized coupling λ_R through the error propagation expression with three sources:

$$\sigma_{\lambda_R} = \sqrt{\left(\frac{\partial \lambda_R}{\partial \chi_4}\right)^2 \sigma_{\chi_4}^2 + \left(\frac{\partial \lambda_R}{\partial \tilde{G}}\right)^2 \sigma_{\tilde{G}}^2 + \left(\frac{\partial \lambda_R}{\partial \tilde{G}_*}\right)^2 \sigma_{\tilde{G}_*}^2} \quad (\text{A.4.7})$$

where σ_{χ_4} , $\sigma_{\tilde{G}}$ and $\sigma_{\tilde{G}_*}$ are outputs from the simulations. By deriving Eq.(6.4.2) with respect to χ_4 , $\tilde{G}$ and $\tilde{G}_*$, we obtain:

$$\frac{\partial \lambda_R}{\partial \chi_4} = -\frac{1}{\tilde{G}^2} (p_*)^d \left(\frac{\tilde{G}_*}{\tilde{G} - \tilde{G}_*} \right)^{d/2} \quad (\text{A.4.8})$$

$$\frac{\partial \lambda_R}{\partial \tilde{G}} = \frac{\chi_4}{\tilde{G}^2} (p_*)^d \left(\frac{\tilde{G}_*}{\tilde{G} - \tilde{G}_*} \right)^{d/2} \left[\frac{1}{\tilde{G}} + \frac{d}{2} \frac{1}{(\tilde{G} - \tilde{G}_*)} \right] \quad (\text{A.4.9})$$

$$\frac{\partial \lambda_R}{\partial \tilde{G}_*} = -\frac{d}{2} \frac{\chi_4}{\tilde{G}^2} (p_*)^d \left(\frac{\tilde{G}_*}{\tilde{G} - \tilde{G}_*} \right)^{d/2} \left(\frac{1}{\tilde{G}_*} + \frac{1}{\tilde{G} - \tilde{G}_*} \right) \quad (\text{A.4.10})$$

These formulas can be simplified to:

$$\frac{\partial \lambda_R}{\partial \chi_4} = \frac{\lambda_R}{\chi_4} \quad (\text{A.4.11})$$

$$\frac{\partial \lambda_R}{\partial \tilde{G}} = -\lambda_R \left[\frac{1}{\tilde{G}} + \frac{d}{2} \frac{1}{(\tilde{G} - \tilde{G}_*)} \right] \quad (\text{A.4.12})$$

$$\frac{\partial \lambda_R}{\partial \tilde{G}_*} = \frac{d}{2} \lambda_R \left(\frac{1}{\tilde{G}_*} + \frac{1}{\tilde{G} - \tilde{G}_*} \right) \quad (\text{A.4.13})$$

Therefore, the final expression for the error estimation in measuring λ_R is:

$$\sigma_{\lambda_R} = \lambda_R \sqrt{\frac{1}{\chi_4^2} \sigma_{\chi_4}^2 + \left[\frac{1}{\tilde{G}} + \frac{d}{2} \frac{1}{(\tilde{G} - \tilde{G}_*)} \right]^2 \sigma_{\tilde{G}}^2 + \frac{d^2}{4} \left(\frac{1}{\tilde{G}_*} + \frac{1}{\tilde{G} - \tilde{G}_*} \right)^2 \sigma_{\tilde{G}_*}^2} \quad (\text{A.4.14})$$

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