The Gaussian Model

An Exploration into the Foundations of Quantum Field Theory

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Preface

This is the first of a series of a few short books about the foundations of quantum field theory. It is not meant as a traditional textbook on that subject. Its intention is not to exhaust the subject, but to probe deeply into just a few essential topics of a conceptual nature. These topics are treated in a way that is mathematically more solid than what is usually the case in the subject without, however, any intention to aim at extreme generality or extreme mathematical rigor. The use of the mathematics is kept as elementary as possible throughout the text.

This first volume has as its subject the Gaussian model, which is the Euclidean version of the theory of the free scalar field. This model is treated mostly by analytical means, which are within reach of anyone with a solid background in physics. Only a very limited use of computation is involved, mostly in an auxiliary role. Since the Gaussian model is the only model that can be solved completely by analytical means, in all the space-time dimensions we will be interested in, it is essential that we take maximum advantage of it, in our exploration of the conceptual foundations of the theory.

The second volume of the series will address some non-linear models of scalar fields which can be understood as generalizations of the Gaussian model, namely the polynomial models and the sigma models. In this second volume the ideas and techniques developed in the present volume will be applied to these more complex models, in the same spirit in which they are used here, to probe into the foundations of the theory. Since in these non-linear models no exact analytical solutions can be found, the use of numerical computation will have a much more extensive role to play in the second volume.

The strong dependence on the use of rather large computational resources for the very large scale stochastic simulations needed to deal with this subject is a serious stumbling block for its teaching and dissemination. In fact, one of the criteria for the contents of the current volume is that they do not depend on such large-scale stochastic simulations. A third volume of the series will eventually cover the technical aspects of programming and of the use of computers and of free software, which are essential for the acquisition of a real measure of technical control over the subject.

This subject is still an open and incomplete chapter of physics, and is full of misunderstandings and misconceptions. The line of thought developed here is meant to point a way out of the state of confusion in which one currently finds the subject. However, this line of thought is very far from finished, and it is likely that most of the

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Chapter 1

Conceptual Foundations

In this chapter we will discuss some preliminary philosophical points, dealing with what should be required of the definition of a physical theory in the quantum domain. We will also introduce the most basic foundational objects of the mathematical structure of the theory as it is presented in this book, that is, we will discuss the basic nature of the lattice and introduce the notion of fields defined on it, as well as the notion of functionals of these fields. Special attention will be paid to the notion of the lattice as a representation of space-time, in particular with respect to its geometrical aspects.

The somewhat philosophical points which we will discuss in the first section are nevertheless important to guide the analysis of the mathematical structure of the physical theory, dealing with quantum fields, to be discussed in the other chapters. Although these points are not exactly physical principles, their discussion here is not idle, because they will play a crucial role when the time comes to make some fundamental choices about the mathematical structure of the physical theory, as will be discussed in the last chapter of this book.

The first section is not needed for the understanding of many of the detailed technical aspects presented in the other chapters, except for the discussion in the last chapter, and could be skipped without trouble on a first reading.

1.1 Philosophical Preliminaries

The first thing we must do here is to point out an important duality of nature, according to which all things that exist in nature can be classified either as belonging to what has been termed the world of atoms, or as belonging to what can be described as the world of bits. By the first of these two general classes what is meant here is really the set of all physical objects. To put it in a more precise and fundamental way, this consists of matter and radiation. The name "world of atoms" is too restrictive for our purposes, and maybe one should use "world of energy" instead, since the energy is the one concept common to all forms of matter and radiation. This world of energy is the set of objects which are the subject of the physical sciences, and comprises what one usually understands in physics as objective physical reality.

serve. We will therefore *not* require the physical theory to contain exclusively the elements of objective physical reality, but rather require that it also make life easy for the mind. In other words, physical theory will be allowed to contain elements which are not mandated by objective physical reality, and that are allowed in for the convenience of the mind.

The next subject we must tackle here relates to the issue of the mathematical definition of the structure of the physical theory. At risk of stating the obvious, we must say here that the mathematical structure of the theory should be clearly and completely defined. Theoretical physics is a very difficult subject, and it leads to a strong tendency towards unbridled speculation. Although this may be a good and healthy thing, and can be an important tool of discovery, it should not become an end in itself. After all the speculations are proposed, examined, and possibly discarded, a well-structured mathematical theory should emerge. Too much wild speculation for too long can not only lead to loss of contact with physical reality, it may also lead to loss of contact with mathematical reality, and even to loss of contact with logic.

Besides requiring that the mathematical structure of the theory be stated clearly and completely, we must further require that this definition be *constructive*, that is, ultimately built without gaps from basic things such as the arithmetic of integer and real numbers. One way to interpret this requirement is to say that the definition should allow for an algorithmic realization. What this means is that, given a definite physical question within the theory, it should be possible to derive from its definition a set of rules and chained operations that would make it possible to answer that question, at least in principle, by the use of a program running on a digital computer. The proviso "at least in principle" is included because obtaining an infinitely precise answer might require the use of an infinitely powerful computer, being therefore impossible in practice. A less strict but sufficient requirement would be that the answer can be obtained within a finite and limited level of precision, given a sufficiently powerful computer and sufficient time to run the program on it.

Note that we do *not* regard as a requirement that it be possible to execute the necessary calculations with the unaided human mind, or by the use of the traditional analytical methods of mathematics. The ability to use a digital computer may be an essential element for the utilization of a physical theory as we understand it here. Although it is conceivable that the future may bring new analytical methods in mathematics, which may find use in the most important calculations in the theoretical physics described here, no such analytical methods are known at present, and it may even turn out that none exist. We do not, therefore, require that purely analytical methods be applicable to the theory, and regard direct numerical methods as sufficient.

The next subject to be discussed here has to do with the nature of the limits involved in the mathematical definition of the theory. Although the mathematical structures involved in the theory will, by the end of the definition process, become *continuum* mathematical structures, we will require that such continuum structures be obtainable by means of limiting procedures starting from *finite* mathematical

freedom constantly, and we will arrive at a fairly complete definition of the observables only very slowly, using our mathematical and computational probes into the inner workings of the theory along the way.

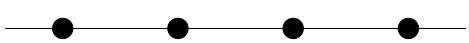
The last issue we would like to address here is that of the *closure* of the theory. By this we mean that, once it is defined completely in a concise way, all physical elements which are needed to describe objective physical reality must be contained within its structure, either directly as fundamental elements or as higher-level constructs derived from them. It should not be necessary to call on any external elements in order to complete the description. Although this may sound as somewhat self-evident, it is important to state it here, for clarity of definition. The role of this property will become evident in the subsequent chapters, but its most important consequences only come into play much later on, when one discusses the geometry of space-time, and are therefore outside the scope of this book.

The closure of the theory has a role to play in the very difficult issue of the physical measurement process. Measurement apparata are part of physical reality and are of course subject to the same physical laws they are meant to probe. The definition of the observables within the theory if of course closely tied to the definition of the process of physical measurement, by which information is created out of physical processes involving energy, and is therefore equally difficult. In the chapters that follow we will attempt to narrow down gradually the definition of an observable, but no complete description of the physical measurement process will be possible within the confines of the Gaussian model, which contains only free, non-interacting fields.

The complete description of the measurement process, including what is usually referred to as the reduction of the wave packet, and hence the complete definition of the physical observables, is probably only possible in the context of a complete and interacting theory, in which there are stable bound states. This is so because without bound states it would not be possible to store the bits of information generated by the measurement process. Such a complete and realistic theory is certainly a very difficult object to deal with, and we are not currently in a position to describe a complete model having all these properties.

1.2 The Euclidean Lattice

The object we will call the *Euclidean lattice* consists of a finite set of points with a certain relation of *neighborhood* established among them. The type and structure of this relation of neighborhood will determine the *dimension* of the lattice, a whole number that, for us, will always be between 1 and 5. The points will be called *sites* and the neighborhood relations will be represented by connections among the points, which we will call *links*. A simple example of a lattice could be



We have here four sites and five links in sequence, connecting sites which are neighbors to each other. Another lattice similar to this one could be obtained interconnecting the two loose ends of the outer links, resulting in the lattice

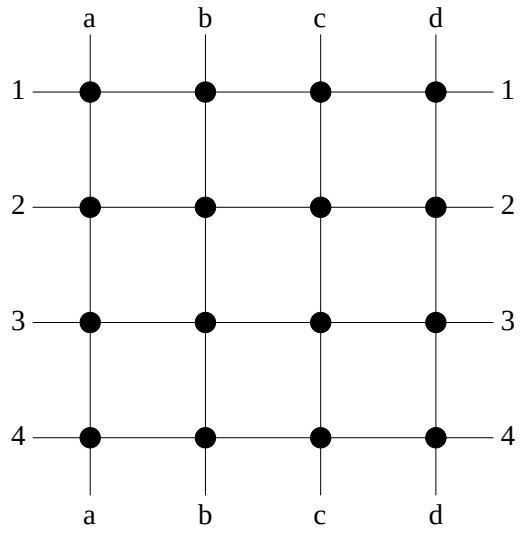


Figure 1.2.1: The basic elements of a typical two-dimensional lattice.

leaving as implicitly understood the connections of the links at the boundary with those on the opposite side.

If we somehow associate physical lengths to the links, we may understand these lattices as rough representations of a finite volume of space (in the case $d = 3$) or of space-time (in the case $d = 4$), in this case in an *Euclideanized* version. What we mean by this is that this is not really the usual space-time, since there is here no temporal direction that differs fundamentally from the other three. However, it is possible to establish a relation between the Euclidean space of dimension 4 and the space-time of physics. Further along we will come back to the issue of the relation between real space-time and its Euclideanized version.

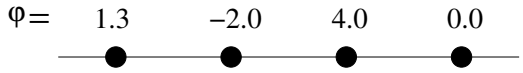
It is clear that, in order to obtain a finer representation of the space, whatever its dimension, we must increase the number of sites in our lattice of that same dimension. The purely mathematical issue of the representation of a continuous space by a scheme based on lattices of increasing size is quite complex and, as it turns out, not relevant for our purposes here, so it will not be further discussed and will be left at this intuitive level. Anyway, it is clear that we will be interested in the properties of lattice systems when the number of sites they contain increases without bound. The examples we drew in the figures of this section have $N = 4$, where N is the number of *vertices*, that is, the number of consecutive sites, according to the relations of neighborhood established by the links, in each one of the d directions of the lattice. The total number of sites of the lattice is given by N^d where d is its dimension.

Our strategy is, then, to study the properties of lattices of finite but arbitrary size, with the purpose of eventually discovering to what these properties tend when N tends to infinity. We will refer to this limit, using its traditional name, as the *continuum limit*. As we shall see, this limit contains the central mathematical difficulty of the theory. It is within it that we find the main problems and the deepest

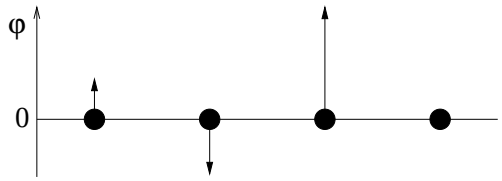
1.3 Fields on the Lattice

The fundamental variables of our structure will be *fields*, that is, functions defined on the lattice, for example with real values. The notion of *particle* will not be an elementary notion in our theory. Instead, it will appear later, as a notion derived from the structure of the theory. We will make, on the other hand, extensive use of the notion of wave. However, the physical interpretation of these waves will still be kept at an imprecise and intuitive level, serving mostly to guide our intuition regarding the identification, for closer examination, of the most important elements of the structure.

A scalar field φ is a function that associates, to each one of the N^d sites of the lattice, a real number. Since a single real value is associated to each site, we say that this is a field with a single *component*. A particular one-component real field in our first example lattice could be represented as

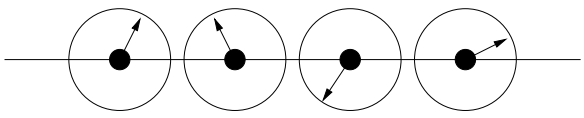


It is usual to represent this field by means of a set of arrows located at the sites, pointing along a real axis $\mathbb{R}$, with lengths given by the values associated by the field to each site,



Note that the values of the field at each site are not discrete, they exist within a continuous set, the real line. Occasionally one may be interested in fields with discrete values, but this is not the case in general. In this book we will consider only real fields with continuous values. Note also that this field is *dimensionless*, its values are real numbers without units, because so far there is no physical dimension associated to the fields.

In later parts of the development of the theory one may be interested in scalar fields with values in spaces which are larger and more complex than the real line $\mathbb{R}$. For example, fields which n components may have values in $\mathbb{R}^n$, and one may have fields with values in other spaces, not necessarily flat, such as the circle and the sphere. A field with values on the circle may be represented by arrows oriented along it,



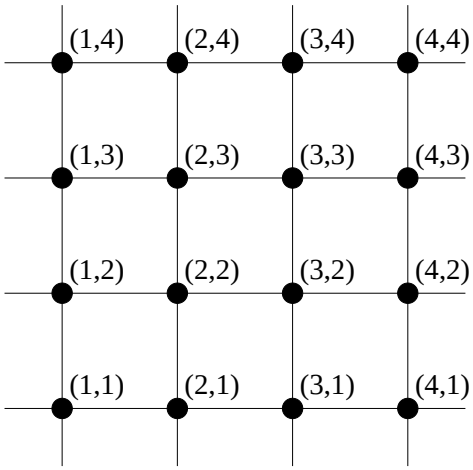


Figure 1.3.1: A system of integer coordinates in a typical two-dimensional lattice.

the system of integer coordinates which indexes the sites in the way indicated in figure 1.3.1.

A particularly important functional, which will be used to define completely each particular model to be considered in the theory, is the one we will call the *action*, usually denoted by $S[\varphi]$. From the physical standpoint, we will say that this functional determines the *dynamics* of a given model within the scope of the theory. In order for this to be possible this functional must satisfy some basic properties. First, it must be bounded from below, that is, there must exist a real number S_m such that $S[\varphi] \geq S_m$ for any configuration φ and for any lattice size N. Second, it must involve only sums of functions of the field at each site and sums of functions of products of fields at neighboring sites, that is, there is a veto against any dependence on products of fields at sites which are not neighbors, according to the relations of neighborhood established by the links of the lattice.

The first of these two conditions we call the *stability condition* of the model, for reasons to be made clear later. The second one we call the *locality condition*, for it means that this fundamental functional cannot depend on the product of values of the field which are associated to sites which are mutually distant from each other, in terms of the number of links that it is necessary to cross to go from one site to the other, in terms of the neighborhood relations of the lattice. This second condition may also be called the *next-neighbor condition*. It corresponds, in the continuum limit, to the inclusion in the action of terms containing derivatives of at most second order on the fields.

A possible example of an action S would be given by

$$S[\varphi] = \sum_s \varphi^2(s).$$

This functional satisfies the two conditions, because it depends only on a function (the square) of the field at each site, and because there is a number $S_m = 0$ such that $S[\varphi] \geq S_m$ for any configuration φ and for any value of N. However, this

where $\alpha_0 \geq 0$. The model defined by this action is called the *Gaussian model* or the *free scalar field*. As we shall see, this is the sole type of model over which we have complete analytical control for any value of the lattice size N in any of the dimensions d in which we are interested. For this reason, it will be extensively studied here as a way to probe into the concepts, issues and problems within the theory.

In terms of the physical interpretation, we may say that the non-Euclidean version of this model in $d = 4$ represents the dynamics of non-interacting plane waves, or of *free particles*, which do not interact with each other. Despite this limitation in scope, we will see that many important and useful things can be learned from this model, which in fact holds a few surprises for us, and will help to clarify the very foundations of the theory. A careful and complete understanding of this model is also essential as a preparation for the future study of interacting fields.

Problems

1.3.1. Show that, if $\alpha_0 < 0$, then the action S_0 of the theory of the free field has no lower bound.

1.3.2. Determine the range of values of the parameters α and λ for which the functional

$$S[\varphi] = \frac{1}{2}\sum_{\ell}(\Delta_\ell\varphi)^2 + \frac{\alpha}{2}\sum_{s}\varphi^2(s) + \frac{\lambda}{4}\sum_{s}\varphi^4(s)$$

satisfies the conditions for an action functional. Determine the value of the lower bound of this action as a function of α and λ.

Chapter 2

Classical Field Theory

In this chapter we will give a complete definition on the lattice of the classical theory of the free scalar field, showing by means of a few simple examples that one recovers in this way the familiar results of the usual approach to the theory. Some concepts and techniques which are important for the subsequent treatment of the quantum theory will also be introduced and explored, such as the treatment of the boundary conditions, the finite difference operators and their eigenvalues, the space of field configurations, the finite Fourier transforms and the transformation to momentum space, and the introduction and treatment of external sources.

It is important to observe that, although from the technical point of view this may be seen as a preliminary exercise for the work in the quantum theory, it is *not* a prerequisite to the quantum theory on a conceptual level. Conceptually, one should first define the quantum theory and only afterwards derive the classical theory from it, as the classical limit of that quantum theory. Although using the classical theory as an intuitive guide for the construction of the quantum theory may be a very good idea, the conceptual derivation must be from the quantum theory to the classical one, and *not* the other way around. In other words, while the "quantization" of a classical theory belongs to the realm of imaginative guesswork, the derivation of the classical limit of a quantum theory should be precise deductive work.

The main objective of this chapter, besides introducing useful concepts and techniques and establishing a standard notation for them, is to establish that the lattice formalism can be used as a mathematically complete and precise way to define the familiar structure of the classical theory of fields, including a careful discussion of the continuum limit and of the introduction of a physical length scale leading to the geometry of space-time.

2.1 Definition of the Classical Theory

We will now use the action S_0 to illustrate the relation that exists between our mathematical structure on the lattice and the classical (non-quantum) theory of fields. It should be noted here that our approach to the subject, unlike the traditional one, in both the classical and quantum cases, will not be based on equations of

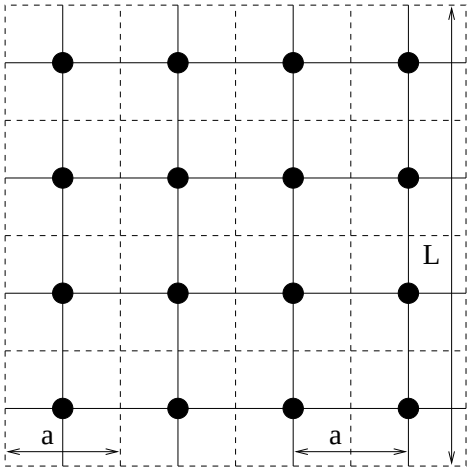


Figure 2.1.1: The geometrical elements of a periodical two-dimensional lattice.

way. In addition to this we will assume that the lattice remains symmetrical and homogeneous from the point of view of the lengths induced by the introduction of the external scale L into the theory. With all these assumptions made, we may now define dimensionfull versions of each one of the original dimensionless elements of our structure. For example, all the links of the lattice now have the same length, which we will denote by a, which is related to L by $L = Na$, and which goes to zero in the limit $N \to \infty$. The volume of the box which contains the lattice may now be divided into N^d disjoint cubes of volume a^d, whose union reconstitutes the total volume, as shown in figure 2.1.1.

We may now write the action S_0 in the form

$$S_0[\varphi] = \frac{1}{2}\sum_s a^d \sum_\mu \left[\frac{a^{(2-d)/2}\Delta_\mu \varphi(s)}{a}\right]^2 + \frac{\alpha_0}{2a^2}\sum_s a^d \left[a^{(2-d)/2}\varphi(s)\right]^2,$$

where all the factors of a that we introduced cancel out. Note that the sums over the sites combined with the factors a^d approach Riemannian integrals over the volume of the box. In order to make α_0 go to zero in the limit, as mentioned before that we must, we choose the relation $\alpha_0 = (m_0 a)^2$ for some finite m_0. Besides this, we define the dimensionfull version ϕ of the field as $\phi = a^{(2-d)/2}\varphi$, with which we may write for S_0, still on a finite lattice,

$$S_0[\phi] = \frac{1}{2}\sum_s a^d \sum_\mu \left[\frac{\Delta_\mu \phi(s)}{a}\right]^2 + \frac{m_0^2}{2}\sum_s a^d \phi^2(s).$$

At this point it becomes clear that, since in the $N \to \infty$ limit with constant L we have $a \to 0$, the sums indeed approach integrals over the volume of the lattice, with integration element $dv = \mathrm{d}^d x = a^d$, while the ratios between the finite differences of the field and a approach partial derivatives $\partial_\mu \equiv \partial/\partial x_\mu$. In short, we may write for S_0, in this limit, the expression

If we now impose the condition of minimum for S_0, that is, that $\delta S_0 = 0$ to first order for *any* variation $\delta\phi(\vec{x})$, we obtain the relation

$$-\partial^2\phi + m_0^2\phi = 0, \tag{2.1.1}$$

where $\partial^2 = \sum_\mu \partial_\mu\partial_\mu$ is the Laplacian operator in d dimensions. We refer to this equation, using the usual terminology of physics, as the *equation of motion*, although it may have nothing to do with movement, for example in the three-dimensional case, in which there is no temporal coordinate. The non-Euclidean version of this equation, in the case $d = 4$, is known as the Klein-Gordon equation and is related to the relativistic dynamics of free particles with mass m_0 and spin zero.

Observe that it is also possible to derive an equation corresponding to this one on finite lattices, because the integration by parts which is used for the derivation of this equation in the classical continuum theory has an exact counterpart on finite lattices. In order to see this we write explicitly the term containing the derivatives, for simplicity in only one dimension,

$$\begin{aligned}
&\sum_l (\Delta_\ell\varphi)^2 \\
&= \ldots + (\varphi_{n-1} - \varphi_n)^2 + (\varphi_n - \varphi_{n+1})^2 + \ldots \\
&= \ldots + \varphi_{n-1}^2 - 2\varphi_{n-1}\varphi_n + \varphi_n^2 + \varphi_n^2 - 2\varphi_n\varphi_{n+1} + \varphi_{n+1}^2 + \ldots \\
&= \ldots + \varphi_{n-1}^2 - \varphi_{n-1}\varphi_n - \varphi_n\varphi_{n-1} + 2\varphi_n^2 - \varphi_n\varphi_{n+1} - \varphi_{n+1}\varphi_n + \varphi_{n+1}^2 + \ldots \\
&= \ldots + \varphi_{n-1}^2 - \varphi_{n-1}\varphi_n - \varphi_n(\varphi_{n-1} - 2\varphi_n + \varphi_{n+1}) - \varphi_{n+1}\varphi_n + \varphi_{n+1}^2 + \ldots \\
&= -\sum_n \varphi_n(\varphi_{n-1} - 2\varphi_n + \varphi_{n+1}),
\end{aligned}$$

where we denoted the dependency on the position by means of indices, for simplicity of notation. With a detailed examination of the algebraic passages illustrated above it becomes clear that the regrouping of the terms can be done all around the circle, resulting in the final form, which relates a sum over links with a sum over sites,

$$\sum_l (\Delta_\ell\varphi)^2 = -\sum_s \varphi(s)\Delta^2\varphi(s),$$

where the Laplacian operator on finite one-dimensional lattices is defined as

$$\Delta^2\varphi(n) = \varphi(n-1) - 2\varphi(n) + \varphi(n+1).$$

Note that the Laplacian has values naturally defined on sites, like the field, not on links. The generalization of this definition to lattices of higher dimensions is immediate, the algebraic operation described can be repeated on all the directions and therefore it suffices to add a sum over the directions,

$$\Delta^2\varphi(\vec{n}) = \sum_\mu [\varphi(n_\mu - 1) - 2\varphi(n_\mu) + \varphi(n_\mu + 1)]. \tag{2.1.2}$$

2.2 Fixed Boundary Conditions

In order to illustrate in a more familiar form the analogy between the $d = 3$ classical field theory as defined here and electrostatics, it is necessary to change the boundary conditions. We will do this, defining what we will call *fixed* boundary conditions, first of all on finite lattices. This type of boundary condition and other similar types, derived from it, will also have a role to play in the quantum theory, as we may see in a future opportunity, but in the scope of this book we will use them only in this chapter. We will represent a finite lattice with fixed boundary conditions in the form shown in figure 2.2.1, where the sites marked with crosses are the one in the external border. These sites have a different role from the others, which we will call internal sites, being for this reason marked in a different way. Note that each one of them connects to a single internal site, independently of the dimension d of the lattice.

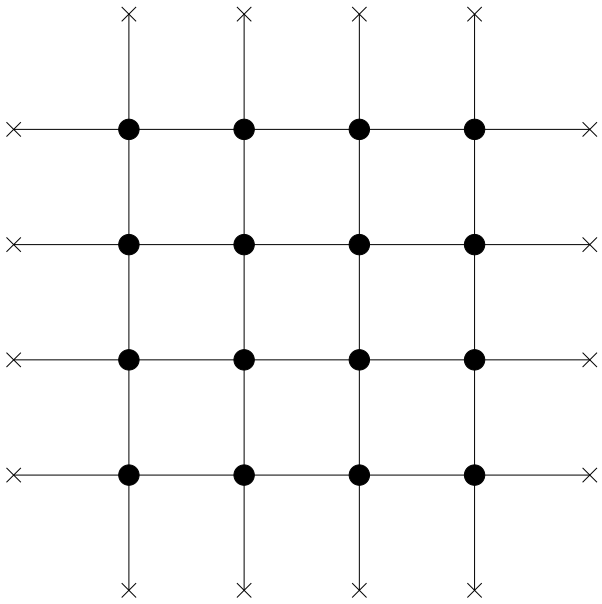


Figure 2.2.1: A two-dimensional lattice with fixed boundary conditions.

In the scope of the classical theory we assume that *the values of the fields are fixed* and given a-priori at these border sites. The form of the action we considered before in equation (1.3.1) does not change, except for the fact that the sum over links includes now the links connecting the internal sites to the border. The sum over sites does not change at all, it remains running over the internal sites. Under these conditions the classical finite equation of motion in equation (2.1.3) also does not change form. It applies to all internal sites, but not to the border sites, for two reasons. For one thing, it is not necessary that it determine the values of the field at these sites, since they are given a-priori. For another, it is not possible to calculate the value of the Laplacian at these sites, because of the lack of sufficient data.

In order to see this, it is necessary to derive the equation in detail on a finite lattice. Note that the action itself changes slightly in form, because in this case we have,

$$\delta S_0 = \Delta_{\ell_{b-}}\varphi\delta(\Delta_{\ell_{b-}}\varphi) + \sum_{\ell_i}\Delta_{\ell_i}\varphi\delta(\Delta_{\ell_i}\varphi) + \Delta_{\ell_{b+}}\varphi\delta(\Delta_{\ell_{b+}}\varphi) + \alpha_0\sum_{n=1}^{N}\varphi(n)\delta\varphi(n).$$

It is easy to verify (problem 2.2.1) that, on any of the links,

$$\delta(\Delta_\ell\varphi) = \Delta_\ell\delta\varphi(s),$$

and we therefore have

$$\delta S_0 = \Delta_{\ell_{b-}}\varphi\Delta_{\ell_{b-}}\delta\varphi + \sum_{\ell_i}\Delta_{\ell_i}\varphi\Delta_{\ell_i}\delta\varphi + \Delta_{\ell_{b+}}\varphi\Delta_{\ell_{b+}}\delta\varphi + \alpha_0\sum_{n=1}^{N}\varphi(n)\delta\varphi(n).$$

We write now, explicitly, the part of the sum with the first terms containing derivatives close to one of the ends of the lattice, recalling that $\delta\varphi(0) = \delta\varphi(N+1) = 0$,

$$\begin{aligned}
&(\varphi_1-\varphi_0)\delta\varphi_1 + (\varphi_2-\varphi_1)(\delta\varphi_2-\delta\varphi_1) + (\varphi_3-\varphi_2)(\delta\varphi_3-\delta\varphi_2)+\ldots\\
&= \varphi_1\delta\varphi_1 - \varphi_0\delta\varphi_1 + \varphi_2\delta\varphi_2 - \varphi_1\delta\varphi_2 - \varphi_2\delta\varphi_1 + \varphi_1\delta\varphi_1\\
&\quad +\varphi_3\delta\varphi_3 - \varphi_2\delta\varphi_3 - \varphi_3\delta\varphi_2 + \varphi_2\delta\varphi_2 + \ldots\\
&= -\varphi_0\delta\varphi_1 + 2\varphi_1\delta\varphi_1 - \varphi_2\delta\varphi_1 - \varphi_1\delta\varphi_2 + 2\varphi_2\delta\varphi_2 - \varphi_3\delta\varphi_2 + \ldots\\
&= -\delta\varphi_1(\varphi_0 - 2\varphi_1 + \varphi_2) - \delta\varphi_2(\varphi_1 - 2\varphi_2 + \varphi_3) + \ldots.
\end{aligned}$$

With this we see that the variation of the action may be written as

$$\delta S_0 = -\sum_{n=1}^{N}[\Delta^2\varphi(n)]\delta\varphi(n) + \alpha_0\sum_{n=1}^{N}\varphi(n)\delta\varphi(n) = \sum_{n=1}^{N}[-\Delta^2\varphi(n) + \alpha_0\varphi(n)]\delta\varphi(n).$$

Se now see that, for δS_0 to vanish for any function $\delta\varphi(n)$ it is necessary that, for all n,

$$-\Delta^2\varphi(n) + \alpha_0\varphi(n) = 0,$$

which is the equation of motion for this case. We see that its form does not change, we have the same equation, although with different boundary conditions, of course.

Note that in this type of lattice there are N internal sites in each direction, but a larger number, $N+1$, of links in each direction. In order to take the continuum limit we proceed in a way similar to the one used before, but this time the relation between the size L of the box and the length a of the links is $L = (N+1)a$. The volume of the integration element is the same as before, a^d, but there are now surface terms to consider in the integrals. The new representation of the lattice with all these elements is shows in figure 2.2.2.

In the continuum limit the equation of motion is the same differential equation we obtained before for periodic boundary conditions, shown in (2.1.1). What changes, naturally, are the boundary conditions. When $m_0 = 0$ and $d = 3$ this equation

the derivatives that appear in this expression have finite values, it now becomes clear that in this limit the surface terms only vanish in the case in which the field is kept equal to zero at the external surface. Hence, we see that the form of the action changes by the addition of surface terms both on finite lattices and in the continuum limit of the classical theory, while the equation of motion does not change, the difference remaining implicitly only in the boundary conditions to be used to solve the equation.

It is important to observe here that this kind of boundary condition will *not* have a *fundamental* role to play in the quantum theory. This is due to the fact that in the quantum theory the value of the field at sites is neither an observable nor a controllable quantity that one can fix at a constant value without fluctuations. The boundary conditions discussed here will be associated, in the context of the quantum theory, to an approximation scheme, namely the so-called *mean-field method*. In any case we do see here, by means of these examples, that our discrete structure on the lattice reduces in fact to known cases of classical field theories in the continuum limit, when we introduce into the structure a dimensional scale which is *external* to the structure of our theory on the lattice.

Problems

2.2.1. If $f(s)$ is an arbitrary function of the sites, s_+ and s_- are the sites at the two ends of a link ℓ, $\Delta_\ell f = f(s_+) - f(s_-)$ is the finite difference of the fields at these sites, and assuming that an infinitesimal variation $\delta\varphi(s)$ at each site s of the lattice is made, show that

$$\delta(\Delta_\ell \varphi) = \Delta_\ell \delta\varphi.$$

2.2.2. Show, on finite lattices in d dimensions, for an arbitrary position $\vec{n}$ in the interior of the lattice, that the equation $\Delta^2\varphi(\vec{n}) = 0$ implies that $\varphi(\vec{n})$ is equal to the average value of its $2d$ nearest neighbors.

2.2.3. ($\star$) Write a program that uses the relaxation method, which is based on the result of problem 2.2.2, to find the field $\varphi(s)$ that satisfies the equation $\Delta^2\varphi = 0$ on a two-dimensional lattice in which $\varphi = 1$ at two opposite sides of the border and $\varphi = -1$ at the other two opposite sides of the border.

2.3 Finite-Difference Operators

We will now elaborate a little the notion of operators that act on the lattice, related to finite differences of the fields. In the usual numerical methods for the solution of differential equations these operators are looked at as approximations on finite

Our action functional S_0 depends only on the field and its first derivatives (or rather, finite differences), therefore we are ready to write it in a more explicit way. It can be verified that from the use of either the $\Delta_\mu^{(+)}$ form or the $\Delta_\mu^{(-)}$ form of the finite-difference operator results the same action on the lattice, with only next-neighbor couplings among the values of the field at the various sites,

$$S_0[\varphi] = \frac{1}{2}\sum_\ell \left[\Delta_\ell^{(+)}\varphi\right]^2 + \frac{\alpha_0}{2}\sum_s \varphi^2(s) = \frac{1}{2}\sum_\ell \left[\Delta_\ell^{(-)}\varphi\right]^2 + \frac{\alpha_0}{2}\sum_s \varphi^2(s).$$

In both these cases, expanding the square of the finite-difference operator, one may write S_0 as (problem 2.3.1)

$$S_0[\varphi] = -\sum_\ell \left[\varphi(\vec{x})\varphi(\vec{x}+a\hat{x}_\ell)\right] + \left(d + \frac{\alpha_0}{2}\right)\sum_s \varphi^2(\vec{x}).$$

What is understood by "next-neighbor couplings" is that, in the terms of the action which involve products of values of the field at different sites, the values involved are in adjacent sites, connected by a link. Note that the inter-site interaction that appears above is similar to an interaction between two spins at neighboring sites, such as the one that appears in the Ising model of magnetism. This elementary interaction among neighboring sites should not be confused with what is usually referred to in the theory as "interaction terms", which supposedly couple together the Fourier modes of the fields and thus cause plane waves to interact with each other, giving rise to scattering processes in the non-Euclidean version of the theory. These interaction terms will be discussed in a future volume, but are outside the scope of this book.

The use of the realization $\Delta_\mu^{(c)}$, however, produces from the continuum action a lattice action with more than interactions between next-neighbor sites. The association of the finite-difference operator with links is intuitive and very attractive, as well as closely related to the realization of the lattice of gauge theories, as will be seen in a future volume. This fact, plus the simplicity of having to deal only with couplings between next neighbors, would be sufficient to decide the question as to the type of finite-differencing scheme to choose for the definition of the theory on the lattice. But we will see in what follows, in a direct way, that the use of $\Delta_\mu^{(c)}$ may also be reduced to exactly the same theory on the lattice, and that the finite-difference operator is inevitably defined on links.

In order to see this we consider the integration by parts of the first term of the action S_0 which, as commented previously, is only a not too appropriate name for an algebraic operation involving sums of differences along the lattice. In this way we may write the action as

$$S_0[\varphi] = -\frac{1}{2}\sum_{s,\mu} \varphi(\vec{x})\Delta_\mu^2\varphi(\vec{x}) + \frac{\alpha_0}{2}\sum_s \varphi^2(\vec{x}) = \frac{1}{2}\sum_s \left[-\varphi(\vec{x})\Delta^2\varphi(\vec{x}) + \frac{\alpha_0}{2}\varphi^2(\vec{x})\right].$$

In spite of the fact that in order to do this with the usual mathematical language of the continuum it may seem necessary to interpret the term $(\Delta_\mu\varphi)^2$ in a mixed

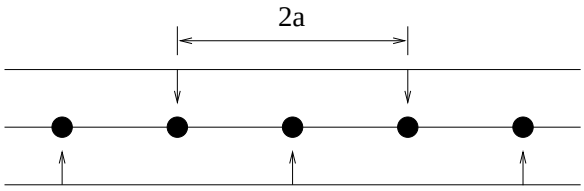


Figure 2.3.1: A one-dimensional double lattice.

verify that, in d dimensions with even N and periodical boundary conditions, the use of $\Delta_\mu^{(c)}$ and $\Delta_{(c)}^2$ corresponds *exactly* to the representation on the lattice of 2^d simultaneous and non-interacting copies of the same model, with a lattice spacing parameter rescaled by two, equal therefore to $2a$. For odd N the use of the central finite-difference operator will produce a multiple cover of the torus and we end up with a single realization of the model wrapped up 2^d times around the torus, with both a and L rescaled by a factor of two. Figure 2.3.1 may help in the visualization of these facts in the case $d = 1$. In the figure the lines with arrows point to the two subsets of sites which are related by the dynamics of the theory. In one dimension one of the two sets is the set of sites with even integer coordinates, and the other is the set of sites with odd integer coordinates. According to the dynamics of the theory, each one of these two sets interacts internally, but each one of them does not interact at all with the other one (problems 2.3.4 and 2.3.5).

Observe that this realization by means of $\Delta_\mu^{(c)}$ does complicate the counting of the degrees of freedom of the models. Where we thought we had a single field value per site we end up with 2^d independent field values, which are non-interacting or interacting only through the boundary conditions. It is interesting to observe that the realization on the lattice of fermionic fields also involves multiplications of the spectrum of particles by factors of 2^d, a phenomenon that remains as one of the main open problems for that type of field. In that case the problem appears in momentum space rather than position space, but it seems likely that in that case too the problem may reduce to the question of counting degrees of freedom.

We see therefore that in these realizations the finite-difference operator ends up once more associated in a natural way to links, now with length $2a$, a fact that leads us to think that the association of finite differences to links has a certain character of inevitability. The same is true for more complex models such as, for example, the polynomial models and the sigma models, so long as consistent use is made in them of either the $[\Delta_\mu^{(\pm)}, \Delta^2]$ or the $[\Delta_\mu^{(c)}, \Delta_{(c)}^2]$ realizations. Since we do not have any interest in having to deal with several identical copies of the same model sharing the same lattice, in what follows we will restrict the discussion to only the case of next-neighbor couplings.

Problems

2.3.1. Show, by expanding the term that contains the square of the finite-difference operator, that the action S_0 of the free scalar field can be written as

2.4 Space of Field Configurations

Linear operators and the spaces on which they act can in general be represented by matrices and vectors, respectively. Having constructed the Laplacian operator both on finite lattices and in the continuum limit, we will now show how to represent it in matrix form on finite lattices. We will have in this way a very concrete representation both of the operators and of the vectors that constitute the space on which they act. This representation is very useful as a concrete mental image of the objects under study, as well as a computational tool, which can be used to good advantage in the context of the stochastic methods which constitute the main calculational approach to the quantum theory.

In order to do this we will introduce and develop to some extent the concept of the space of field configurations, which will be of great importance for the quantum theory. The space of configurations, as previously defined, is the space of all possible field-functions on the lattice. This is in fact a different space for each lattice size, so we are actually talking here of a set or sequence of spaces. For a real field with a single component on a lattice of N^d sites in d dimensions this space is $\mathbb{R}^{(N^d)}$.

For simplicity we will do the construction for the case of periodical boundary conditions. We shall start with the case $d = 1$, which is very simple. In this case we can represent each configuration of the field by the collection of its values at the sites along the lattice, in the order in which they appear on the linear chain defined by it,

$$\begin{bmatrix} \varphi_1 \\ \cdot \\ \cdot \\ \cdot \\ \varphi_i \\ \cdot \\ \cdot \\ \cdot \\ \varphi_N \end{bmatrix} .$$

Any function defined on the lattice can be represented by a vector like this one, with absolutely no additional restriction imposed on the nature of the functions. The $n = N^1$ components of the vector are the n values assumed by the function on the n sites existent on the lattice. In this simple case the index i of the vector that represents the field is simply the integer coordinate n_1 of the one-dimensional lattice. Further along the development of the theory one may have scalar fields φ_a with more than a single component, that is, vectors $\vec{\varphi}$ in some internal symmetry space of the fields, but one may still use this kind of representation for the fields in the space of configurations. One will simply have several vectors like the one illustrated above, one for each field component in the internal space. The ideas involved in the representation of the field as a function over the lattice do not change, the field simply acquires an additional index that does not mix with those referring to space-time.

In this way we see that both the pair (n_1, n_2) and the index ι determine uniquely a site. We may now use ι as the index of the vector that will represent the field on a two-dimensional lattice,

$$\begin{bmatrix} \varphi_1 \\ \cdot \\ \cdot \\ \cdot \\ \varphi_\iota \\ \cdot \\ \cdot \\ \cdot \\ \varphi_{N^2} \end{bmatrix},$$

that is, we may represent the function $\varphi(n_\mu)$ by the vector with components φ_ι.

This method can be immediately generalized to any dimension d. For example in three dimensions, with integer coordinates (n_1, n_2, n_3), the index is given by

$$\iota = 1 + (n_1 - 1) + (n_2 - 1)N + (n_3 - 1)N^2,$$

and the inversion operations are (problem 2.4.2)

$$\begin{aligned} n_3 &= 1 + \frac{(\iota - 1)}{N^2}, \\ n_2 &= 1 + \frac{(\iota - 1) - (n_3 - 1)N^2}{N}, \\ n_1 &= 1 + (\iota - 1) - (n_3 - 1)N^2 - (n_2 - 1)N. \end{aligned}$$

At this point it is already possible to see the pattern and imagine how to generalize this. In general the index, on a lattice in d dimensions with integer coordinates n_μ, will be given by

$$\iota = 1+(n_1-1)+(n_2-1)N+\ldots+(n_{d-1}-1)N^{d-2}+(n_d-1)N^{d-1} = 1+\sum_{\mu=1}^{d}(n_\mu-1)N^{\mu-1},$$

where ι varies from 1 a N^d along all the extent of the lattice and the recursive inversion operations are an immediate generalization of the relations for the three-dimensional case, given above. For $n_1 = \ldots = n_d = 1$ we immediately have $\iota = 1$ and for $n_1 = \ldots = n_d = N$ we have $\iota = N^d$, as we may verify by inspection,

$$\left.\begin{array}{rc} & (n_d-1)N^{d-1} \\ + & (n_{d-1}-1)N^{d-2} \\ + & (n_{d-2}-1)N^{d-3} \\ & \vdots \\ + & (n_3-1)N^2 \\ + & (n_2-1)N^1 \\ + & (n_1-1)N^0 \end{array}\right\} = \left\{\begin{array}{rccc} & N^d & - & N^{d-1} \\ + & N^{d-1} & - & N^{d-2} \\ + & N^{d-2} & - & N^{d-3} \\ & \vdots & & \vdots \\ + & N^3 & - & N^2 \\ + & N^2 & - & N \\ + & N & - & 1 \end{array}\right\} = N^d.$$

which has a non-zero determinant so long as the mass is not zero. This corresponds to the fact that only the theory of the free field with *zero mass* has a zero mode on the torus and, potentially, problems due to the occurrence of divergences in the infra-red limit, in which one makes the size L of the box tend to infinity, thus including into the structure of the models arbitrarily large wavelengths and, therefore, arbitrarily low frequencies.

Still for periodical boundary conditions, the forward difference operator $\Delta_\mu^{(+)}$ has the matrix representation

$$\Delta_\mu^{(+)} = \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 \end{bmatrix},$$

and the backward difference operator $\Delta_\mu^{(-)}$ the representation

$$\Delta_\mu^{(-)} = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 \\ -1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 1 \end{bmatrix}.$$

It can be easily verified (problem 2.4.5), in this one-dimensional case, that they are related to Δ^2 by

$$\Delta^2 = \Delta^{(+)}\Delta^{(-)} = \Delta^{(-)}\Delta^{(+)}.$$

In this way the treatment, both of the fields and of the action on them of linear operators such as the Laplacian, can always be reduced in an explicit way to operations with vectors and matrices in a space with a large but finite dimension, the space of field configuration on the lattice. This is specially useful in programs for the execution of stochastic simulations of models in the quantum theory.

Problems

2.5 Momentum Space

We will now define a concept which will be of great importance both for the solution of the mathematical problems of the theory and in relation to its physical interpretation, even when it is not possible to find exact solutions. This is the concept of *momentum space*. The fields, as defined so far, are written as functions of the sites s and hence of their integer coordinates $\vec{n}$. As we saw before, we refer to the space of all possible fields as the space of field configurations. We will call this representation of the fields, as functions of the sites, by the name *position space*. Another representation of the fields exists in *momentum space*, which is obtained by means of a linear transformation that effects a change of basis in the space of configurations. The integer coordinates $\vec{n}$ of the sites will be mapped on a new set of integer coordinates $\vec{k}$ that index what we will call the *modes* of the lattice, in a way similar to the indexing of the sites by $\vec{n}$. The name originates from the classical concept of normal modes of oscillation.

We will begin by showing a simple property of exponentials with discrete arguments involving integers. Let $1 \leq n \leq N$ be an integer and consider the exponential function

$$e^{\imath 2\pi n/N}$$

for the set of N possible values of the argument. We have here complex phases, which means that this function assumes values along the unit circle of the complex plane. As n varies from 1 to N the function goes around the circle, defining along it N equally spaced points. In figure 2.5.1 we have an example with $N = 8$, with the N values of n marked for each phase.

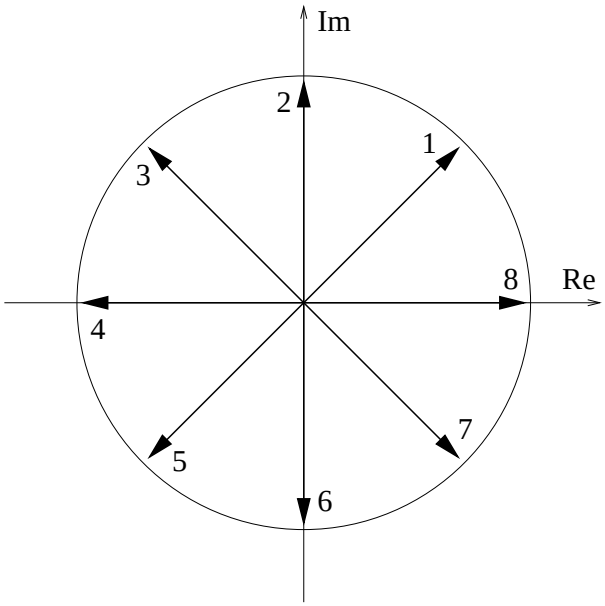


Figure 2.5.1: Example of a complex unit circle for $N = 8$.

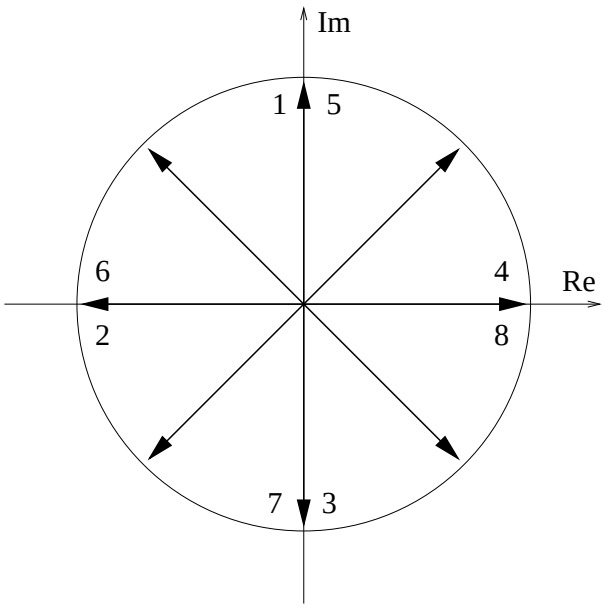


Figure 2.5.3: A double lap on the complex unit circle with $N = 8$.

$$\sum_{n=1}^{N} e^{\imath 2\pi kn/N} = 0.$$

The same is valid for any other values of k in the interval under consideration, except for $k = 0$. In this case we always have, very simply, N times the positive real phase $\exp(0) = 1$, so that we may write for our sum of phases

$$\sum_{n=1}^{N} e^{\imath 2\pi kn/N} = N\delta(k, 0),$$

where $\delta(k, 0)$ is the Kronecker delta, equal to 1 if $k = 0$, equal to 0 if $k \neq 0$. In order to convince oneself of the truth of this fundamental relation, which will give rise to the relations of *orthogonality* and *completeness* that we will frequently use, one may try out a certain number of particular cases, until one acquires a practical understanding of how the sum of phases works. We may also verify it in a simple and elegant way using the formula for the sum of a geometrical progression[1], although the numbers involved are complex rather than real. The extension of this formula to the complex domain is a simple process of analytical extension and its validity can be verified algebraically (problem 2.5.1). If we have as the initial element of the progression $a_1 = \exp(\imath 2\pi k/N)$ and as the ratio $q = \exp(\imath 2\pi k/N) \neq 1$, with $k \neq 0$, we will also have $a_N = \exp(\imath 2\pi k) = 1$ for any k, and the sum is given by

$$\frac{a_N q - a_1}{q - 1} = \frac{e^{\imath 2\pi k} e^{\imath 2\pi k/N} - e^{\imath 2\pi k/N}}{e^{\imath 2\pi k/N} - 1} = e^{\imath 2\pi k/N} \frac{e^{\imath 2\pi k} - 1}{e^{\imath 2\pi k/N} - 1} = 0.$$

[1]This idea was proposed by Mr. Arnaldo Gomes de Oliveira Filho.

We may now write the relations above in a slightly different form, that we will name *relation of orthogonality*,

$$\sum_{n=1}^{N} e^{\imath \frac{2\pi}{N} n(k-k')} = N\delta_{k,k'}, \tag{2.5.1}$$

and *relation of completeness*,

$$\sum_{k=k_m}^{k_M} e^{\imath \frac{2\pi}{N} k(n-n')} = N\delta_{n,n'}, \tag{2.5.2}$$

where k_m and k_M are the minimum and maximum limits of the interval of values of k in each case. Once these relations are established for the one-dimensional case as we have done here, their extensions to higher dimensions is immediate, achieved by means of the use of the properties of the exponential function (problem 2.5.3). Hence in d dimensions we have the relations

$$\begin{aligned} \sum_{n_1=1}^{N} \cdots \sum_{n_d=1}^{N} e^{\imath \frac{2\pi}{N} \vec{n}\cdot(\vec{k}-\vec{k}')} &= N^d \delta_{k_1,k_1'} \ldots \delta_{k_d,k_d'}, \\ \sum_{k_1=k_m}^{k_M} \cdots \sum_{k_d=k_m}^{k_M} e^{\imath \frac{2\pi}{N} \vec{k}\cdot(\vec{n}-\vec{n}')} &= N^d \delta_{n_1,n_1'} \ldots \delta_{n_d,n_d'}. \end{aligned}$$

The first relation establishes a definition of scalar product between modes, according to which they are all orthogonal to one another. The exponential functions $\exp(\imath 2\pi \vec{k} \cdot \vec{n}/N)$ are called the *mode functions* of these Fourier modes. This scalar product is defined as a sum over position space of products of two mode functions, which are characterized by $\vec{k}$ and $\vec{k}'$. The second relations involves a sum over momentum space and establishes that any function of the sites on the lattice can be written as a linear superposition of these mode functions, which therefore constitute a complete set of functions on the lattice (problem 2.5.4).

Problems

2.5.1. Derive algebraically the expression for the sum of a geometrical progression of N terms with $q \neq 1$ and show that the result is valid independently of q and the first term a_1 being real or complex.

2.5.2. Show that the modes corresponding to k_1 and $k_1 + N$ are in fact the same mode, that is, that the corresponding mode functions, $\exp(\imath 2\pi kn/N)$, have the same values at all the lattice sites.

2.5.3. Using the properties of the exponential function, derive the orthogonality and completeness relations in d dimensions from the one-dimensional relations given in equations (2.5.1) and (2.5.2).

2.6 Finite Fourier Transforms

We are now in a position to define the *finite Fourier transform* of our field, as well as its inverse. As we shall see, the orthogonality of the modes we defined establishes that this transform will take us to the *normal modes of oscillation* of the field within the box. On our cubic N-lattice with periodical boundary conditions we define the finite Fourier transform of the field $\varphi(\vec{n})$ as

$$\widetilde{\varphi}(\vec{k}) = \frac{1}{N^d} \sum_{\vec{n}} e^{\imath \frac{2\pi}{N} \vec{k}\cdot\vec{n}} \varphi(\vec{n}).$$

This is a linear transformation of coordinates in the space of field configurations, taking us from the N^d coordinates $\varphi(\vec{n})$ to the also N^d coordinates $\widetilde{\varphi}(\vec{k})$. The inverse transform, taking us back to the coordinates in terms of site positions, is given by

$$\varphi(\vec{n}) = \sum_{\vec{k}} e^{-\imath \frac{2\pi}{N} \vec{k}\cdot\vec{n}} \widetilde{\varphi}(\vec{k}),$$

where the sum is over all the momenta, that is, an abbreviation such as

$$\sum_{\vec{k}} \equiv \sum_{k_1=k_m}^{k_M} \cdots \sum_{k_d=k_m}^{k_M} .$$

Note that, as defined here, φ and $\widetilde{\varphi}$ are both dimensionless. The fact that the two operations defined above are the inverses of one another is a consequence of the orthogonality and completeness relations, as you will have a chance to show in one of the problems (problem 2.6.1). Observe that all these relations are exact on finite lattices, that they do not involve any kind of approximation. What we have here is simply a linear transformation in a finite-dimensional vector space. As we shall see further along, this linear transformation allows us to solve exactly the Gaussian model, which is the Euclidean version of the theory of the free scalar field.

Let us examine now how these transformations behave in the continuum limit. As we did before in section 2.1, in order to take this limit we will introduce an external dimensional scale into our system. Once more we assume that the system is contained in a cubic box of size L in this external system of units. When we make $N \to \infty$ with constant L, the lattice spacing $a = L/N$ of the lattice goes to zero and the sum that defines the Fourier transform approaches a Riemann integral over the box of volume $V = L^d$. In this case we may write this relation, in the limit, as

$$\widetilde{\varphi}(\vec{p}\,) = \frac{1}{V} \int_V \mathrm{d}^d x \; e^{\imath \vec{p}\cdot\vec{x}} \varphi(\vec{x}),$$

where $\vec{x} = a\vec{n}$ are the coordinates that describe positions within the continuous box and $\vec{p} = 2\pi\vec{k}/L$ are the discrete momenta associated to the vectors with integer components $\vec{k}$. Since we are now within a continuous but still finite box, these modes

where we see that, in this case, the divergent factors of V cancel out. It is clear that the normalization factors involving V are not at all convenient in the case of the infinite box and, therefore, we will change the normalizations, so that we may in fact take the limits and obtain the Fourier transforms in their usual form, in which $\widetilde{\phi}_\infty$ and ϕ have different dimensions,

$$\begin{aligned}
\widetilde{\phi}_\infty(\vec{p}) &= \int \mathrm{d}^d x \, e^{\imath \vec{p}\cdot\vec{x}} \phi(\vec{x}), \\
\phi(\vec{x}) &= \int \frac{\mathrm{d}^d p}{(2\pi)^d} \, e^{-\imath \vec{p}\cdot\vec{x}} \widetilde{\phi}_\infty(\vec{p}), \\
\int \mathrm{d}^d x \, e^{\imath \vec{x}\cdot(\vec{p}-\vec{p}')} &= \delta^d\left(\vec{p}-\vec{p}'\right), \\
\int \frac{\mathrm{d}^d p}{(2\pi)^d} \, e^{\imath \vec{p}\cdot(\vec{x}-\vec{x}')} &= \delta^d\left(\vec{x}-\vec{x}'\right).
\end{aligned}$$

All the relations examined in this section also have their equivalent counterparts in non-Euclidean space. In particular, the complex exponentials $\exp(\imath\vec{p}\cdot\vec{x})$ are, in their non-Euclidean version, plane waves that propagate in infinite space. These plane waves will have an important role to play also in the quantum theory, where they will be associated to free particles. We see here that the Fourier transformation may also be understood as a decomposition of functions of position in terms of plane waves.

We wrote here the equations relating to infinite space only for reference, since in these notes we will seldom be working in an infinite box. With few exceptions it will suffice to consider the definition of quantum field-theoretical models inside finite boxes. The normalization we chose to adopt for the case of finite lattices is appropriate for this case. In fact, note that with this normalization the zero-momentum ($\vec{k}=\vec{0}$) transform of the field is its average value inside the box,

$$\widetilde{\varphi}(\vec{0}) = \frac{1}{N^d} \sum_{\vec{n}} \varphi(\vec{n}) = \overline{\varphi}.$$

This average is also called the *zero mode* of the field and it will play a special role in the subsequent development of the theory.

Problems

2.6.1. Show, on finite lattices, that the inverse Fourier transform really recovers the original function from its Fourier components.

2.6.2. Assuming that $\vec{x} = a\vec{n}$, show that the product $a^{-d}\delta^d(\vec{n},\vec{n}')$, where $\delta^d(\vec{n},\vec{n}')$ is the d-dimensional Kronecker delta, transforms into the d-dimensional Dirac delta function $\delta^d(\vec{x}-\vec{x}')$ in the continuum limit. In order to do this, build on the lattice expressions that, in the continuum limit, converge to integrals of $\delta^d(\vec{x}-\vec{x}')$ over $\vec{x}$ in domains that may or may not include the point $\vec{x}'$, showing that they have the values one would expect of a Dirac delta function.

$$\rho_\mu(k_\mu) = 2\sin\left(\frac{\pi}{N}\vec{k}\cdot\hat{n}_\mu\right) = 2\sin\left(\frac{\pi k_\mu}{N}\right), \tag{2.7.1}$$

the remaining factors are simply the imaginary unit $\imath$ that comes from the finite differentiation and a phase

$$e^{\imath\frac{\pi}{N}\vec{k}\cdot\hat{n}_\mu} = e^{\imath\vec{p}\cdot\hat{x}_\mu a/2},$$

indicating that the natural location of the result is the middle of the link that points in the positive μ direction starting from the site in question! The dimensionfull quantity $p_\mu^{(N)} = \rho_\mu(k_\mu)/a$ is the quantity on the lattice that really corresponds to the physical linear momentum of the states and particles of the theory. We will also refer to the quantities $\rho_\mu(k_\mu)$ as the dimensionless momenta on the lattice. The lattice momenta $p_\mu^{(N)}$ reduce in the continuum limit to the continuum momenta p_μ, so long as these are finite in the limit, that is, for modes with integer coordinates k_μ that are much smaller than N on large lattices,

$$p_\mu^{(N)} = \frac{2}{a}\sin\left(\frac{\pi k_\mu}{N}\right) \simeq \frac{2\pi k_\mu}{Na} = \frac{2\pi k_\mu}{L} = p_\mu, \quad \text{for} \quad k_\mu \ll N.$$

In the case of the operator Δ^2 (problem 2.7.2) we have for each finite second-difference Δ_μ^2 (with no sum over μ),

$$\Delta_\mu^2 e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}} = -\left[2\sin\left(\frac{\pi}{N}\vec{k}\cdot\hat{n}_\mu\right)\right]^2 e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}.$$

Hence we see that the eigenvalues of Δ_μ^2 are $-\rho_\mu^2$ and we have, therefore,

$$\Delta^2 e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}} = -\rho^2 e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}, \tag{2.7.2}$$

where ρ^2 is given by

$$\rho^2 = \sum_\mu \rho_\mu^2 = 4\left[\sin^2\left(\frac{\pi k_1}{N}\right) + \ldots + \sin^2\left(\frac{\pi k_d}{N}\right)\right].$$

In this case the eigenvalues are real and we have a Hermitian operator. Again, the eigenvalues are related to the dimensionless versions of the momenta on the lattice, $\rho_\mu(k)$. All the quantities that we will calculate in the theory will end up written in terms of these quantities, more often in terms of ρ^2.

Note that the fact that the complex exponentials are eigenvectors of the Laplacian implies that some of them are also solutions of the classical theory in its non-Euclidean version. In order to see this it suffices to directly apply the equation to the functions, resulting in

$$(-\Delta^2 + \alpha_0)e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}} = (\rho^2 + \alpha_0)e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}},$$

With the use of fixed boundary conditions, in which the values of the field at the border are given beforehand and kept fixed, the appropriate mode functions for the transformation to momentum space are no longer the usual complex phases, used with periodical boundary condition in the Fourier transformations. They are instead the real eigenfunctions $f_{\vec{k}}(\vec{n})$ of the Laplacian operator that satisfy the boundary conditions imposed on the box. In principle the field can be kept fixed at arbitrary and independent values at each one of the sites of the external border. This is the situation which is typically of interest in the classical theory, for example when we study techniques to determine the electric potential inside a box when its walls are kept at arbitrarily given values of the potential.

Another type of boundary condition of interest in the classical theory are those in which, instead of the field itself, it is the derivatives of the field that are kept at arbitrarily given values at the border. This is relevant, for example, in situations where the electric field rather than the electric potential is known at the border. The case in which the derivatives are zero at the border is also known by the name of "free" boundary conditions, since in this case we may simply eliminate form the model the values of the field at the border and the links that connect the interior to the border, which is equivalent to fixing at zero the value of the normal derivative at the border. This type of boundary condition is often used for models in statistical mechanics, which is mathematically quite similar to the quantum theory of fields, as a simpler alternative to periodic boundary conditions.

However, when we study in more detail the question of the boundary conditions in the quantum theory, later on, we will see that this type of situation is not of much interest in that case, in which the important aspects of the boundary conditions are of another nature. Since our study of fixed boundary conditions here is meant mostly at illustrating how to deal with them, we will limit ourselves here to the case of null boundary conditions, in which we make $\varphi = 0$ at all the border sites. This type of boundary condition will be of some use in the development of the quantum theory, and it can be easily generalized, in all situations of interest, to the case in which φ is kept constant at some non-zero single value over the whole border. On finite lattices, for boundary conditions $\varphi = 0$, it can easily be shown (problems 2.8.1 and 2.8.2) that the eigenfunctions of the finite-difference Laplacian which vanish at the border are given by

$$f^N_{\vec{k}}(\vec{n}) = 2^{d/2} \sin\left(\frac{\pi k_1 n_1}{N+1}\right) \ldots \sin\left(\frac{\pi k_d n_d}{N+1}\right), \tag{2.8.1}$$

where the integer coordinates $k_\mu = 1, \ldots, N$, $\mu = 1, \ldots, d$ are the coordinates that identify each one of the discrete eigenmodes of the Laplacian in momentum space.

Observe that in this case, unlike the case of periodical boundary conditions, we cannot make $k_\mu = 0$ for any value of μ, since the corresponding eigenfunction would be identically zero. Besides this, for any μ the change $k_\mu \to -k_\mu$ will only change the sign of the eigenfunction and therefore does not produce an independent eigenfunction. Due to this, we do not have here the freedom we had in the periodical case, of choosing the range of variation of k_μ, which must be as given above. This

It is also not difficult to show (problem 2.8.1) that the eigenvalues of the finite-difference Laplacian for the base of functions defined in equation (2.8.1) are given by

$$\rho_f^2 = 4\left\{\sin^2\left[\frac{\pi k_1}{2(N+1)}\right] + \ldots + \sin^2\left[\frac{\pi k_d}{2(N+1)}\right]\right\}. \tag{2.8.4}$$

Observe however that, unlike what happened in the periodical case, the functions given in (2.8.1) are *not* eigenfunctions of the finite-difference operator Δ_μ (problem 2.8.3). This is related to the fact that the finite-difference operator acts over the lattice functions as a generator of translations and, since the boundary conditions are fixed, it is not possible to execute such translations without violating the boundary conditions. As we shall see in future volumes, just as in the case of periodical boundary conditions, also in this case all quantities of physical interest on finite lattices will be functions of $\vec{k}$ *only* through the combination $\rho_f^2(\vec{k})$.

In the limit $N \to \infty$ each one of these quantities approaches the corresponding continuum-limit quantity. Assuming as always the existence of an external dimensional scale in which the side of the box is given by L, in this limit the eigenfunctions of the Laplacian are given by

$$f_{\vec{k}}(\vec{x}) = 2^{d/2}\sin\left(\frac{\pi k_1 x_1}{L}\right)\ldots\sin\left(\frac{\pi k_d x_d}{L}\right), \tag{2.8.5}$$

where $x_\mu = n_\mu a$, $a = L/(N+1)$, $n_\mu = 0, \ldots, N+1$ define the continuum coordinates x_μ within the box, which in the limit are defined in the interval $[0, L]$. These functions satisfy the orthogonality and completeness relations (problem 2.8.5)

$$\int_0^L \mathrm{d}x_1 \ldots \int_0^L \mathrm{d}x_d \; f_{\vec{k}}(\vec{x}) f_{\vec{k}'}(\vec{x}) = \delta^d(\vec{k}, \vec{k}'), \tag{2.8.6}$$

$$\sum_{\vec{k}} f_{\vec{k}}(\vec{x}) f_{\vec{k}}(\vec{x}') = V\delta^d(\vec{x} - \vec{x}'), \tag{2.8.7}$$

where the integer coordinates k_μ extend now from 1 to ∞ and $\delta^d(\vec{x}-\vec{x}')$ is the Dirac delta function in d dimensions. The eigenvalues of the Laplacian corresponding to these eigenfunctions are given (problem 2.8.5) by the limits of the quantities ρ_f^2/a^2. In the limit the values of the dimensionfull momenta are given by $p_\mu = \pi k_\mu / L$ and the eigenvalues of the Laplacian are

$$p^2 = \frac{\pi^2}{L^2}\left(k_1^2 + \ldots + k_d^2\right). \tag{2.8.8}$$

In the continuum the transformation of the field from position space to momentum space and its inverse are written as

$$\widetilde{\varphi}(\vec{k}) = \frac{1}{V}\int_V \mathrm{d}^d x f_{\vec{k}}^N(\vec{x})\varphi(\vec{x}),$$

$$\varphi(\vec{x}) = \sum_{\vec{k}} f_{\vec{k}}^N(\vec{x})\widetilde{\varphi}(\vec{k}).$$

$$\frac{1}{2}f_\kappa(0)f_{\kappa'}(0) + \sum_{n=1}^{N} f_\kappa(n)f_{\kappa'}(n) + \frac{1}{2}f_\kappa(N+1)f_{\kappa'}(N+1),$$

reflecting the fact that the sites at the border are associated to integration elements with half the volume of the integration elements associated to the internal sites.

2.8.7. ($\star$) Find, if at all possible, a subset of N of the functions given in problem 2.8.6 that is complete for the representation of functions $\varphi(n)$ of the N sites in the interior of the lattice, given two independent fixed values $\varphi(0)$ and $\varphi(N+1)$ at the two ends of the lattice[2].

2.9 Basis Transformations in Configuration Space

The whole formalism of Fourier transformation can be applied in identical form both to the dimensionless field φ and to the dimensionfull field ϕ, as well as to any other quantity of the theory that is a function of position on the lattice, whatever the boundary conditions may be. In fact, the transformation to momentum space is a fundamental operation, not only in the classical theory but in the quantum theory as well, because, as we shall see in more detail later, it corresponds to a transformation from a representation in terms of point-like quantities, whose quantum expectation values cannot be observed directly, to a representation in terms of extended quantities, whole expectation values are associated in a more direct way to the quantities that are in fact physically observable.

Any operation that is linear on the fields and that involves an integration (in the continuum case) or sum (in the discrete case) over the whole lattice, as is the case for the Fourier transforms, may be understood as a matrix multiplication operation on a vector. This is true both for periodical and for fixed boundary conditions. The Fourier transformation itself, for periodical boundary conditions, which is given by

$$\widetilde{\varphi}(\vec{k}) = \frac{1}{N^d}\sum_{\vec{n}} e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\varphi(\vec{n}),$$

may be written as a matrix operation so long as we represent the positions $\vec{n}$ of the sites by means of the index ι, as discussed in section 2.4, at the same time that we exchange the integer coordinates $\vec{k}$ of momentum space for another index κ defined in an analogous way. Once we have "piled up" in this way both the $\vec{n}$ and the $\vec{k}$ coordinates into indices of vectors of dimension N^d, we may write the transformation as

[2]Note: the answer to this problem is currently unknown.

where $I_{\iota'\iota} = \delta_{\iota'\iota}$ is the unit matrix. Again, this is just a consequence of the orthogonality and completeness relations satisfied by the mode functions. One can get the transformation to become truly unitary with the normalization

$$F^{(\mathrm{u})}_{\kappa\iota} = \frac{1}{N^{d/2}} e^{\imath \frac{2\pi}{N} \vec{k}\cdot\vec{n}}.$$

As we shall see later on, in the quantum theory it will be necessary to consider the determinant of this transformation. Since the transformation is linear its determinant is a constant, in the sense that it does not depend on the fields. One can easily show in the one-dimensional case (problem 2.9.3) that, with our usual normalization, we have

$$\det(\mathbb{F}) = \begin{cases} N^{-N/2}\ \imath^{(N+2)/2} & \text{if } N \text{ is even, and} \\ N^{-N/2}\ \imath^{(1-N)/2} & \text{if } N \text{ is odd,} \end{cases} \tag{2.9.1}$$

while for the inverse transformation we have $\det(\mathbb{F}^{-1}) = 1/\det(\mathbb{F})$, naturally. For larger dimensions the calculation is more complex but the result still has the all-important property that it does not depend on the fields.

Problems

2.9.1. Write explicitly the matrix $\mathbb{F}$ in the one-dimensional case $d = 1$ for the following lattice sizes: $N = 2$, $N = 4$ and $N = 6$. Write also the matrix for the two-dimensional case $d = 2$ with $N = 2$.

2.9.2. If $\mathbb{F}$ is the Fourier matrix with our usual normalization and $\mathbb{I}$ is the unit matrix, show that $\mathbb{F}^{-1} = N^d \mathbb{F}^\dagger$, that is, show that

$$N^d \mathbb{F}^\dagger \mathbb{F} = \mathbb{I}.$$

2.9.3. Calculate the determinant of $\mathbb{F}$ in the one-dimensional case, for an arbitrary N, obtaining the result given in equation (2.9.1).

2.9.4. ($\star$) Calculate the determinant of $\mathbb{F}$ in the two-dimensional case, for an arbitrary N.

2.10 External Sources and Green Functions

In this section we will introduce a new fundamental element, still in the context of the classical theory. This is the concept of an *external source* for the field. This new object will have great importance also in the quantum theory. In our paradigmatic

$$
\begin{aligned}
&= \left[\sum_{\ell}(\Delta_\ell\varphi)\delta(\Delta_\ell\varphi) + \alpha_0\sum_s \varphi(s)\delta\varphi(s) - \sum_s j(s)\delta\varphi(s)\right] \\
&= \sum_s\left[\sum_{\mu}(\Delta_\mu\varphi)\Delta_\mu(\delta\varphi) + \alpha_0\varphi(s)\delta\varphi(s) - j(s)\delta\varphi(s)\right] \\
&= \sum_s\left\{-\left[\Delta^2\varphi(s)\right]\delta\varphi(s) + \alpha_0\varphi(s)\delta\varphi(s) - j(s)\delta\varphi(s)\right\} \\
&= \sum_s \delta\varphi(s)\left[-\Delta^2\varphi(s) + \alpha_0\varphi(s) - j(s)\right],
\end{aligned}
$$

were we made the "integration by parts" for periodical boundary conditions as was already explained before in section 2.1. If we now impose that $\delta S_0 = 0$ for *any* $\delta\varphi(s)$, we obtain the equation of motion

$$
\begin{aligned}
-\Delta^2\varphi(s) + \alpha_0\varphi(s) - j(s) &= 0 \Rightarrow \\
\left[-\Delta^2 + \alpha_0\right]\varphi(s) &= j(s).
\end{aligned}
$$

This is the non-homogeneous version of the equation of motion obtained before for this same model, where the non-homogeneous term is the external source. We can find the general solution of this equation using the usual techniques of the theory of linear differential equations. The general solution of a non-homogeneous linear equation is always obtained as the sum of the general solution of the homogeneous equation with a particular solution of the non-homogeneous equation. However, we are not interested here in writing explicitly the general solution, but rather in finding the solution for the particular type of boundary condition that we adopted. This solution can be obtained by the use of the finite Fourier transforms. In order to do this, we write the field and the external source in terms of their Fourier transforms as

$$
\begin{aligned}
\varphi(\vec{n}) &= \sum_{\vec{k}} e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\widetilde{\varphi}(\vec{k}), \\
j(\vec{n}) &= \sum_{\vec{k}} e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\widetilde{\jmath}(\vec{k}).
\end{aligned}
$$

The substitution of these expressions in the equation of motion (2.1.3) result in

$$
\sum_{\vec{k}}\widetilde{\varphi}(\vec{k})(-\Delta^2 + \alpha_0)e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}} = \sum_{\vec{k}} e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\widetilde{\jmath}(\vec{k}).
$$

Since the exponentials are eigenfunctions of the Laplacian with eigenvalues given by $-\rho^2(\vec{k})$, as we saw in equation (2.7.2), we obtain

$$
\sum_{\vec{k}} e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\left\{\widetilde{\varphi}(\vec{k})\left[\rho^2(\vec{k}) + \alpha_0\right] - \widetilde{\jmath}(\vec{k})\right\} = 0.
$$

We may simplify a little these expressions by choosing the position $\vec{n}' = \vec{0}$ for the point source, which can always be done by means of an adequate choice of the intervals of variation of the integer coordinates of the sites. These solutions represent the response of the system to the presence of a point source. The function of the momenta that appears in these solutions,

$$\widetilde{g}(\vec{k}) \equiv \frac{1}{N^d \left[\rho^2(\vec{k}) + \alpha_0\right]},$$

is called the *propagator* or the *Green function* of the system, written in momentum space. Its finite inverse Fourier transform, which can be written as

$$g(\vec{n} - \vec{n}') = \sum_{\vec{k}} \frac{1}{N^d \left[\rho^2(\vec{k}) + \alpha_0\right]} e^{-\imath \frac{2\pi}{N} \vec{k} \cdot (\vec{n} - \vec{n}')},$$

is the Green function in position space, the response of the theory to the presence of a unit point source, with $j_0 = 1$. Observe that this is a kind of double inverse transform, where the two factors $\exp(-\imath 2\pi \vec{k} \cdot \vec{n}/N)$ and $\exp(\imath 2\pi \vec{k} \cdot \vec{n}'/N)$ appear, since in general the function g is a function of two points, $g(\vec{n}, \vec{n}')$. The fact that g is a function only of the difference $\vec{n} - \vec{n}'$ is a specific property of the periodical boundary conditions, for which we have discrete translation invariance on the lattice. These lattice versions of the Green functions are both dimensionless. Our solutions for the point charge may now be written as

$$\begin{aligned} \widetilde{\varphi}(\vec{k}) &= j_0 \widetilde{g}(\vec{k}) e^{\imath \frac{2\pi}{N} \vec{k} \cdot \vec{n}'}, \\ \varphi(\vec{n}) &= j_0 g(\vec{n} - \vec{n}'), \end{aligned}$$

which, for $\vec{n}' = \vec{0}$, simplify to

$$\begin{aligned} \widetilde{\varphi}(\vec{k}) &= j_0 \widetilde{g}(\vec{k}), \\ \varphi(\vec{n}) &= j_0 g(\vec{n}). \end{aligned}$$

In addition to this, the solution for an arbitrary external source in momentum space may now be written as

$$\widetilde{\varphi}(\vec{k}) = N^d \widetilde{j}(\vec{k}) \widetilde{g}(\vec{k}), \tag{2.10.2}$$

and the corresponding solution in position space, with a little more work (problem 2.10.3) and the use of the orthogonality and completeness relations, as

$$\varphi(\vec{n}) = \sum_{\vec{n}'} j(\vec{n}') g(\vec{n} - \vec{n}'). \tag{2.10.3}$$

Let us consider quickly the continuum limit of this expression. It is easy to verify (problem 2.10.4) that, in order for the complete action in the continuum limit to be written as

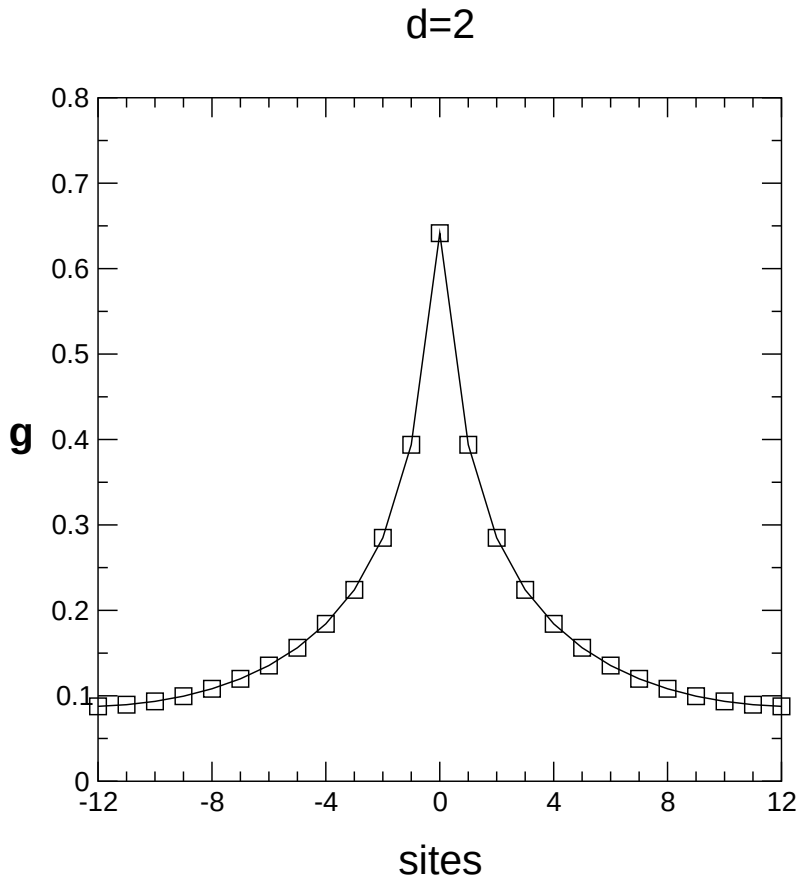


Figure 2.10.2: Periodical Green function in the case $d = 2$.

the solution in the presence of an arbitrary external source in terms of the Green function becomes, in the continuum limit,

$$\phi(\vec{x}) = \int \mathrm{d}^d x \; J(\vec{x}')G(\vec{x} - \vec{x}'). \tag{2.10.5}$$

We see therefore that G is in fact the Green function of the non-homogeneous equation of motion in the usual sense in which the term is used in the theory of linear differential equations. Note that, due to the existence of a zero mode on the torus, for which $\rho^2 = 0$, this Green function is well defined only if $\alpha_0 > 0$.

We may acquire an intuitive idea of how the response of the system to the presence of a point source looks, in position space, drawing a few graphs of this function around the point where the external point source is located. Figure 2.10.1 shows the function g for dimension $d = 1$, mass parameter $\alpha_0 = 3$ and external source $j_0 = 1$ on a lattice with $N = 25$. We see here that the field assumes non-zero values along all the lattice, with a maximum at the position of the source. This is the solution which we denominate qualitatively as the "circus tent", given its form. The same happens in larger dimensions. A similar example for $d = 2$ can be found

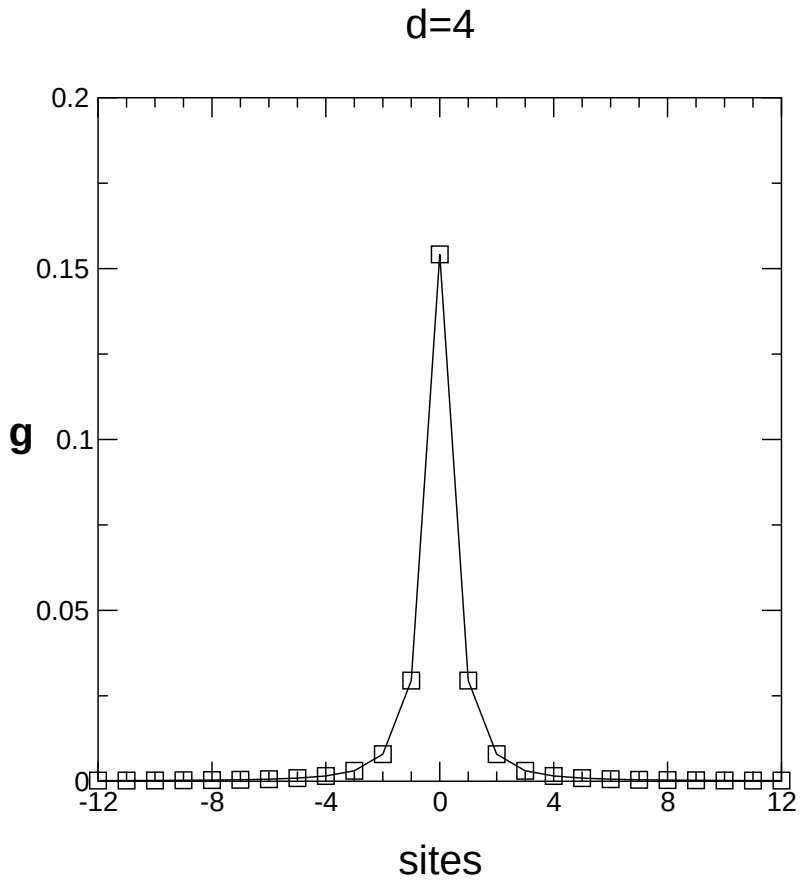


Figure 2.10.4: Periodical Green function in the case $d = 4$.

proportional to its magnitude and, in general, a finite range. This range depends on α_0, as one can verify by drawing other graphs of the functions (problem 2.10.6), a fact that will be of great importance in the quantum theory.

Problems

2.10.1. Show that, on a finite lattice with periodical boundary conditions and a constant external source j_0, the minimum value of the action $S_0[\varphi]$ is achieved for a field $\varphi(s) = \varphi_0$, which is constant over the whole lattice.

2.10.2. ($\star$) Show that the action $S_0[\varphi]$ given in equation (2.10.1) has a lower bound, for any finite external source j, so long as $\alpha_0 > 0$. In order to do this, write the action in terms of the Fourier transforms $\widetilde{\varphi}(\vec{k})$ of the field and $\widetilde{\jmath}(\vec{k})$ of the external source, then complete a square in order to show that the dependence on the field is contained solely within a manifestly positive term of the resulting expression for the action. Determine also the value of the lower bound as a function of the external source.

$$\begin{aligned}\varphi(\vec{n}) &= \sum_{\vec{k}} f^N_{\vec{k}}(\vec{n})\widetilde{\varphi}(\vec{k}),\\ j(\vec{n}) &= \sum_{\vec{k}} f^N_{\vec{k}}(\vec{n})\widetilde{\jmath}(\vec{k}).\end{aligned}$$

Substituting these expressions in (2.11.1) we have

$$(-\Delta^2+\alpha_0)\sum_{\vec{k}} f^N_{\vec{k}}(\vec{n})\widetilde{\varphi}(\vec{k}) = \sum_{\vec{k}} f^N_{\vec{k}}(\vec{n})\widetilde{\jmath}(\vec{k}).$$

Since the functions $f^N_{\vec{k}}(\vec{n})$ are eigenvectors of the Laplacian with eigenvalues $-\rho_f^2$, we have

$$\sum_{\vec{k}} f^N_{\vec{k}}(\vec{n})\left[\widetilde{\varphi}(\vec{k})(\rho_f^2+\alpha_0)-\widetilde{\jmath}(\vec{k})\right]=0.$$

We see therefore that, once more, the differential equation reduces to an algebraic equation for the components of the field in momentum space, in fact, the very *same* equation we had before,

$$\widetilde{\varphi}(\vec{k})\left[\rho_f^2(\vec{k})+\alpha_0\right]=\widetilde{\jmath}(\vec{k}),$$

the sole difference being that both the transforms and the eigenvalues ρ_f^2 relate now to the eigenfunctions of the Laplacian with fixed boundary condition. We have now solutions that are similar to the ones we had before,

$$\begin{aligned}\widetilde{\varphi}(\vec{k}) &= \frac{\widetilde{\jmath}(\vec{k})}{\rho_f^2(\vec{k})+\alpha_0},\\ \varphi(\vec{n}) &= \sum_{\vec{k}} f^N_{\vec{k}}(\vec{n})\frac{\widetilde{\jmath}(\vec{k})}{\rho_f^2(\vec{k})+\alpha_0}.\end{aligned}$$

For the case of the point source we have for the external source and its transform

$$\begin{aligned}j(\vec{n}) &= j_0\delta^d(\vec{n},\vec{n}'),\\ \widetilde{\jmath}(\vec{k}) &= \frac{1}{(N+1)^d}\sum_{\vec{n}} f^N_{\vec{k}}(\vec{n})j_0\delta^d(\vec{n},\vec{n}')\\ &= \frac{j_0}{(N+1)^d}f^N_{\vec{k}}(\vec{n}'),\end{aligned}$$

which implies that the solutions of the classical theory may be written as

$$\begin{aligned}\widetilde{\varphi}(\vec{k}) &= j_0\widetilde{g}_f(\vec{k})f^N_{\vec{k}}(\vec{n}'),\\ \varphi(\vec{n}) &= j_0\sum_{\vec{k}}\widetilde{g}_f(\vec{k})f^N_{\vec{k}}(\vec{n}')f^N_{\vec{k}}(\vec{n}),\end{aligned}$$

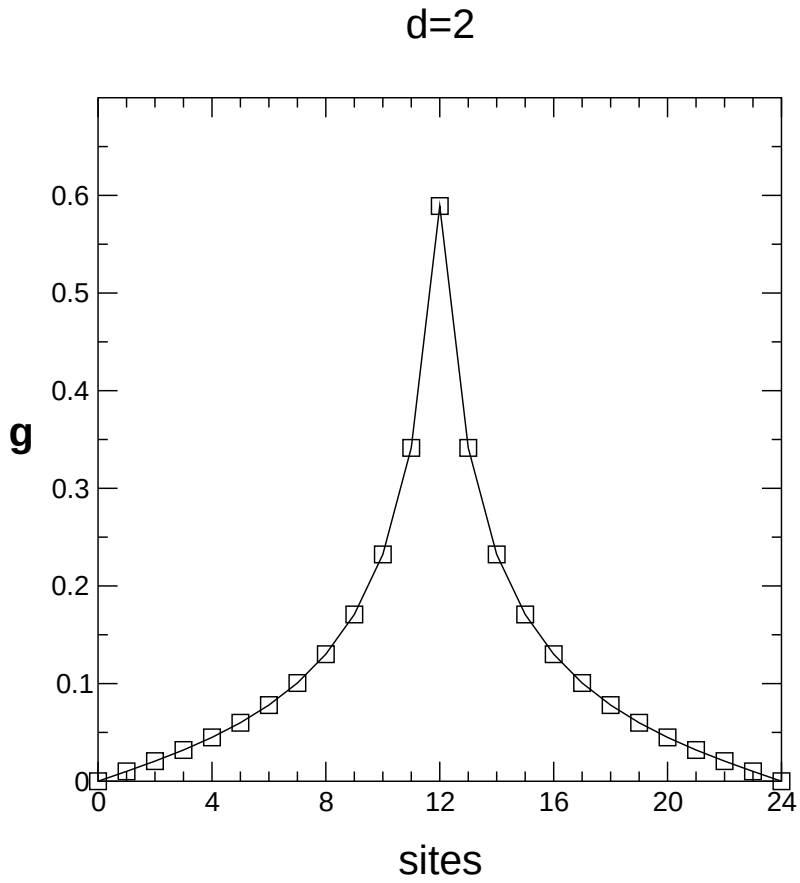


Figure 2.11.2: Green function with fixed boundary conditions for $d = 2$.

$$\varphi(\vec{n}) = \sum_{\vec{n}'} j(\vec{n}') g_f(\vec{n}, \vec{n}').$$

The expression for the Green function in position space may be somewhat simplified if we choose the position of the source right in the middle of the lattice, so that $n' = (N+1)/2$, which can be done without difficulty for the case of odd N. In figures from 2.11.1 to 2.11.4 we show the Green function on a lattice with $N = 23$ and this value of n', in dimensions from 1 to 4. As one can see, the behavior is similar to that of the case of periodical boundary conditions, with the exception that in our case here the functions are always zero at the boundary.

Using the usual rescalings of all quantities in terms of the lattice spacing a, we may write dimensionfull versions of all these quantities. As before, we define the dimensionfull version $\widetilde{G}_f$ in momentum space as $\widetilde{G}_f = a^{2-d}\widetilde{g}_f$, resulting in

$$\widetilde{G}_f(\vec{k}) = \frac{1}{L^d \left[\rho_f^2(\vec{k})/a^2 + \alpha_0/a^2\right]},$$

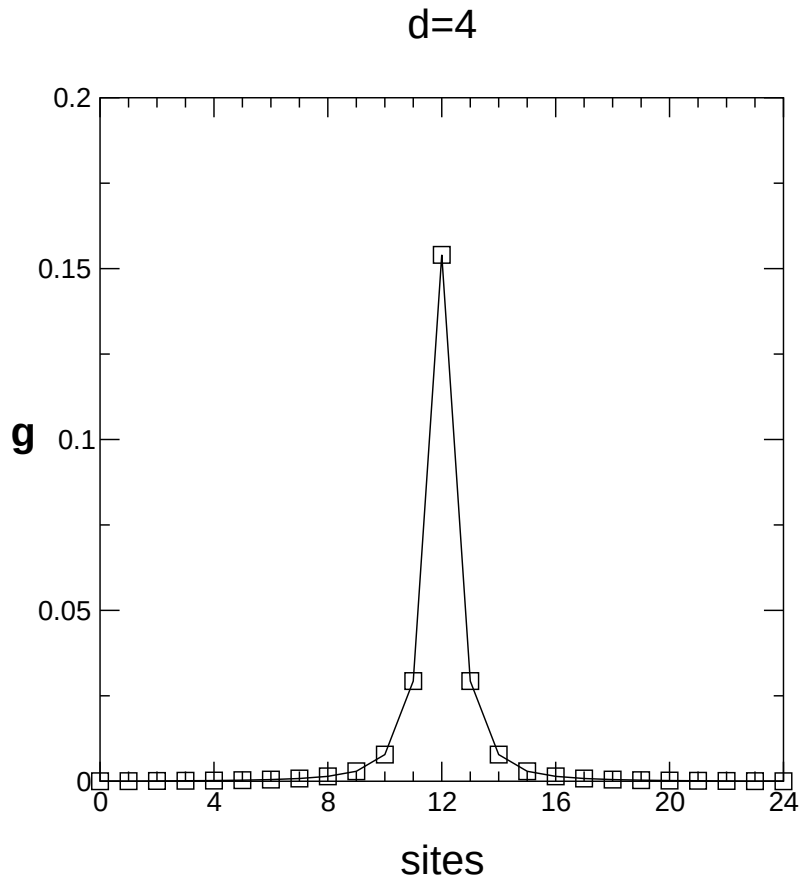


Figure 2.11.4: Green function with fixed boundary conditions for $d = 4$.

we go to infinite space. This fact will be of particular importance for the correlation functions to be defined in the quantum theory, of which the Green function discussed here is an example.

Clearly, despite the fact that the imposition of the condition $\varphi = 0$ at the border changes the detailed form of the results of the theory in position space, both on finite lattices and in the continuum limit inside a finite box, it does not prevent us from seeing the basic structure of the continuum theory in infinite space, so long as we use the representation of the theory in momentum space, when we deal with the theory on finite lattices. In addition to this, the fact that the Green function is a function of the coordinates k_μ only through the combination $\rho_f^2(\vec{k})$ is clearly related to the underlying rotational invariance of the Euclidean theory in infinite space which, in this form, may be indirectly detected from within a finite continuous box or even from within the confines of a discrete lattice. These two properties allow us to treat models in a very specific and practical way, in any particular set of boxes and lattices that we may be using, without loosing sight of the invariances that the theory should have when one goes to infinite continuous space.

Chapter 3

Quantum Field Theory

In this chapter the basic definition of the quantum theory of fields will be presented, following what are essentially traditional lines. The point of view adopted here regarding the nature of the quantum theory is essentially the traditional one, on a conceptual level, although the mathematical tools used are not those commonly employed in the usual presentation of the subject. It is important to point out that this point of view is provisional, and will have to be changed, to some extent, later on.

Later analysis will show that this definition is not complete, due to the fundamental difficulties in dealing with the concepts of the physical observables and of the process of measurement, within the structure of the theory. Due to this some of the statements made here are provisional and will have to be somewhat changed later, such as the statement that the set of n-point correlation functions of a model determine all the physics of the model, which is a standard point of view of the traditional approach to the subject.

The formal relation of the theory with the mathematical structure of the statistical mechanics of lattice systems will be pointed out. A detailed mathematical development leading to the tools needed for the solution of the Gaussian model will be presented. This simple model will be solved in detail, including a complete discussion of its correlation functions. The same tools and ideas used here in the solution of this model will also be of much use in the future, for dealing with more complex models by means of approximative schemes such as perturbation theory, the mean-field method and the Gaussian approximation.

The introduction of external sources in the quantum theory will also be discussed in detail. These sources are interpreted as representations of classical objects within the theory, and will lead to the concept of the functional generators of the correlation functions, and ultimately to the important concept of the effective action. Unlike the usual treatment, all these objects will be defined directly on the Euclidean lattice. The physical interpretation of the effective action, as well as its relation to the classical limit of the theory, will be discussed in detail.

The main objective of this chapter is to establish that the quantum theory of fields can be defined and analyzed on the Euclidean lattice on essentially traditional

For example, in the case of the free scalar field we have for these factors

$$e^{-S_0[\varphi]}.$$

The set of field configurations with these associated probabilities is referred to as the *ensemble* of configurations or as the *distribution* of configurations of the model. The definition would be the same for any other model, with any number and types of fields, defined by some action functional S. Given a certain functional $\mathcal{O}[\varphi]$ of the field, the *expectation value* of the observable associated to it on a lattice of size N is defined as the average

$$\langle \mathcal{O} \rangle_N = \frac{\displaystyle\int_{-\infty}^{\infty} \prod_s \mathrm{d}\varphi(s)\ \mathcal{O}[\varphi]\ e^{-S_0[\varphi]}}{\displaystyle\int_{-\infty}^{\infty} \prod_s \mathrm{d}\varphi(s)\ e^{-S_0[\varphi]}}, \tag{3.1.1}$$

where the integration element is

$$\prod_s \mathrm{d}\varphi(s) = \prod_{n_1=1}^{N} \ldots \prod_{n_d=1}^{N} \mathrm{d}\varphi(\vec{n})$$

and the integral extends over all possible values of the field, on all the sites. In our case here, the value of the field at each site ranges over the whole real line. This is a ratio of two multiple integrals of large but finite dimension, being therefore a well-defined and familiar mathematical object. The conditions imposed before on the action and the fact that it appears as the argument of a decreasing exponential imply that, for all reasonably well-behaved functionals $\mathcal{O}$, we do not need to worry about the convergence of such integrals on finite lattices. We see now that the conditions imposed on $S[\varphi]$ so that it may be used in the role of an action functional have the objective of making sure that these integral exist for a large set of observables, including those of physical interest for the theory of fields. From now on we will simplify a little the notation of these integrals, denoting $\prod_s \mathrm{d}\varphi(s)$ simply by $[\mathbf{d}\varphi]$. In more general cases, in which the field may have several components, this notation will refer to the integration over all independent field components at all the sites. For example, if we have a field $\vec{\varphi}$ with several components φ_i, the complete definition would be

$$[\mathbf{d}\varphi] \equiv \prod_s \prod_i \mathrm{d}\varphi_i(s).$$

Usually we will also omit the extremes of integration, since it is always understood that the integrals extend over the full image of the field functions. The structure including the functional integration element and the distribution of statistical weights, in which the observable is integrated in order to produce the expectation value,

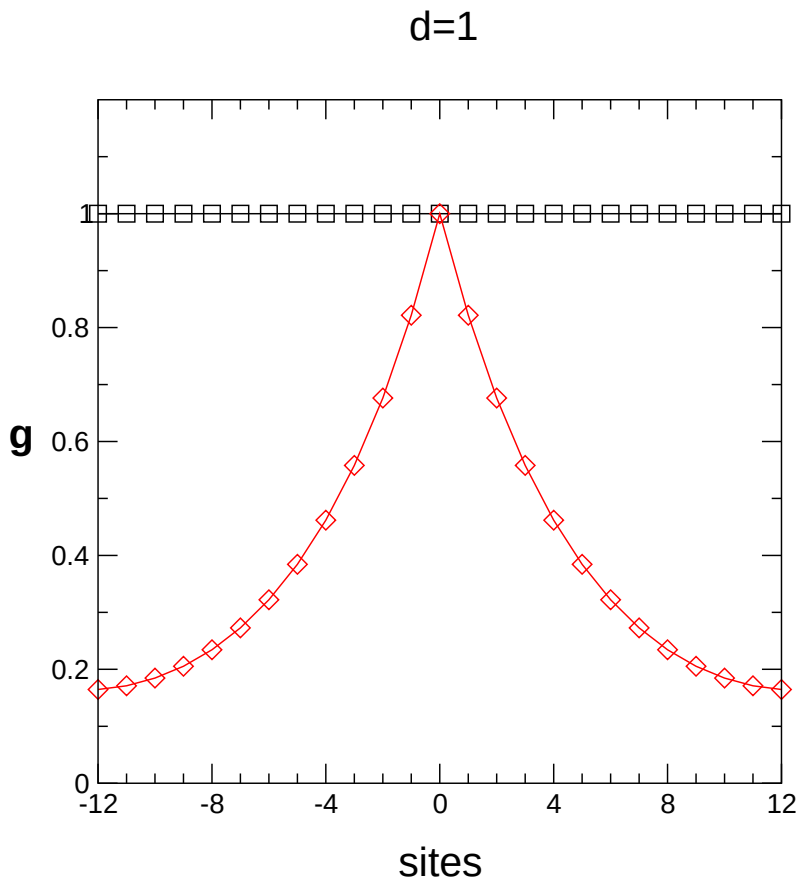


Figure 3.1.1: Periodical two-point correlation functions for $d = 1$.

role to play in a future volume, when we discuss the phenomenon of *spontaneous symmetry breaking*.

The two-point function $\langle\varphi(s_1)\varphi(s_2)\rangle$, which we will also call the *propagator* of the theory, has a particularly important role to play. It is the simplest observable that gives us relations between different sites of the lattice, which may be arbitrarily distant from one another. Hence, it is the simplest observable by means of which we may look at *propagation* phenomena along the lattice. As we shall see later on in specific examples, in general this function decreases when we increase the distance between the two sites involved, measured in discrete terms, that is, in terms of the minimum number of links that it is necessary to cross in order to go from one site to the other. We say that the two-point function measures the *correlations* between the values of the field associated to the two sites, and that these correlations *decay* with the distance along the lattice.

This decaying behavior of the two-point function may be, in general, of one of two different types, polynomial or exponential. If the decay is polynomial we say that there are in the model correlations with an infinite range, and that it does not establish a scale of distances. However, if the decay is exponential, then the rate of

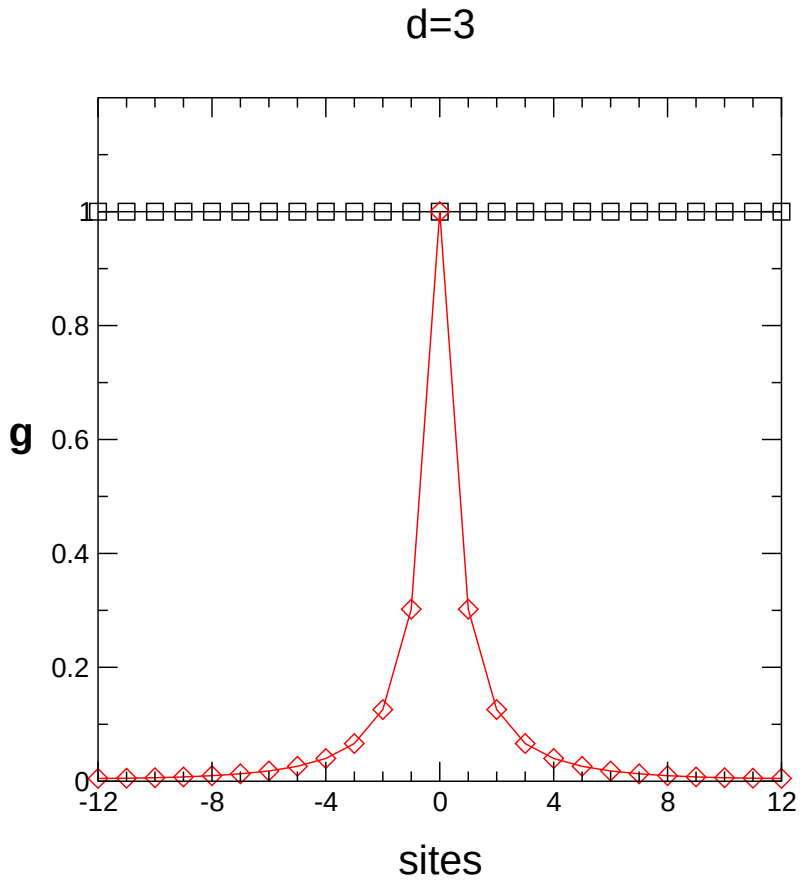


Figure 3.1.3: Periodical two-point correlation functions for $d = 3$.

$\alpha_0 = 10^{-66}$ to illustrate the polynomial decay because, due to the existence of a zero mode on the torus, we cannot use the value zero for α_0. Later on we will discuss how to make such calculations.

One can show that in $d = 1$ the quantum theory of fields defined by S_0 is formally identical to the quantum mechanics of the harmonic oscillator (problem 3.1.2). However, the situation with the correlations in larger dimensions is similar to this one. A similar example with $d = 2$ can be found in figure 3.1.2, for the same value of N, where the same values of the parameter α_0, and hence of the range of the correlations, were used. The difference between the two correlation functions is a bit more pronounced in this case, and it becomes even bigger in larger dimensions. In the graphs contained in figures 3.1.3 and 3.1.4 one can see similar examples for $d = 3$ and $d = 4$. Note the clear similarity of these graphs with the graphs of the Green functions of the classical theory, which were examined in section 2.10. In fact, as we shall see later on, in the free theory the two-point correlation function is always equal to the Green function of the classical theory, in any dimension.

We will refer to this distance, within which the correlations are appreciable, as the *range* of the correlations or as the *correlation length*. If the decay of the two-

states and what are their properties, in short, all the elements needed to determine both the nature of the structure of matter and the nature of the physical interactions among the elementary entities of which it is composed. Another correlation function of particular importance, besides the propagator, is the four-point function, because it will be related to the existence or not of *interactions* among particles within the theory. For the time being we cannot give examples of this, because the free theory we are using as an example, exactly because it is a theory of free fields, does not contain interactions between particles. This means that we may calculate the four-point function in this model, but it will decompose into sums of products of pairs of two-point functions. Later on we will present a complete analysis of the structure of the correlation functions in the free theory.

Having defined the quantum theory of our model on each finite lattice, we are now in a position to define completely the quantum field theory associated to this action, in the continuum limit. Since it is the n-point functions that define the physics of the model, it would suffice to define them in this limit, but we can do this in a somewhat more general form, for an arbitrary observable. We say then that the values of all observables of the quantum field theory in the continuum limit are the values obtained by means of the limits

$$\langle \mathcal{O}[\varphi] \rangle = \lim_{N \to \infty} \langle \mathcal{O}[\varphi] \rangle_N .$$

To solve exactly a quantum field theory means to manage to calculate exactly these limits for all observables of physical interest. The quantum theory of the model in question will be well-defined if these limits exist and are finite. Note that it is not necessary that the limits be finite for all possible observables, but only for that set, say the n-point functions, that define completely the physics of the model. In addition to this, we will see later on that, in order for these limits to exist and have acceptable physical properties, in general it is necessary to impose additional conditions on the dimensionless parameters that appear in the model, regarding their behavior in the limit.

One of the especially important conditions to satisfy in the continuum limit is that the *correlation length* of the model have a non-zero limit, because otherwise we would have no correlations at all left in the theory after the limit, which would thus become physically meaningless. A zero correlation length in the limit corresponds to the existence of particles with infinite physical mass m, a case in which there is no possibility of propagation in the theory, since the movement of such particles would require infinite energy. Usually we will impose that at least one of the correlation lengths of the model have a finite and non-zero limit, since it should define in the limit the physical scale associated to the intrinsic system of physical units on the theory. All other correlation lengths must be non-zero (but possibly infinite) in the limit. In order to put it in a more precise way, if ξ is the dimensionless correlation length and $\chi = a\xi = 1/m$ the corresponding dimensionfull correlation length, in general we will impose that, in the limit, the ratio χ/L have a finite and non-zero limit, or at least that the ratio a/χ go to zero in the limit, characterizing it as a continuum limit.

ematical structure of the theory correspond to observables. In fact, the definition of physical observable as statistical averages given here should be understood as a provisional definition. While all physical observables must be statistical averages of functionals of the fields as defined here, not all the possible statistical averages of functionals of the fields will be interpretable as physical observables. For example, although statistical averages of functionals of the field, $\langle \mathcal{O}[\varphi] \rangle$, may be observables according to our provisional definition, the field φ itself is *not* an observable. The field is a random variable whose fluctuations constitute a representation within the theory of the uncertainty principle or, to put it in a more general form, of the observability limits of nature.

These fluctuations behave exactly like thermal fluctuations in statistical mechanics, but their physical interpretation is completely different. The real quantum fluctuations of the theory are those that can be observed on the expectation values of superpositions of the fields within finite boxes with non-zero extension in all dimensions of space-time, measured in successive times. These *block variables* are very important for the physical interpretation of the theory, as we shall see in the next chapter. They are related to additional restrictions on the nature of the quantities that can be associated to observables of the theory. As we shall see later on, only variables associated to superpositions within these blocks can in fact be observed. Note that the Fourier transforms may be understood as a kind of weighted average over the whole lattice, hence characterizing them as a certain type of block variable. Therefore, the Fourier components of the fields are related in a more direct way with the physical observables of the theory.

The content of the remaining part of this book may be classified in a rough way as composed of two main parts. From the mathematical point of view it consists of the discussion and development of methods and means of calculation of these ratios between multiple integrals. From the physical point of view it consists of the development of the physical interpretation of the elements of this mathematical structure. In the remainder of this chapter the mathematical aspects will be addressed, which will enable us to review the interpretation of the structure on the next chapter. In future volumes we intend to consider the extension of these ideas to other types of fields and will examine other quantum-field-theoretical models.

Problems

3.1.1. Show that in the theory of the free scalar field defined by S_0 the expectation value of the field $\varphi(s_0)$ at an arbitrary site s_0 is zero. Use symmetry and parity arguments to evaluate the necessary functional integrals, in particular the fact that the action S_0 is invariant by changes of sign of the field, $\varphi \to -\varphi$, when these are made in an homogeneous way over the whole lattice.

3.1.2. Starting from the action S_0 for the free scalar field in one dimension in the continuum limit,

an analogy with respect to the physical aspects of the theory, however this analogy is extremely useful as a guide for our physical intuition within quantum field theory. Often concepts of statistical mechanics find use in quantum field theory and their nomenclature is used for the corresponding mathematical elements in that theory, but we should not loose sight of the great differences of physical interpretation that exist between the two theories.

We will make here a few comparisons between terms and concepts of each theory, relating each element of our structure to the corresponding elements of statistical mechanics. We will also point out the main differences of interpretation between the two theories, in addition to introducing some concepts that are of great importance and usefulness. Without intending to develop the subject in detail or to show objective evidences of the facts mentioned, we will try to describe the main facts relating to the aspects of statistical mechanics that are most important for quantum field theory, specially those related to the phenomenology of systems that display phase transitions and critical behavior.

In statistical mechanics the lattice usually represents some real crystalline structure, which implies, in particular, that in this case there is a natural length scale in the system, defined by the lattice spacing of this crystalline structure as measured in terms of the atomic and molecular parameters of matter. The paradigmatic topic for the use of the lattice in statistical mechanics is the study of crystalline substances with magnetic properties. In this case the fields $\varphi(s)$ associated to each site are representations of the *spins* of the components of matter, and of their magnetic moments. In this context the quantity that plays the role of the action is the energy, represented by the Hamiltonian function H of the system of spins, the relative statistical weights being given by the usual Boltzmann distribution $\exp(-\beta H[\varphi])$, where $\beta = 1/(kT)$ is the usual factor involving the temperature T of the system. A simple model that is very popular for this type of study is the Ising model, in which we have at each site a one-dimensional spin φ that can assume only two discrete values, 1 and -1. The energy of the system is given by

$$H[\varphi] = -\sum_{\ell} \varphi_{(-)}\varphi_{(+)} - j\sum_{s} \varphi(s).$$

In future volumes we will see that there are indeed close relations between this model and the models of scalar fields in quantum field theory. Observe that this Hamiltonian causes it to be energetically favorable for neighboring spins to have the same sign, that is, for them to align with each other. The denominator that appears in (3.1.1) corresponds in this case to the partition function of the statistical model,

$$Z = \sum_{\mathcal{C}} e^{-\beta H[\varphi]},$$

where the indicated sum is over all the *configurations* $\mathcal{C}$ of the system, that is, all possible combinations of 1 or -1 at all the sites of the lattice. This model was created and is widely used for the study of *critical phenomena* in statistical mechanics, which are associated to *phase transitions* in the materials. Processes such as the boiling

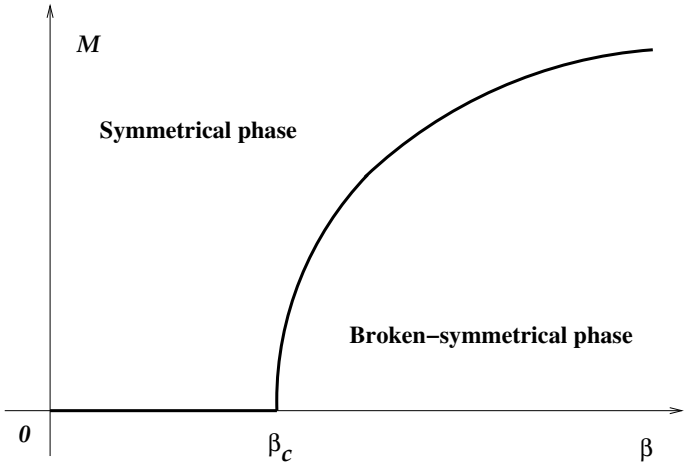


Figure 3.2.1: Qualitative diagram of the magnetization as a function of β.

the variables are discrete, but all the fundamental facts relative to the behavior close to the critical point are similar. First, we define a quantity $\vec{M}$, which we refer to here as the magnetization, which is simply the sum of all spins,

$$\vec{M} = \sum_s \vec{\varphi}(s).$$

In the case of the quantum theory of fields, we would be more interested in the average value of the fields over the lattice,

$$\overline{\vec{\varphi}} = \frac{1}{N^d} \sum_s \vec{\varphi}(s),$$

which is basically the same quantity with a different normalization. We say that the modulus of the average value of $\vec{M}$ is the *order parameter* of the system, because its behavior characterizes the two phases in which the system can exist. For high temperatures T, that is, for small β, the model has a phase that is denominated *symmetrical* or *disordered* and that is characterized by the value

$$M = |\langle \vec{M} \rangle| = 0$$

for the quantity shown, which we name the scalar magnetization M, where the statistical average is defined by

$$\langle \vec{M} \rangle = \frac{\displaystyle\int_{S_{(2)}} [\mathbf{d}\sigma]\ \vec{M}\ e^{-\beta H[\vec{\varphi}]}}{\displaystyle\int_{S_{(2)}} [\mathbf{d}\sigma]\ e^{-\beta H[\vec{\varphi}]}}.$$

For low temperatures T and hence large β the model has an *ordered* or *broken-symmetrical* phase, in which $M \neq 0$. These two regions of values of T are separated

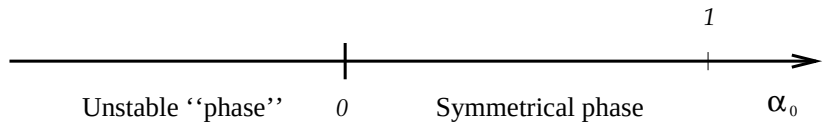


Figure 3.2.2: Critical diagram for the theory of the free field.

speaking, because the model only exists at all in one of the two regions of the α_0 real line separated by the critical value, the half-axis in which $\alpha_0 > 0$. In the other half-axis the model is unstable, in the sense that in this region it is not possible to define it by means of the Euclidean lattice as we did here. We may denominate this region as the *unstable "phase"*, a name that comes from the fact that the computer simulations, that one may try to execute in this region, are in fact unstable, making the dimensionless fields φ diverge randomly to infinity. The phase that does exist is denominated "symmetrical phase" for reasons the will become clear in future volumes when we examine the polynomial models of scalar fields. We can represent all this situation by means of a *critical diagram* like the one in figure 3.2.2, as we will do in future volumes for less trivial models than this one. In statistical mechanics the free theory is called the *Gaussian model* and the critical point $\alpha_0 = 0$ is called the *Gaussian critical point*.

One of the most fundamental differences between statistical mechanics and quantum field theory relates to the types of limits that are of interest in each case. In both cases we are interested in the limit $N \to \infty$, but in statistical mechanics this limit is taken in a way that does not characterize it as a continuum limit, but rather as the thermodynamical limit in which we make the volume of the system tend to infinity. This is due to the fact that in this case the lattice spacing a does not go to zero, but instead of this is kept constant, which implies that the size L of the box must become infinite in the limit. This is the limit that corresponds to the study of macroscopic samples of materials whose structure is a lattice at the atomic level, where the lattice spacing a establishes the physically relevant scale. In the case of quantum field theory we may either make the volume tend to infinity or keep it finite, but what is important is that in either case the lattice spacing a be made to go to zero in comparison to the length scales that are relevant to the physics of the model. Hence, when we consider some finite and non-zero length in the case of statistical mechanics, it will always correspond to a *finite* number of consecutive links. In quantum field theory a finite and non-zero length will always correspond to an *infinite* number of consecutive links. This difference regarding the nature of the limits is one of the main conceptual differences between statistical mechanics and quantum field theory.

In these statistical systems we may define a function, which we will call the *correlation function*, that measures the range of the correlations among the spins at the various sites, as a function of the distances among them. Assuming that the model is such that the averages of the variables φ at the sites are zero, $\langle\varphi\rangle = 0$, while the variables undergo statistical fluctuations with a certain characteristic magnitude around this value, we may define this function, relating two sites s_1 e s_2, as

where $\mathfrak{f}_0$ and r_0 are positive constants and p is a positive integer or half-integer power. The constant r_0 defines the range of the correlations, since for $r < r_0$ there will be appreciable correlations, while for $r > r_0$ the correlations vanish very quickly. We call r_0 the *correlation length* of the statistical system. As measured here, in terms of number of links and therefore using as the unit of length the lattice spacing a, this is the correlation length of interest for statistical mechanics. The statistical systems that display second-order critical behavior are characterized by the fact that the correlation length r_0 goes to infinity when we approach the critical point, which means that $\mathfrak{f}(r)$ ceases to display an exponential decay and acquires a polynomial decay at this point. We say then that the system has acquired long-range order. In these systems the exponential decay of $\mathfrak{f}(r)$ is characteristic of the symmetrical or disordered phases, while the polynomial decay is characteristic of the broken-symmetrical or ordered phases. In the context of quantum field theory, on the other hand, a r_0 that is a finite multiple of the lattice spacing a represents a correlation length that goes to zero in the continuum limit, because by definition a goes to zero in this limit. Hence, in the quantum theory only the situation in which r_0 tends to infinity in terms of a are of any interest. It is due to this that in the quantum theory of fields we are interested only in the critical points, which are the points where r_0 behaves in this way.

We close with an observation regarding the concept of temperature in the context of quantum field theory. Observe that the statistical-mechanic quantity that really corresponds to the action S of quantum field theory is the product βH. In many important models such as, for example, the gauge theories, it is possible to change variables in the action so that it ends up multiplied by a parameter such as this β. In these models we tend to refer to this parameter as the inverse of a temperature, since the analogy with the temperature of statistical mechanics is very useful to guide our intuition regarding the statistical inner workings of the model. However, it is necessary to emphasize that this parameter is in no way related to the thermodynamical temperature of the physical system described by the model defined by S. Usually the parameter is related to what we call the non-renormalized or bare coupling constant of the theory, and not to the true physical temperature. Of course there is a concept of thermodynamical temperature that can be defined as part of our models of quantum field theory, but it is not related to this parameter and it is important to keep in mind a clear distinction between the two concepts, since one involves the real thermodynamical temperature and the other is only a very useful mathematical analogy.

Problems

3.2.1. Consider the Ising model in one dimension, as defined in the text, on finite lattices of size N. Write a program to calculate directly, summing over all possible configurations, the quantities $M = |\langle \vec{M} \rangle|$ and $M' = \langle |\vec{M}| \rangle$, given a value of β. Plot M and M' as functions of β for a few values of N, up to the

$$\begin{aligned} I_0^2(\alpha) &= 2\pi \int_0^\infty \mathrm{d}r\ r\ e^{-\alpha r^2} \\ &= 2\pi \left(\frac{-1}{2\alpha}\right) e^{-\alpha r^2} \Big[_0^\infty \\ &= \pi \frac{1}{\alpha}, \end{aligned}$$

so that the original integral is

$$I_0(\alpha) = \sqrt{\frac{\pi}{\alpha}}.$$

This result can be generalized to integral of products of polynomials with the Gaussian exponential. First of all, one can see that integrals involving odd powers of x are zero by means of symmetry arguments, because in this case the integrand is an odd function and the domain of integration is symmetrical. If $i \geq 0$ is a non-negative integer,

$$I_{2i+1}(\alpha) = \int_{-\infty}^{\infty} \mathrm{d}x\ x^{2i+1} g(x) \equiv 0.$$

If we have even powers of x, we can derive the integrals I_{2i} successively starting from our result for I_0. For example we have, differentiating the original expression for I_0 with respect to α,

$$\partial_\alpha I_0(\alpha) = \int_{-\infty}^{\infty} \mathrm{d}x\ \partial_\alpha e^{-\alpha x^2} = -\int_{-\infty}^{\infty} \mathrm{d}x\ x^2\ e^{-\alpha x^2} = -I_2(\alpha),$$

while, differentiating in the same way the explicit result that we obtained, we have

$$\partial_\alpha I_0(\alpha) = \sqrt{\pi} \left(-\frac{1}{2}\right) \sqrt{\frac{1}{\alpha}}^3.$$

Comparing these two expressions we obtain the result for I_2,

$$I_2(\alpha) = \frac{\sqrt{\pi}}{2} \sqrt{\frac{1}{\alpha}}^3.$$

This procedure can now be iterated in order to obtain the general result for I_{2i},

$$I_{2i} = \sqrt{\pi} \frac{(2i-1)!!}{2^i} \sqrt{\frac{1}{\alpha}}^{(2i+1)}.$$

Another kind of generalization in which we are interested is the one for integrals in larger dimensions. Assuming that we have n real variables x_i with $i = 1, \ldots, n$, in this case the form of the argument of the exponential will be that of a quadratic form $\mathbb{Q}$ with coefficients Q_{ij}, and the integral will be written as

$$S_0[\varphi] = \frac{1}{2}\sum_{\vec{n}}\left\{\sum_{\mu}[\Delta_\mu\varphi(\vec{n})]^2 + \alpha_0\varphi^2(\vec{n})\right\}.$$

Writing the field in terms of its Fourier transform, using two different momenta $\vec{k}$ and $\vec{k}'$, because all the terms are quadratic in the field, we obtain

$$\begin{aligned} S_0[\widetilde{\varphi}] &= \frac{1}{2}\sum_{\vec{n}}\left[\sum_{\mu}\sum_{\vec{k}}\sum_{\vec{k}'}\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}')(\Delta_\mu e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}})(\Delta_\mu e^{\imath\frac{2\pi}{N}\vec{k}'\cdot\vec{n}})\right. \\ &\qquad \left. + \alpha_0\sum_{\vec{k}}\sum_{\vec{k}'}\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}')e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}e^{\imath\frac{2\pi}{N}\vec{k}'\cdot\vec{n}}\right]. \end{aligned}$$

Since the complex exponentials are eigenvectors of the finite-difference operator, we obtain

$$\begin{aligned} S_0[\widetilde{\varphi}] &= \frac{1}{2}\sum_{\vec{k}}\sum_{\vec{k}'}\left(\sum_{\vec{n}}e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}e^{\imath\frac{2\pi}{N}\vec{k}'\cdot\vec{n}}\right)\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}') \\ &\qquad \times\left[\sum_{\mu}\imath\rho_\mu(\vec{k})e^{\imath\frac{\pi}{N}k_\mu}\imath\rho_\mu(\vec{k}')e^{\imath\frac{\pi}{N}k'_\mu} + \alpha_0\right]. \end{aligned}$$

As one can see, we may now execute the sum over the positions $\vec{n}$ using the orthogonality and completeness relations, obtaining

$$S_0[\widetilde{\varphi}] = \frac{1}{2}\sum_{\vec{k}}\sum_{\vec{k}'}N^d\delta^d_{\vec{k},-\vec{k}'}\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}')\left[-\sum_{\mu}\rho_\mu(\vec{k})e^{\imath\frac{\pi}{N}k_\mu}\rho_\mu(\vec{k}')e^{\imath\frac{\pi}{N}k'_\mu} + \alpha_0\right].$$

Using now the delta function to execute the sum over the momenta $\vec{k}'$ the expression simplifies considerably and we obtain

$$S_0[\widetilde{\varphi}] = \frac{N^d}{2}\sum_{\vec{k}}\left[-\sum_{\mu}\rho_\mu(\vec{k})\rho_\mu(-\vec{k}) + \alpha_0\right]\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(-\vec{k}).$$

Finally, we have that $\rho_\mu(-\vec{k}) = -\rho_\mu(\vec{k})$ and, since the field is real, that $\widetilde{\varphi}(-\vec{k}) = \widetilde{\varphi}^*(\vec{k})$, so that we obtain the final result

$$S_0[\widetilde{\varphi}] = \frac{N^d}{2}\sum_{\vec{k}}\left[\rho^2(\vec{k}) + \alpha_0\right]|\widetilde{\varphi}(\vec{k})|^2. \tag{3.3.2}$$

In this expression the degrees of freedom are indexed by the coordinates $\vec{k}$ in momentum space. As one can see, there are no terms that contain products of fields

While the domain of integration is clear in the space of the φ, where each $\varphi(\vec{n})$ goes from $-\infty$ to ∞, the same is not true in the space of the $\widetilde{\varphi}$, because it is necessary to find a path in the complex plane of each $\widetilde{\varphi}$ such that these constraints are satisfied. The integral that we want to calculate may be understood as an integral over a N^d-dimensional surface embedded in the $2N^d$-dimensional space generated by the set of all the $\mathfrak{R}$ and $\mathfrak{I}$ variables. We may calculate the integral over the surface by integrating over the whole space an expression involving Dirac delta functions that have support over the surface. In this way we will be explicitly implementing the constraints by means of the Dirac delta functions and we may then extend the integration to all variables $\mathfrak{R}$ and $\mathfrak{I}$, each one of them going from $-\infty$ to ∞, which makes much clearer the treatment of the limits of integration. A simple example of this kind of operation can be found in problem 3.3.4. Using these ideas and performing a careful counting of the modes in momentum space, in order to build a consistent pairing of those that have their real and imaginary part related (problem 3.3.5), we may write the integral in the form

$$\begin{aligned} I &= \int \left[\prod_{\vec{k}} \mathrm{d}\mathfrak{R}(\vec{k})\mathrm{d}\mathfrak{I}(\vec{k})\right] \left\{\prod_{\vec{k}=\mathcal{P}(\vec{k})} \delta\left[\mathfrak{I}(\vec{k})\right]\right\} \\ &\quad \times \left\{\prod_{(\vec{k},\mathcal{P}(\vec{k})),\vec{k}\neq\mathcal{P}(\vec{k})} \delta\left[\frac{\mathfrak{R}(\vec{k})-\mathfrak{R}(-\vec{k})}{\sqrt{2}}\right] \delta\left[\frac{\mathfrak{I}(\vec{k})+\mathfrak{I}(-\vec{k})}{\sqrt{2}}\right]\right\} \\ &\quad \times [\mathfrak{R}(\vec{k}')+\imath\mathfrak{I}(\vec{k}')][\mathfrak{R}(\vec{k}'')+\imath\mathfrak{I}(\vec{k}'')]e^{-S_0[\mathfrak{R},\mathfrak{I}]}, \end{aligned}$$

where $\prod_{\vec{k}=\mathcal{P}(\vec{k})}$ is a product that runs over the real modes, $\prod_{(\vec{k},\mathcal{P}(\vec{k})),\vec{k}\neq\mathcal{P}(\vec{k})}$ is a product that runs over one half of the complex modes existing in momentum space, that is, over pairs of complex modes which are paired up by the pairing operator $\mathcal{P}$, and this pairing operator is such that $\mathcal{P}(\vec{k}) = -\vec{k}$ unless one or more of the components of $-\vec{k}$ are outside their standard range of variation, in which case one must add N to them in order to bring them back into the correct range. When this happens $\mathcal{P}(\vec{k})$ is not equal to $-\vec{k}$, since only some of its components change sign. For odd N the only mode for which $\vec{k} = \mathcal{P}(\vec{k})$ is the zero mode $\vec{k} = \vec{0}$, but for even N there are 2^d such modes. In addition to this, S_0 may be written in a simple form in terms of the $\mathfrak{R}$'s and $\mathfrak{I}$'s,

$$S_0[\mathfrak{R},\mathfrak{I}] = \frac{N^d}{2}\sum_{\vec{k}}[\rho^2(\vec{k})+\alpha_0][\mathfrak{R}^2(\vec{k})+\mathfrak{I}^2(\vec{k})],$$

where, naturally, $\mathfrak{I} = 0$ for the real modes. In this way it becomes much simpler to deal with these integrals, because now we may treat all the variables as independent.

In order to verify in which cases our integral is equal to zero or not, let us start by the case in which we have

$$\vec{k}' \neq \vec{k}'' \quad \text{and} \quad \vec{k}' \neq -\vec{k}'',$$

Once more, we may use the delta functions to obtain

$$\begin{aligned} I &= 2I' \times \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}') \\ &\quad \times \left[\Re^2(\vec{k}') - \Im^2(\vec{k}') + 2\imath\Re(\vec{k}')\Im(\vec{k}')\right] \\ &\quad \times e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\Re^2(\vec{k}')+\Im^2(\vec{k}')\right]}. \end{aligned}$$

For the third term of the bracket the same parity argument used in the previous case is valid, and therefore it is zero. As for the first two terms, we may change the names of the integration variables in one of them, thus verifying that they cancel out. Therefore, in the case $\vec{k}' = \vec{k}''$ we also have $I = 0$.

There remains to be examined the case $\vec{k}' = -\vec{k}''$. Once more we collect the appropriate factors, obtaining

$$\begin{aligned} I &= I' \times \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Re(-\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(-\vec{k}') \\ &\quad \times \delta\left[\frac{\Re(\vec{k}') - \Re(-\vec{k}')}{\sqrt{2}}\right] \delta\left[\frac{\Im(\vec{k}') + \Im(-\vec{k}')}{\sqrt{2}}\right] \\ &\quad \times \left[\Re(\vec{k}')\Re(-\vec{k}') - \Im(\vec{k}')\Im(-\vec{k}') + \imath\Re(\vec{k}')\Im(-\vec{k}') + \imath\Re(-\vec{k}')\Im(\vec{k}')\right] \\ &\quad \times e^{-\frac{N^d}{2}[\rho^2(\vec{k}')+\alpha_0]\left[\Re^2(\vec{k}')+\Im^2(\vec{k}')\right]}\ e^{-\frac{N^d}{2}[\rho^2(-\vec{k}')+\alpha_0]\left[\Re^2(-\vec{k}')+\Im^2(-\vec{k}')\right]}. \end{aligned}$$

Using the delta functions to do the integrals over $\Re(-\vec{k}')$ and $\Im(-\vec{k}')$ we obtain

$$I = 2I' \times \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}') \left[\Re^2(\vec{k}') + \Im^2(\vec{k}')\right] e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\Re^2(\vec{k}')+\Im^2(\vec{k}')\right]}.$$

where the facts that $\Re(\vec{k}') = \Re(-\vec{k}')$ and that $\Im(\vec{k}') = -\Im(-\vec{k}')$ imply the cancelling of the two imaginary terms in the bracket. The two other terms no longer cancel out as was the case in the previous case, so that it becomes now clear that in this case the integral I is *not* zero. We have then the result

$$\begin{aligned} &\int \prod_{\vec{k}} \mathrm{d}\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}')\widetilde{\varphi}(\vec{k}'')e^{-S_0[\widetilde{\varphi}]} \\ &\quad = 2I' \times \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}') \left[\Re^2(\vec{k}') + \Im^2(\vec{k}')\right] e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\Re^2(\vec{k}')+\Im^2(\vec{k}')\right]}. \end{aligned}$$

In analogous fashion, we also have the integral, with the same I',

$$\int \prod_{\vec{k}} \mathrm{d}\widetilde{\varphi}(\vec{k})e^{-S_0[\widetilde{\varphi}]} = 2I' \times \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}')\ e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\Re^2(\vec{k}')+\Im^2(\vec{k}')\right]},$$

so that we may now use these results to calculate the ratio of integrals that appears in the expectation value that defines the propagator in momentum space,

$$\int [\mathbf{d}\widetilde{\varphi}] e^{-S_0[\widetilde{\varphi}]} = \int [\mathbf{d}\widetilde{\varphi}] e^{-\frac{N^d}{2}\sum_{\vec{k}}[\rho^2(\vec{k})+\alpha_0]|\widetilde{\varphi}(\vec{k})|^2} = \prod_{\vec{k}} \sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k})+\alpha_0]}}, \qquad (3.3.4)$$

because all the other relevant integrals, with even powers of the fields, can be obtained from this one by means of differentiation with respect to the quantity $-N^d[\rho^2(\vec{k})+\alpha_0]/2$.

The fact that expectation values of the type $\langle\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k'})\rangle$ are zero when $\vec{k'} \neq -\vec{k}$ is related directly to the conservation of momentum during the propagation of field waves and, indirectly, also during the propagation of particles. It means that if a wave or particle enters (we adopt the convention that "enters" means sign "+" for the momentum) into a propagation process, which is a kind of interaction of the object with itself, then it must exit (in this convention "exit" means sign "−" for the momentum) with the same vector $\vec{k}$, that is, it propagates with a constant momentum, in a given mode of the lattice in momentum space. This is, of course, a specific characteristic of periodical boundary conditions, for which we have discrete translation invariance.

For fixed boundary conditions nothing essential changes regarding the calculation of the Gaussian integrals. In that case the eigenmodes of the Laplacian are associated to stationary waves within the box, not to travelling plane waves. Due to this the components in momentum space are all real rather than complex, which implies that the transformation to momentum space really diagonalizes the quadratic form in the action, instead of anti-diagonalizing it as happened here. This actually makes the calculation of the integrals more straightforward than in the periodical case, because there is no additional complication of having complex components as integration variables. In this case a modified versions of equation (3.3.4) holds (problem 3.3.6),

$$\int [\mathbf{d}\widetilde{\varphi}] e^{-S_0[\widetilde{\varphi}]} = \int [\mathbf{d}\widetilde{\varphi}] e^{-\frac{(N+1)^d}{2}\sum_{\vec{k}}[\rho_f^2(\vec{k})+\alpha_0]\widetilde{\varphi}^2(\vec{k})} = \prod_{\vec{k}} \sqrt{\frac{2\pi}{(N+1)^d[\rho_f^2(\vec{k})+\alpha_0]}},$$

starting from which we can calculate other integrals using the same procedures of differentiation with respect to a parameter, in this case the quantity

$$-(N+1)^d[\rho_f^2(\vec{k})+\alpha_0]/2,$$

as we already discussed above for the periodical case.

In order to finish the development of this section it is still necessary that we relate these integrals over the Fourier components of the field with the original integrals over the fields in position space, by means of which we defined the theory. We have already seen how to transform the action from one field coordinate system to the other, but the same must be done with the integration element in configuration space. As we saw before in section 2.9, with our usual normalization we have for the determinant of the transformation matrix of the finite Fourier transform $\det(\mathbb{F}) =$

3.3.4. (a) Consider the square of vertices $(0,0)$, $(0,1)$, $(1,0)$, and $(1,1)$ in the plane (x,y), a function $f(x,y)$ on this plane and the curve in the plane defined by $f(x,y)=0$. Let us denote by C the part of the curve that is inside the square. Show that the line integral over the curve C that gives its arc length can be written in terms of an integral over the plane in the following way,

$$\int_C \mathrm{d}\ell = \int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y\ \delta\left(\frac{x\partial_x f + y\partial_y f}{\sqrt{(\partial_x f)^2+(\partial_y f)^2}}\right),$$

where the Dirac delta function appears. Hint: make, at each point along the curve, a transformation of variables from (x,y) to (u,v), where u varies along the tangent to the curve and v varies along the line perpendicular to it, that is, $\mathrm{d}u=\mathrm{d}\ell$; remember that $\mathrm{d}f\equiv 0$ along the curve.

(b) Verify the result above for the particular cases $f(x,y)=x^2+y^2-1$ and $f(x,y)=x-y$. Show that this last case, in which f is linear on x and y, is the one used in the text, in which the expression of the integral over the plane reduces to

$$\int_C \mathrm{d}\ell = \int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y\ \delta\left(\frac{x-y}{\sqrt{2}}\right).$$

3.3.5. Consider the definition of the pairing operator $\mathcal{P}(\vec{k})$, which is that $\mathcal{P}(\vec{k})=-\vec{k}$ unless one or more of the components of $-\vec{k}$ falls outside the allowed range of values, when they must be brought back into the range by the addition of N.

(a) Show that a real mode, for which the imaginary part of the Fourier transform of the field is zero, is one for which $\vec{k}=\mathcal{P}(\vec{k})$. Examine then the situation with these real modes and define the product $\prod_{\vec{k}=\mathcal{P}(\vec{k})}$ used in the text. Show that for odd N the product has just one factor, the zero mode $\vec{k}=\vec{0}$, while for even N it contains 2^d factors.

(b) Show that, excluding the real modes, it is possible to pair up all the remaining Fourier modes in momentum space so that each pair has equal real parts $\mathfrak{R}$ and imaginary parts $\mathfrak{I}$ that differ only by the sign. Use the pairing operator $\mathcal{P}$ in order to do the pairing and define, in this way, the product $\prod_{(\vec{k},\mathcal{P}(\vec{k})),\vec{k}\neq\mathcal{P}(\vec{k})}$ used in the text. Write a detailed definition of this product, and show that for odd N it consists of N^d-1 factors, while for even N it consists of N^d-2^d factors.

3.3.6. Calculate the basic Gaussian integral of the free theory in the case of fixed boundary conditions, that is, show that

$$\int [\mathbf{d}\widetilde{\varphi}] e^{-S_0[\widetilde{\varphi}]} = \prod_{\vec{k}} \sqrt{\frac{2\pi}{(N+1)^d[\rho_f^2(\vec{k})+\alpha_0]}},$$

$$\widetilde{g}(\vec{k}_1, \ldots, \vec{k}_{2i+1}) = \langle \widetilde{\varphi}(\vec{k}_1) \ldots \widetilde{\varphi}(\vec{k}_{2i+1}) \rangle = 0.$$

In the case of momentum space we may refine a little this argument, extending its reach, if we take into account the fact that in this space the modes of the model are decoupled. Due to this, one can easily show (problem 3.4.2) that the expectation value of the product of two fields corresponding to distinct modes factors into the product of the expectation values of each one of the two fields. Since the components $\vec{k}_\mu$ assume both positive and negative values, in this case we must worry also about modes related by a change in the sign of $\vec{k}$. For example, for the case of two factors we have that, if $\vec{k}_1 \neq \pm\vec{k}_2$, then

$$\langle \widetilde{\varphi}(\vec{k}_1)\widetilde{\varphi}(\vec{k}_2) \rangle = \langle \widetilde{\varphi}(\vec{k}_1) \rangle \langle \widetilde{\varphi}(\vec{k}_2) \rangle.$$

Hence, even if the number of fields multiplied together is even, the expectation value is still zero unless the fields are paired up in each mode, with an even number of factors in each one. In addition to this, as we saw in the case of the propagator in section 3.3, it is necessary the fields be paired up in such a way that they organize as a set of squared absolute values. This is a general fact, valid for all the correlation function in momentum space, associated to the fact that all the correlation functions are real. It can be remembered by means of the rule of association of momenta that we saw before: momentum conservation on the periodical lattice implies that each momentum that "goes into" the expectation value, associated to $\widetilde{\varphi}(\vec{k})$, must be equal and opposite to the one that "exits", associated to $\widetilde{\varphi}(-\vec{k}) = \widetilde{\varphi}^*(\vec{k})$. Hence, we have that each factor $\widetilde{\varphi}(\vec{k})$ must be paired up with another factor $\widetilde{\varphi}(-\vec{k})$ in order for the expectation value not to be zero. For example, the expectation value $\langle \widetilde{\varphi}(\vec{k}_1)\widetilde{\varphi}(\vec{k}_2) \rangle$ is zero if $\vec{k}_1 \neq -\vec{k}_2$, as we saw before in section 3.3.

In this way, in momentum space we may quickly reduce the number of different possibilities for correlation functions potentially different from zero. The ones that remain to be discussed are those of the types $\langle |\widetilde{\varphi}(\vec{k}_1)|^2 \rangle$, $\langle |\widetilde{\varphi}(\vec{k}_1)|^2 |\widetilde{\varphi}(\vec{k}_2)|^2 \rangle$, $\langle |\widetilde{\varphi}(\vec{k}_1)|^4 \rangle$, $\langle |\widetilde{\varphi}(\vec{k}_1)|^4 |\widetilde{\varphi}(\vec{k}_2)|^2 \rangle$, etc, where only even powers of absolute values of the Fourier components appear. As a non-trivial example of factorization, it is not difficult to verify (problem 3.4.3) that, for $\vec{k}_1 \neq \pm\vec{k}_2$,

$$\langle |\widetilde{\varphi}(\vec{k}_1)|^2 |\widetilde{\varphi}(\vec{k}_2)|^2 \rangle = \langle |\widetilde{\varphi}(\vec{k}_1)|^2 \rangle \langle |\widetilde{\varphi}(\vec{k}_2)|^2 \rangle.$$

It is important to emphasize that, although it is true that, for $\vec{k}_1 \neq -\vec{k}_2$,

$$\langle \widetilde{\varphi}(\vec{k}_1)\widetilde{\varphi}(\vec{k}_2) \rangle = \langle \widetilde{\varphi}(\vec{k}_1) \rangle \langle \widetilde{\varphi}(\vec{k}_2) \rangle, \tag{3.4.1}$$

the analogous relation is *not* true in position space, that is, even if $\vec{x}_1 \neq \vec{x}_2$ we have that

$$\langle \varphi(\vec{x}_1)\varphi(\vec{x}_2) \rangle \neq \langle \varphi(\vec{x}_1) \rangle \langle \varphi(\vec{x}_2) \rangle. \tag{3.4.2}$$

for which we may write, in the case in which $\widetilde{\varphi}(\vec{k})$ is real,

$$\begin{aligned}
\langle|\widetilde{\varphi}(\vec{k})|^4\rangle &= \frac{\left(\dfrac{-2\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \displaystyle\int [\mathbf{d}\widetilde{\varphi}]\; e^{-S_0[\widetilde{\varphi}]}}{\displaystyle\int [\mathbf{d}\widetilde{\varphi}]\; e^{-S_0[\widetilde{\varphi}]}} \\
&= \frac{\left(\dfrac{-2\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \displaystyle\prod_{\vec{k}'} \sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}{\displaystyle\prod_{\vec{k}'} \sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}} \\
&= \frac{(-2)^2\left(-\dfrac{1}{2}\right)\left(-\dfrac{3}{2}\right)\dfrac{1}{\sqrt{N^d[\rho^2(\vec{k})+\alpha_0]}^5}}{\dfrac{1}{\sqrt{N^d[\rho^2(\vec{k})+\alpha_0]}}} \\
&= 3\frac{1}{\{N^d[\rho^2(\vec{k})+\alpha_0]\}^2}.
\end{aligned}$$

In this way, comparing this result with the fundamental result of equation (3.3.3), we obtain the factorization relation

$$\langle|\widetilde{\varphi}(\vec{k})|^4\rangle = 3\langle|\widetilde{\varphi}(\vec{k})|^2\rangle^2,$$

for the case $\vec{k}=\vec{0}$ and other purely real modes, showing that the four-point function factors into two two-point functions. The same is true for higher-order functions, as one can verify without difficulty. For example, one can obtain for the purely real modes (problem 3.4.5) a more general factorization formula,

$$\langle|\widetilde{\varphi}(\vec{k})|^{2n}\rangle = (2n-1)!!\langle|\widetilde{\varphi}(\vec{k})|^2\rangle^n,$$

for any integer n, involving a double factorial $(2n-1)!! = (2n-1)(2n-3)(2n-5)\ldots 1$.

In the case in which $\widetilde{\varphi}(\vec{k})$ has a non-zero imaginary part we have

$$\begin{aligned}
\langle|\widetilde{\varphi}(\vec{k})|^4\rangle &= \frac{\left(\dfrac{-\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \displaystyle\int [\mathbf{d}\widetilde{\varphi}]\; e^{-S_0[\widetilde{\varphi}]}}{\displaystyle\int [\mathbf{d}\widetilde{\varphi}]\; e^{-S_0[\widetilde{\varphi}]}} \\
&= \frac{\left(\dfrac{-\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \displaystyle\prod_{\vec{k}'} \sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}{\displaystyle\prod_{\vec{k}'} \sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}
\end{aligned}$$

Problems

3.4.1. Show, using the same ideas that were suggested for problem 3.1.1, that the correlation function of an odd number of points in position space is zero, that is, that for any $i = 0, \ldots, \infty$ and any $\vec{x}_i$,

$$g(\vec{x}_1, \ldots, \vec{x}_{2i+1}) = \langle \varphi(\vec{x}_1) \ldots \varphi(\vec{x}_{2i+1}) \rangle = 0.$$

3.4.2. Show, using the explicit form of the action $S_0[\widetilde{\varphi}]$ and the definition of the functional integral in momentum space, that the expectation value of two Fourier components of the field with different momenta factors into the product of the expectation values of each component, that is, that for $\vec{k}_1 \neq \pm\vec{k}_2$ we have

$$\langle \widetilde{\varphi}(\vec{k}_1)\widetilde{\varphi}(\vec{k}_2) \rangle = \langle \widetilde{\varphi}(\vec{k}_1) \rangle \langle \widetilde{\varphi}(\vec{k}_2) \rangle.$$

3.4.3. Show, using the same ideas used in problem 3.4.2, that for $\vec{k}_1 \neq \pm\vec{k}_2$ we have the factorization

$$\langle |\widetilde{\varphi}(\vec{k}_1)|^2 |\widetilde{\varphi}(\vec{k}_2)|^2 \rangle = \langle |\widetilde{\varphi}(\vec{k}_1)|^2 \rangle \langle |\widetilde{\varphi}(\vec{k}_2)|^2 \rangle.$$

3.4.4. Show that equation (3.4.2) holds. In other words show that, unlike what happens in momentum space as described by equation (3.4.1), this type of factorization does not happen in position space. In order to do this, first show that $\langle \varphi(\vec{x}) \rangle = 0$, so that the right-hand side of equation (3.4.2) is zero. Then apply Fourier transformations to the left-hand side of equation (3.4.1) and obtain the result given in equation (3.4.3) for the two-point function in position space. Finally, show that the right-hand side of this last equation is never zero.

3.4.5. Using the techniques given in the text for the calculation of the functional integrals, demonstrate the factorization formula

$$\langle |\widetilde{\varphi}(\vec{k})|^{2n} \rangle = (2n-1)!! \langle |\widetilde{\varphi}(\vec{k})|^2 \rangle^n,$$

for the case of purely real modes $\widetilde{\varphi}(\vec{k})$, while for the case of modes in which $\widetilde{\varphi}(\vec{k})$ has a non-zero imaginary part, demonstrate the factorization relation

$$\langle |\widetilde{\varphi}(\vec{k})|^{2n} \rangle = n! \langle |\widetilde{\varphi}(\vec{k})|^2 \rangle^n,$$

for an arbitrary integer n in either case.

3.4.6. Using previous results already known and/or Fourier transforms, calculate explicitly, at an arbitrary site $\vec{n}$, the quantities $\langle \varphi^4(\vec{n}) \rangle$ and $\langle \varphi^2(\vec{n}) \rangle$, showing in this way that the following factorization formula is valid for them:

$$\langle \varphi^4(\vec{n}) \rangle = 3 \langle \varphi^2(\vec{n}) \rangle^2.$$

$$
\begin{aligned}
= \quad & \frac{1}{2}\sum_{\ell}(\Delta_\ell\varphi')^2 + \frac{\alpha_0}{2}\sum_s \varphi'^2(s) \\
& + \sum_{\ell}(\Delta_\ell v)(\Delta_\ell\varphi') + \alpha_0\sum_s v(s)\varphi'(s) - \sum_s j(s)\varphi'(s) \\
& + \frac{1}{2}\sum_{\ell}(\Delta_\ell v)^2 + \frac{\alpha_0}{2}\sum_s v^2(s) - \sum_s j(s)v(s).
\end{aligned}
$$

Observe that the third line of the second version of this equation contains only terms which are independent of φ. When we exponentiate S_0 these terms become a constant multiplying the functional integral and, since they exist in the integrals both in the numerator and in the denominator, these factors cancel out, in all observables. It is therefore clear that we may discard these terms without changing anything in the quantum theory. We will commit here a small abuse of language and discard the terms without, however, changing the symbol S_0 to reflect the change. The first line of the equation is the action from which we started written for the field φ', while the second contains only terms linear in φ'. If we recall our symmetry arguments leading to the fact that $\langle\varphi\rangle = 0$ in the theory without sources, added to the fact that we are defining v here in such a way that $\langle\varphi'\rangle = 0$, we see that this will only be possible if these linear terms, which are not invariant by the transformation $\varphi' \to -\varphi'$, are in fact zero for any φ'. Clearly, this is a condition which we can use to determine v,

$$
\sum_{\vec{n}}\left[\sum_{\mu}(\Delta_\mu v)(\Delta_\mu\varphi') + \alpha_0 v(\vec{n})\varphi'(\vec{n}) - j(\vec{n})\varphi'(\vec{n})\right] = 0,\ \forall\varphi', \tag{3.5.1}
$$

where we decomposed the sum over ℓ in sums over μ and $\vec{n}$. Since the boundary conditions are periodical, we may write this equation in another, equivalent form, performing an integration by parts in the first term to obtain

$$
\sum_{\vec{n}}\left[-\Delta^2 v + \alpha_0 v(\vec{n}) - j(\vec{n})\right]\varphi'(\vec{n}) = 0,\ \forall\varphi'. \tag{3.5.2}
$$

In any case the important point is that it must be valid for *all* the configurations φ' that exist in the ensemble of the quantum theory. Note that this equation does not have a classical limit, because φ' is an arbitrary configuration of the quantum theory, and therefore it is not necessarily a continuous function in the continuum limit. While $\varphi'(\vec{n})$ is a completely arbitrary function on the lattice, the quantity within brackets contains only expectation values or classical quantities, all such quantities having well-defined definite values. This is true both for the given external source j and for the expectation value v of the field that results from its introduction. It becomes clear therefore that the only way to satisfy this equation for all φ' is that the quantity within brackets be zero (problem 3.5.1). This equation gives us a condition involving j and v, which determines the relation between these two quantities.

However, since the quantity within the bracket includes a finite-difference operator, it is not so straightforward to solve it as a stand-alone equation in its current

$$\left[-\Delta^2 + \alpha_0\right] v(\vec{n}) - j(\vec{n}) = 0.$$

We have therefore the solution for the expectation value v in the quantum theory,

$$\tilde{v}(\vec{k}) = \frac{\widetilde{j}(\vec{k})}{\rho^2(\vec{k}) + \alpha_0}. \tag{3.5.3}$$

One can verify (problem 3.5.2) that this equation may also be obtained directly from the self-consistency equation $\langle \varphi'(\vec{n}) \rangle = 0$, by direct calculation of the Gaussian integrals involved in this expectation value. Naturally, this is the more direct and straightforward way to obtain the result. The argument presented above is a shortcut based on symmetry arguments.

Note that the solution obtained is exactly the same solution obtained in the classical case for the field in the presence of the external source. It is important to emphasize that this fact is a characteristic *exclusively* of the free theory, due to its linearity, and is *not* valid in general. Having obtained the result in momentum space it is not difficult to write it in position space. One can show directly (problem 3.5.3), taking the inverse Fourier transform of this solution, that

$$v(\vec{n}) = \sum_{\vec{n}'} K(\vec{n}, \vec{n}') j(\vec{n}'), \tag{3.5.4}$$

where $K(\vec{n}, \vec{n}')$ is given by

$$K(\vec{n}, \vec{n}') = \frac{1}{N^d} \sum_{\vec{k}} \frac{e^{-\imath \frac{2\pi}{N} \vec{k} \cdot (\vec{n} - \vec{n}')}}{\rho^2(\vec{k}) + \alpha_0}.$$

One can show also (problem 3.5.4) that $K(\vec{n}, \vec{n}')$ is the propagator in position space,

$$K(\vec{n}, \vec{n}') = \langle \varphi'(\vec{n}) \varphi'(\vec{n}') \rangle.$$

This propagator tells us how the introduction of a source at the point $\vec{n}'$ affects the average value of the field at another point $\vec{n}$, that is, it describes the propagation of relations of cause and effect within the model.

We see in this way that, in a way analogous to what happens in the classical theory, the quantum theory also establishes a functional relation between the expectation value v of the field and the external source j. In the free theory this functional relation is the same that appears in the classical version of the theory, but this is not true in general. The fact that the relation is the same in either case in this simple example is not very important, what really matters is that in the quantum case, in a fashion analogous to what happens in the classical case, the theory establishes a well-defined relation between the external sources and the expectation value of the field. In the classical case we can establish the physical interpretation of the theory in terms of this relation, so that we have here quite a familiar way of doing the

3.6 Functional Generators on the Lattice

We saw in section 3.5 that the quantum theory, in a way analogous to the classical theory, establishes a *functional* relation between the expectation value v of the field and the external source j, which means that in order to calculate v at a given point it is necessary to know j at all points, not only at that particular point. It was mentioned there that this relation can be used to explore the properties of the quantum theory. In this section we will introduce the *functional generators* of the correlation functions of the quantum theory on the lattice, which are the instruments that can be used for this type of analysis. The final objective of this section is to arrive at the concept of the *effective action*. Observe that, differently from what we have been doing up to this point in the discussion of the quantum theory, the development presented in this section is of a very general character. Instead of using the theory of the free scalar field to develop in detail concepts whose qualitative nature may then be generalized, we will make the development directly in the general case, for any arbitrary model of scalar fields.

In this section we will make a temporary change in notation and denote the expectation value of the field by $\varphi_{(c)}$, not by v. We will also refer to φ as the fundamental field, to distinguish it from $\varphi_{(c)}$, which will also be a type of field. In order to develop the formalism we will assume that we have some model of scalar fields defined by an action $S[\varphi]$, without external sources, which has the property that $S[\varphi] = S[-\varphi]$ and, therefore, the property that $\langle\varphi\rangle = 0$. We will then add explicitly to this action a linear term with the external source, given as usual by the product of j and φ,

$$S_{(j)}[\varphi] = S[\varphi] - \sum_{\vec{n}} j(\vec{n})\varphi(\vec{n}).$$

When we do this the source causes the generation of a non-vanishing expectation value for the field, which is a function of $\vec{n}$ and a functional of j,

$$\varphi_{(c)}[j] = \langle\varphi(\vec{n})\rangle_{(j)} = \frac{\displaystyle\int [\mathbf{d}\varphi]\varphi(\vec{n})e^{-S_{(j)}}}{\displaystyle\int [\mathbf{d}\varphi]e^{-S_{(j)}}}. \tag{3.6.1}$$

The index j on the expectation value means that it is calculated in the distribution of the theory with the external source, defined by $S_{(j)}$, instead of that defined only by S. The expectation value $\varphi_{(c)}$ is also referred to as the "classical field" of the quantum theory. This does not mean, however, that it can always be measured directly, because the expectation value of the field at a single site is an ultra-local object, not an extended object on the lattice. For example, for a point source in the theory of the free field $\varphi_{(c)}$ is the Green function and therefore has a divergence at the origin, in the continuum limit. On the other hand, since this "classical field" is an expectation value its value does not fluctuate like the fundamental field, that is, it does behave basically like a classical quantity. By and large we may think of this

that may be changed independently, so that we have for our functional variations

$$\frac{\mathfrak{d} j(\vec{n}_1)}{\mathfrak{d} j(\vec{n}_2)} = \delta^d(\vec{n}_1, \vec{n}_2),$$

where we used the symbol $\mathfrak{d}$ to indicate the functional derivatives. Observe also that only $\varphi_{(c)}$ depends on j, the fundamental field φ is independent of the external sources. Taking n functional derivatives of Z we obtain

$$\frac{\mathfrak{d}^n Z[j]}{\mathfrak{d} j_1 \dots \mathfrak{d} j_n} = \left\langle \varphi_1 \dots \varphi_n e^{\sum_{\vec{n}} j(\vec{n})\varphi(\vec{n})} \right\rangle = \frac{\int [\mathbf{d}\varphi] \varphi_1 \dots \varphi_n e^{-S_{(j)}}}{\int [\mathbf{d}\varphi] e^{-S}},$$

where we denoted the dependencies with the positions $\vec{n}_i$ by means of indices i, for simplicity of notation. Observe that the expectation value is taken in the measure of S, without external sources. For $j = 0$ we recover from this formula the correlation functions of the model in the theory *without* external sources,

$$\frac{\mathfrak{d}^n Z[j]}{\mathfrak{d} j_1 \dots \mathfrak{d} j_n} = \langle \varphi_1 \dots \varphi_n \rangle = g_{1,\dots,n}.$$

However, for $j \neq 0$ we do *not* obtain the true correlation functions in the presence of j, because the expectation values are taken in the measure of S. The true correlation functions in the presence of j are given by the ratios

$$\frac{1}{Z[j]} \frac{\mathfrak{d}^n Z[j]}{\mathfrak{d} j_1 \dots \mathfrak{d} j_n} = \langle \varphi_1 \dots \varphi_n \rangle_{(j)} = \frac{\int [\mathbf{d}\varphi] \varphi_1 \dots \varphi_n e^{-S_{(j)}}}{\int [\mathbf{d}\varphi] e^{-S_{(j)}}} = g_{(j)1,\dots,n},$$

where the index (j) indicates that the expectation value is taken in the measure of $S_{(j)}$ and where we do *not* make $j = 0$. In particular, the expectation value $\varphi_{(c)}$ of the field is given by

$$\varphi_{(c)1}[j] = \frac{1}{Z[j]} \frac{\mathfrak{d} Z[j]}{\mathfrak{d} j_1} = \frac{\mathfrak{d}}{\mathfrak{d} j_1} \ln(Z[j]).$$

This motivates the definition of another functional, related to Z by exponentiation,

$$W[j] = \ln(Z[j]), \quad \text{that is,} \quad Z[j] = e^{W[j]}.$$

The "classical field" $\varphi_{(c)1}$ may now be written as

$$\varphi_{(c)1}[j] = \langle \varphi_1 \rangle_{(j)} = \frac{\mathfrak{d} W[j]}{\mathfrak{d} j_1} = \frac{1}{Z[j]} \frac{\mathfrak{d} Z[j]}{\mathfrak{d} j_1}. \tag{3.6.3}$$

In a way analogous to Z, the functional W also generates correlation functions of the theory. However, we are looking in this case at a different set of functions. While Z

$$\varphi_{(c)}[j] = \frac{\mathfrak{d}W[j]}{\mathfrak{d}j},$$

so that the total variation of W due to variations of j at each point may be written in the form of a *functional differential*

$$\mathbf{d}W = \sum_{\vec{n}} \frac{\mathfrak{d}W[j]}{\mathfrak{d}j(\vec{n})}\mathbf{d}j(\vec{n}) = \sum_{\vec{n}} \varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}),$$

where $\mathbf{d}j$ are the arbitrary variations of j at all points. We may now define a new functional Γ by means of a Legendre transformation applied to W,

$$\Gamma = \sum_{\vec{n}} j(\vec{n})\varphi_{(c)}(\vec{n}) - W[j].$$

Note that the first term is simply the expectation value of $\sum_{\vec{n}} j(\vec{n})\varphi(\vec{n})$ because, since j does not depend on φ, we have

$$\left\langle \sum_{\vec{n}} j(\vec{n})\varphi(\vec{n}) \right\rangle_{(j)} = \sum_{\vec{n}} \langle j(\vec{n})\varphi(\vec{n})\rangle_{(j)} = \sum_{\vec{n}} j(\vec{n})\langle \varphi(\vec{n})\rangle_{(j)} = \sum_{\vec{n}} j(\vec{n})\varphi_{(c)}(\vec{n}).$$

We consider now the variation of Γ due to an arbitrary variation of j, and therefore of $\varphi_{(c)}$, obtaining

$$\begin{aligned}
\mathbf{d}\Gamma &= \sum_{\vec{n}} j(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}) + \sum_{\vec{n}} \varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}) - \mathbf{d}W \\
&= \sum_{\vec{n}} j(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}) + \sum_{\vec{n}} \varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}) - \sum_{\vec{n}} \varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}) \\
&= \sum_{\vec{n}} j(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}),
\end{aligned}$$

where we used the Leibniz rule and the form of the differential of W. The conclusion is that Γ is a functional directly of $\varphi_{(c)}$, because it depends only indirectly on j, its functional derivative being given by

$$\frac{\mathfrak{d}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)}} = j$$

and its functional differential by

$$\mathbf{d}\Gamma = \sum_{\vec{n}} j(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}),$$

showing that Γ is a functional only of $\varphi_{(c)}$. We may now write for our functionals that

$$g_{(c,j)1,2,3} = g_{(j)1,2,3} - g_{(c,j)1,2}\,\varphi_{(c)3} - g_{(c,j)2,3}\,\varphi_{(c)1} - g_{(c,j)3,1}\,\varphi_{(c)2} - \varphi_{(c)1}\,\varphi_{(c)2}\,\varphi_{(c)3},$$

which corresponds to the subtraction from the complete function of all the possible factorizations in terms of the connected functions of smaller number of points.

3.6.3. Show, starting from the definition of $\varphi_{(c)}[j]$ in terms of j in equation (3.6.1), that the variations of $\varphi_{(c)}(\vec{n})$ and $j(\vec{n})$ at the same point $\vec{n}$ are related by

$$\mathbf{d}\varphi_{(c)} = \left[\langle\varphi^2\rangle_{(j)} - \langle\varphi\rangle^2_{(j)}\right]\mathbf{d}j = \sigma^2_{(j)}\mathbf{d}j,$$

where $\sigma_{(j)}$ is the square of the local width of the distribution of values of φ at any given site $\vec{n}$,

$$\sigma^2 = \langle\varphi^2(\vec{n})\rangle - \langle\varphi(\vec{n})\rangle^2.$$

This is always a positive and non-zero number, which shows that, given the sign we chose for the definition of $S_{(j)}$, $\varphi_{(c)}$ always increases with j if both refer to the same point $\vec{n}$.

3.6.4. Repeat the procedure in problem 3.6.3 for the case in which the two quantities involved are at different points, $\varphi_{(c)}(\vec{n}_1)$ and $j(\vec{n}_2)$ with $\vec{n}_1 \neq \vec{n}_2$. Show that $\varphi_{(c)}$ also increases with j in this case, so long as the model at issue has the property that its propagator in position space is always positive, $g_{(c)}(\vec{n}_1, \vec{n}_2) \geq 0$, for any $\vec{n}_1$ and $\vec{n}_2$. If we recall that the propagator is related to the Green function of the classical theory, we see that this is intuitively a very reasonable property for all models that we may want to examine.

3.7 Physical Significance of the Effective Action

As we saw in sections 3.5 and 3.6, both the classical theory and the quantum theory establish well-defined functional relations between $\varphi_{(c)}$ and j. In the classical theory this relation is established by the location of the minimum of the action S as a function of the external source j, while in the quantum theory it is established by the modification of the relative statistical weights $\exp(-S)$ of the field distribution in configuration space, caused by the introduction of j. Unlike what happens in the theory of the free scalar field, in general these two functional relations are different. We may then ask whether there is in the quantum theory a functional whose minimum establishes between $\varphi_{(c)}$ and j, in the fashion of what happens in the classical theory, the functional relation defined by this quantum theory. Clearly, this has to

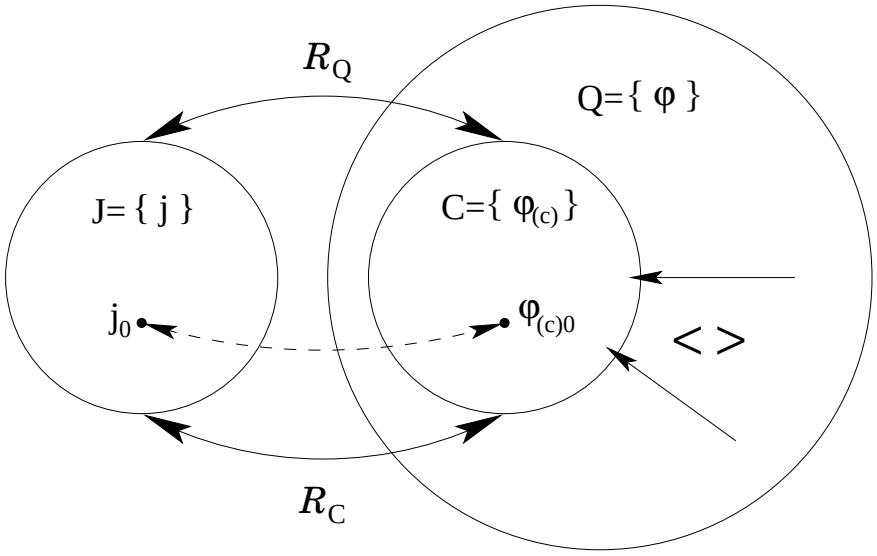


Figure 3.7.1: A diagram of the function spaces involved in the classical and quantum theories.

fields in the classical theory and Q the set of possible configurations of the fields in the quantum theory. The symbols R_{C} and R_{Q} represent the relations established between J and C by the classical and quantum theories, respectively. The symbol $< >$ represents the averaging process of the quantum theory, which takes us from Q into C.

In general, for $j = 0$ we have $\varphi_{(c)} = 0$ and, for each $j \neq 0$ some fairly well-behaved $\varphi_{(c)}$. Se see in this way that the possible configurations for $\varphi_{(c)}$ are determined by the possible configuration of j that we may introduce in the theory. Since j are classical external sources, we may think about the configurations of j as those that we usually associate to distributions of sources or charges in the classical theory, that is, densities represented by continuous and mostly differentiable functions to which we may superpose arbitrary but finite sets of isolated point sources or charges. Once this is settled, from this set of possible sources j the quantum theory determines for each model a certain space of possible classical fields $\varphi_{(c)}$, which is a subspace of Q and which we may take as the space that is relevant in the classical limit of the theory. The classical limit is the limit of large wavelengths in which the quantum fluctuations are ignored and the averages such as $\varphi_{(c)}$ represent what can be observed in the theory.

We see in this way that, starting from the most general possible set of configurations, the dynamical structure of the quantum theory itself automatically defines the subspace of configurations which is relevant for the corresponding classical theory, eliminating any need of imposing by hand the properties of this space in the classical limit of the theory. By and large, we may think of J and C as copies of the same space, the space where classical field-like objects exist. After all, an external source is no more than a representation of an expectation value within some other model or some other part of a more general model, representing a part of the physical world

function $j_0(\vec{n})$ while $\varphi_{(c)}$ varies, but in the first term we should calculate the variation of Γ that comes from its definition. Hence, when we calculate the variation of Γ, the $j[\varphi_{(c)}]$ that appears in the definition, being a functional of $\varphi_{(c)}$, does *not* remain fixed but rather varies with $\varphi_{(c)}$ according to the functional relation established between them by the quantum theory.

Let us calculate then this variation of Γ, making a variation $\varphi_{(c)0} \to \varphi'_{(c)}$ of the classical field around the value $\varphi_{(c)0}$. The variation of Γ is given by

$$\mathbf{d}\Gamma = \Gamma[\varphi'_{(c)}] - \Gamma[\varphi_{(c)0}],$$

so that, using the definition of Γ, we obtain

$$\mathbf{d}\Gamma = -\ln\left\{\frac{\int [\mathbf{d}\varphi]\; e^{\sum_{\vec{n}} j'(\vec{n})\left[\varphi(\vec{n})-\varphi'_{(c)}(\vec{n})\right]}\; e^{-S}}{\int [\mathbf{d}\varphi]\; e^{\sum_{\vec{n}} j_0(\vec{n})\left[\varphi(\vec{n})-\varphi_{(c)0}(\vec{n})\right]}\; e^{-S}}\right\},$$

where the variation of $\varphi_{(c)}$ around $\varphi_{(c)0}$ corresponds to a variation of j around j_0, $j_0 \to j'[\varphi'_{(c)}]$. In general both these variations are dependent on position. We will now write j' as $j' = j_0 + \mathbf{d}j$ and expand to first order the exponential that appears in the denominator, getting

$$e^{\sum_{\vec{n}} j'(\vec{n})\left[\varphi(\vec{n})-\varphi'_{(c)}(\vec{n})\right]} \approx e^{\sum_{\vec{n}} j_0(\vec{n})\left[\varphi(\vec{n})-\varphi'_{(c)}(\vec{n})\right]}\left\{1 + \sum_{\vec{n}}\left[\varphi(\vec{n}) - \varphi'_{(c)}(\vec{n})\right]\mathbf{d}j(\vec{n})\right\},$$

from which it follows that

$$\mathbf{d}\Gamma = -\ln\left\{\frac{e^{-\sum_{\vec{n}} j_0(\vec{n})\varphi'_{(c)}(\vec{n})}\int [\mathbf{d}\varphi]\; e^{\sum_{\vec{n}} j_0(\vec{n})\varphi(\vec{n})}\left\{1 + \sum_{\vec{n}}\left[\varphi(\vec{n}) - \varphi'_{(c)}(\vec{n})\right]\mathbf{d}j(\vec{n})\right\} e^{-S}}{e^{-\sum_{\vec{n}} j_0(\vec{n})\varphi_{(c)0}(\vec{n})}\int [\mathbf{d}\varphi]\; e^{\sum_{\vec{n}} j_0(\vec{n})\varphi(\vec{n})}\; e^{-S}}\right\},$$

where we took off the functional integrals factors that do not depend on φ. Writing this expression in terms of $S_{(j)} = S - \sum_{\vec{n}} j_0(\vec{n})\varphi(\vec{n})$ and manipulating it a little we obtain

$$\begin{aligned}\mathbf{d}\Gamma &= \sum_{\vec{n}} j_0(\vec{n})\left[\varphi'_{(c)}(\vec{n}) - \varphi_{(c)0}(\vec{n})\right] \\ &\quad - \ln\left\{1 + \frac{\int [\mathbf{d}\varphi]\; e^{-S_{(j)}}\sum_{\vec{n}}\left[\varphi(\vec{n}) - \varphi'_{(c)}(\vec{n})\right]\mathbf{d}j(\vec{n})}{\int [\mathbf{d}\varphi]\; e^{-S_{(j)}}}\right\}\end{aligned}$$

derivatives of Z and W with respect to j give us directly all the correlation functions of the theory. Let us now see how the derivatives of Γ can help us to probe the structure of the theory. We already know the first derivative, which is

$$\frac{\mathfrak{d}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}} = j_1[\varphi_{(c)}],$$

where we are using again the notation of the dependency on $\vec{n}_1$ by means of numerical indices. It is tempting to differentiate this a second time directly in terms of $\varphi_{(c)}$, but it is more convenient and clearer, causing less confusion, to proceed in another way. We should always remember that the relation between j and $\varphi_{(c)}$ is not local and that the derivative of the right-hand side of this equation is not as simple as it may seem at first sight. We will differentiate this equation with respect to j first, not with respect to $\varphi_{(c)}$, obtaining

$$\frac{\mathfrak{d}}{\mathfrak{d}j_2}\frac{\mathfrak{d}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}} = \frac{\mathfrak{d}j_1}{\mathfrak{d}j_2} = \delta^d_{1,2}.$$

We now use the chain rule in order to rewrite the derivative in terms of $\varphi_{(c)}$,

$$\frac{\mathfrak{d}}{\mathfrak{d}j_2}\frac{\mathfrak{d}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}} = \sum_3 \frac{\mathfrak{d}\varphi_{(c)3}}{\mathfrak{d}j_2}\frac{\mathfrak{d}^2\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)3}\mathfrak{d}\varphi_{(c)1}} = \delta^d_{1,2}.$$

Now, from equations (3.6.3) and (3.6.4) we have that

$$\frac{\mathfrak{d}\varphi_{(c)3}}{\mathfrak{d}j_2} = \frac{\mathfrak{d}}{\mathfrak{d}j_2}\frac{\mathfrak{d}W}{\mathfrak{d}j_3} = g_{(c,j)3,2},$$

from which it follows that

$$\sum_3 g_{(c,j)3,2}\frac{\mathfrak{d}^2\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)3}\mathfrak{d}\varphi_{(c)1}} = \delta^d_{1,2}. \tag{3.7.2}$$

This result tells us that the second functional derivative of Γ is the inverse of the propagator in position space, both the propagator and its inverse considered as operators in space-time, with matrix representations such as the ones we saw before, in section 2.3, for the finite-difference operators. We will give this new operator a name, which is suggestive in the case of the free theory,

$$\frac{\mathfrak{d}^2\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}\mathfrak{d}\varphi_{(c)2}} = \Box_{(c)1,2}, \tag{3.7.3}$$

where the propagator is the inverse of the operator $\Box_{(c)}$, that is, $g_{(c,j)1,2} = \Box^{-1}_{(c)1,2}$. Let us exemplify this with the theory of the free scalar field. One can show (problem 3.7.1) that, in the theory of the free scalar field defined by the action S_0,

$$S_0[\varphi] = \frac{1}{2}\sum_\ell (\Delta_\ell\varphi)^2 + \frac{\alpha_0}{2}\sum_s \varphi^2(s),$$

which may be written in a more familiar form, in the continuum limit, as a differential equation with a Dirac delta function in the non-homogeneous term, so that we have, in terms of the corresponding dimensionfull quantities,

$$\left(-\sum_{\mu}\partial_{\mu}^{2}+m_{0}^{2}\right)G_{(c)}(x_{1}-x_{2})=\delta^{d}(x_{1}-x_{2}).$$

Observe that, since Γ is quadratic on the fields, any higher-order functional derivative of Γ vanishes, showing that the propagator and hence the phenomenon of propagation are the only physical content of this model. In general these higher-order derivatives are related to the so-called *irreducible* functions with more than two points, that is, with the physical interactions that exist in the models. Their absence in this case is the mathematical translation of the fact that this is a theory of free fields. In future volumes it will be seen that in non-linear models the higher-order derivatives of the effective action will give us directly the renormalized coupling constant, whose value describes the intensity of the physical interactions that exist in the quantum theory.

Problems

3.7.1. Starting from its definition, given in equation (3.7.1), calculate the effective action Γ of the theory of the free scalar field defined by $S = S_0$, obtaining the result given in the text, in equation (3.7.4). In order to do the calculation transform the action to momentum space and use the explicit relation between $\widetilde{\varphi}_{(c)}$ and $\widetilde{\jmath}$ given in equation (3.5.3), which in our current notation may be written as

$$\widetilde{\varphi}_{(c)}(\vec{k})=\frac{\widetilde{\jmath}(\vec{k})}{\rho^{2}(\vec{k})+\alpha_{0}}.$$

3.7.2. Using the explicit form of the effective action Γ of the free theory, given in equation (3.7.4), for the one-dimensional case $d = 1$, calculate its second functional derivative with respect to the classical field, in two positions n_1 and n_2,

$$\frac{\mathfrak{d}^{2}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)}(n_{1})\mathfrak{d}\varphi_{(c)}(n_{2})},$$

showing that the result is $2+\alpha_0$ if $n_2 = n_1$, -1 if $n_2 = n_1 + 1$ or if $n_2 = n_1 - 1$ and 0 in any other case. In this way, it becomes clear that this operation of functional differentiation does in fact recover the matrix elements of the matrix representation of the Euclidean Klein-Gordon operator in configuration space.

Chapter 4

Correlation Structure

In this chapter we will perform a careful and detailed analysis of the two-point correlation function of the Gaussian model. In this way we will be using the calculational techniques described in the previous chapters in order to probe into the fundamental structure of the theory, regarding its correlation functions. This is where we depart from the purely traditional approach to the subject, because we shall see that the results obtained are not part of that traditional approach, and lead to the necessity of a fundamental reinterpretation of the theory. In fact, some aspects of the behavior of the two-point function are quite surprising at first sight.

We will also examine in detail the issue of the mathematical nature of the field configurations that contribute in a dominant way to the expectation values of the theory. The conclusion that we will be led to, that those configurations are not only non-differentiable functions, but that they are in fact discontinuous functions on all the points of their domains, will put the definition of the quantum theory of fields in terms of functional integrals defined on the lattice in sharp contrast to the usual path-integral approach to quantum mechanics. This important fact will have important future consequences for the mathematical treatment of the theory.

We will also introduce and examine in detail the concept of block variables, which will be instrumental in solving the conceptual problems posed by the singular structure of the two-point function. In fact, these variables will turn out to be of central importance for the physical interpretation of the theory. We will see that these variables are closely related to the Fourier components of the field in momentum space, and hence that these Fourier components are quantities more closely related to the observational aspects of the theory, and better instruments than their counterparts in position space for looking into the physical content of the theory.

4.1 Structure of the Two-Point Function

As we saw in section 3.4, the complete solution of the theory of the free scalar field is reducible to the calculation of the propagator, with the consequence that all the physics of the theory is contained in the structure of this propagator. We will

Substituting this "1" in equation (4.1.1) and approximating the discrete lattice quantity $\rho^2(\vec{k}) + \alpha_0$ by $a^2[p^2(\vec{k}) + m_0^2] = L^2[p^2 + m_0^2]/N^2$ we obtain

$$\sigma^2 \sim \frac{1}{N^d} \sum_{\vec{k}} \mathrm{d}^d p \left(\frac{L}{2\pi}\right)^d \frac{N^2}{L^2} \frac{1}{p^2 + m_0^2},$$

so that we may now approximate σ^2 by the integral

$$\sigma^2 \sim \frac{1}{(2\pi)^d} \left(\frac{L}{N}\right)^{d-2} \int \mathrm{d}^d p \, \frac{1}{p^2 + m_0^2}.$$

We must now discuss how to determine the extremes of integration. Note that for $d \geq 3$, due to the factor of N^{d-2} in the denominator, the result can only be non-vanishing in the $N \to \infty$ limit if the integral diverges in that limit. For p near zero the integrand is finite, so long as m_0 is not zero, so that the integral cannot diverge at this extreme. For simplicity, let us assume temporarily that $m_0 \neq 0$, postponing until later the discussion of the case $m_0 = 0$. It follows from these considerations that for $d \geq 3$ the only part of the domain of integration that matters is the one for large absolute values p of the momenta. In any case, we can write the integral in spherical coordinates in momentum space, obtaining

$$\sigma^2 \sim \frac{1}{(2\pi)^d} \left(\frac{L}{N}\right)^{d-2} \Omega_{d-1} \int_0^{N\pi/L} \mathrm{d}p \, \frac{p^{d-1}}{p^2 + m_0^2},$$

where Ω_{d-1} is the complete solid angle in d dimensions and $N\pi/L$ is the largest possible value for the components of the momentum on a lattice with N sites in each direction. Since we are not interested in the lower limit of the integral, we may neglect the m_0 that appears in the denominator and write the integral as

$$\sigma^2 \sim \frac{1}{(2\pi)^d} \left(\frac{L}{N}\right)^{d-2} \Omega_{d-1} \int_{p_m}^{N\pi/L} \mathrm{d}p \, p^{d-3},$$

where p_m is some small and finite but non-vanishing value of the momentum, which we could choose to be m_0 or $2\pi/L$. Recalling that we are discussing all this mostly in the context of the case $d \geq 3$, we see now that for dimensions $d \leq 2$ the factor of p appear in the denominator, so that indeed we will have to examine the cases $d = 1$ and $d = 2$ separately. We may now do the integration for the case $d \geq 3$, obtaining

$$\begin{aligned} \sigma^2 &\sim \frac{1}{(2\pi)^d} \left(\frac{L}{N}\right)^{d-2} \Omega_{d-1} \frac{p^{d-2}}{d-2} \Bigg|^{N\pi/L} \\ &\sim \frac{1}{(2\pi)^d} \left(\frac{L}{N}\right)^{d-2} \Omega_{d-1} \frac{1}{d-2} \left(\frac{N\pi}{L}\right)^{d-2}, \end{aligned}$$

were we neglected the contribution from the lower extreme of the integral, which vanishes in the limit. We see that the factors of N cancel out and that the final result for σ^2 in the limit $N \to \infty$ is

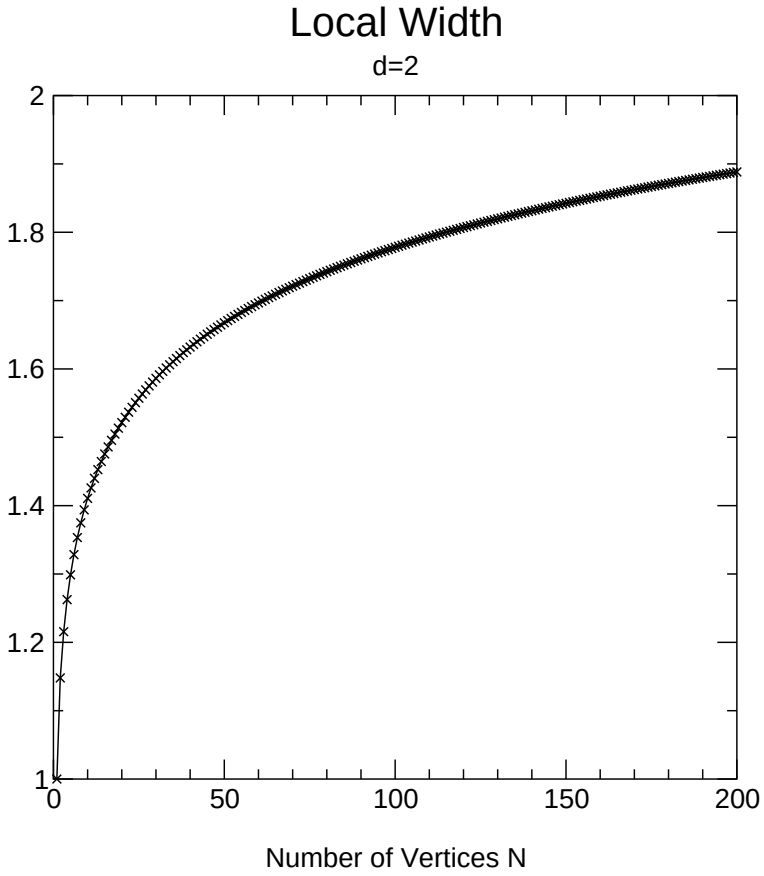


Figure 4.1.2: Behavior of the squared local width σ^2 with N in the case $d = 2$.

of the integral contributes. In this case we have that $\Omega_0 = 2$ and the integral may be written as

$$\sigma^2 \sim \frac{N}{\pi L} \int_{p_m}^{N\pi/L} \frac{\mathrm{d}p}{p^2} \sim \frac{N}{\pi L p_m},$$

so that in this case σ^2 diverges linearly with N. Due to the fact that in these cases the lower extreme contributes significantly to the integral, these are the only cases in which the results depend on p_m, that is, on the details of the choice of the lower integration limit. Since this limit was introduced only to allow us to eliminate m_0 from the integrand and hence facilitate the realization of the integral, this means, in fact, that in these cases the results depend on m_0. In fact, it is possible to improve the analytical calculation in the case $d = 1$ (problem 4.1.1), so as to verify this is an explicit way.

One can perform more careful calculations than these to evaluate the sums that appear in the formulas for σ^2, building integrals that are strict lower bounds and strict upper bounds to the sums (problem 4.1.4), so as to *prove* that σ^2 in fact behaves as a function of N, for large N, in the way given here. In any case, it must

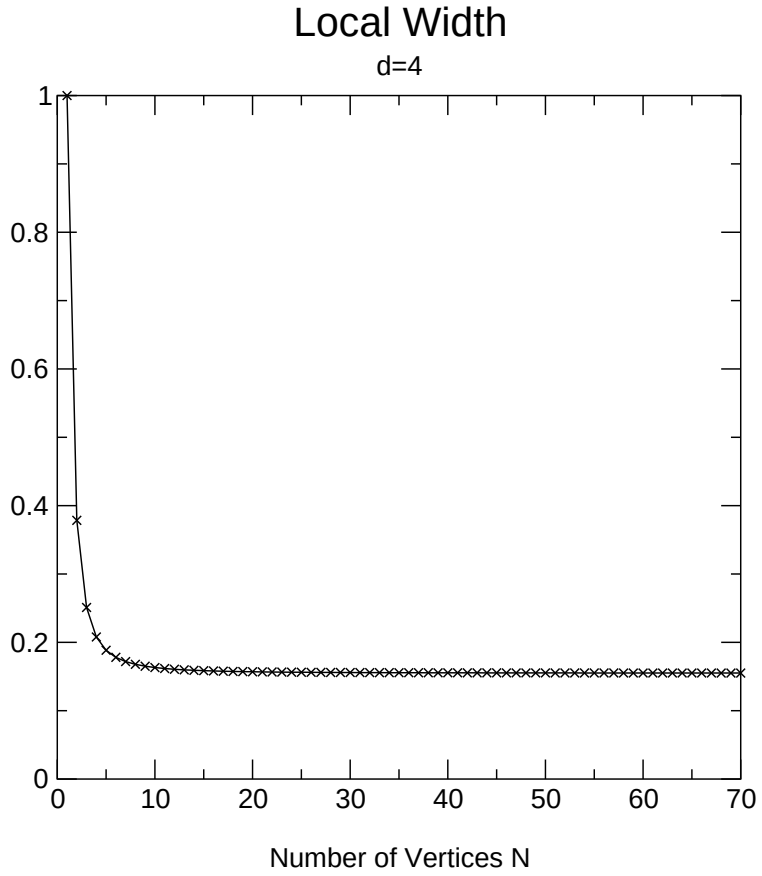


Figure 4.1.4: Behavior of the squared local width σ^2 with N in the case $d = 4$.

of finite lattices in dimensions d from 1 to 5, for the case $m_0 = 1$, obtained by the use of such programs. For $d = 1$ one can see clearly the linear divergence with N. In the case $d = 2$ the logarithmic divergence is also quite clear and it is not difficult to make sure of its nature by simply plotting the graph on an adequate logarithmic scale (problem 4.1.5). Starting with the $d = 3$ case the behavior changes radically, the function $\sigma^2(N)$ becomes a decreasing rather than increasing function of N, approaching a plateau at a finite and non-vanishing value. The flatness of this plateau becomes clearer as the dimension increases, at the same time that its value decreases. In addition to this, as the dimension increases the value of the plateau is approached ever faster, for lattices which are ever smaller in their linear dimensions. Extrapolating these results (problem 4.1.6) to the limit $N \to \infty$ we obtain for σ the final results shown in table 4.1.1.

In all this analysis we see, in a very clear way, that the cases $d = 1$ and $d = 2$ are very special. For $d \geq 3$ we have finite fluctuations of the values of φ at the sites, while for $d = 1$ and $d = 2$ these fluctuations diverge. Observe that in all cases σ^2 is the maximum value of g, because for $\vec{x}_1 \neq \vec{x}_2$ the terms of the sum that defines g are multiplied by numbers with absolute values smaller than 1. This is consistent

d	$\sigma(N \to \infty)$
1	$\simeq \sqrt{1/12 + 1/(m_0 L)^2}\sqrt{N}$
2	$\simeq 0.4095\sqrt{\ln(N)}$
3	$\simeq 0.5027$
4	$\simeq 0.3936$
5	$\simeq 0.3400$

Table 4.1.1: Results for the local width σ for large values of N.

$$G(\vec{x}_1 - \vec{x}_2) = \frac{N^{d-2}}{L^{d-2}N^d} \sum_{\vec{k}} \frac{e^{-\imath \frac{2\pi}{L}\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)}}{\rho^2(\vec{k}) + \alpha_0}.$$

This time our objective is to show that the function G is finite in the continuum limit, so long as $\vec{x}_1 \neq \vec{x}_2$. We will once more approximate the sum by an integral,

$$\begin{aligned} G(\vec{x}_1 - \vec{x}_2) &\sim \frac{1}{L^{d-2}N^2} \sum_{\vec{k}} \left(\frac{L}{2\pi}\right)^d \mathrm{d}^d p \, \frac{e^{-\imath\vec{p}\cdot(\vec{x}_1 - \vec{x}_2)}}{a^2[p^2(\vec{k}) + m_0^2]} \\ &\sim \frac{1}{(2\pi)^d} \int \mathrm{d}^d p \, \frac{e^{-\imath\vec{p}\cdot(\vec{x}_1 - \vec{x}_2)}}{p^2 + m_0^2}. \end{aligned} \tag{4.1.2}$$

Observe that this time there are no divergent terms in front of the integrals. Once more, we must discuss the extremes of integration. Our intention here is to eventually make $L \to \infty$, going in this way from the finite box to infinite space, where G has a simpler form. For the time being, however, we are still doing the integration in the context of a finite position-space volume. For simplicity, we will approximate the momentum-space integral doing it over a spherical domain whose radius is the largest possible value of a momentum component on a d-dimensional lattice with N^d sites. Under these conditions, if we define $\vec{r} = \vec{x}_1 - \vec{x}_2$, we see that G depends only on the modulus r of the vector $\vec{r}$ because, if we make an arbitrary change in the angles of the versor $\hat{r}$, we can make the integral over the momenta return to its previous form doing a corresponding rotation of the integration variables. Hence we can put $\vec{r}$ in the direction of the d^{th} component of $\vec{p}$ and write, for dimensions $d > 2$, without loss of generality,

$$G(r) \sim \frac{1}{(2\pi)^d} \int_{\Omega_{d-1}} \mathrm{d}^{d-1}\Omega \int_0^{N\pi/L} \mathrm{d}p \, p^{d-1} \, \frac{e^{-\imath p r \cos(\theta_{d-2})}}{p^2 + m_0^2}, \tag{4.1.3}$$

where θ_{d-2} is the angle between the vector $\vec{p}$ and its d^{th} component and the angular integration is over the solid angle Ω_{d-1} of the d-dimensional space, with integration element given by

$$\mathrm{d}^{d-1}\Omega = \mathrm{d}\phi \sin(\theta_1)\mathrm{d}\theta_1 \sin^2(\theta_2)\mathrm{d}\theta_2 \ldots \sin^{d-2}(\theta_{d-2})\mathrm{d}\theta_{d-2},$$

equal to $(-2\pi\imath)$ times the value of the residue of the integrand in the lower pole, that is,

$$G(x>0) = \frac{1}{2\pi}(-2\pi\imath)\frac{e^{-m_0 x}}{-2\imath m_0} = \frac{e^{-m_0 x}}{2m_0}.$$

If $x<0$ we should close the contour by the other side, the factor multiplying the residue is $(2\pi\imath)$, and hence we obtain in this case

$$G(x<0) = \frac{1}{2\pi}(2\pi\imath)\frac{e^{m_0 x}}{2\imath m_0} = \frac{e^{m_0 x}}{2m_0}.$$

Defining $r=|x|$, we can join the two answers in the final result

$$G(r) = \frac{e^{-m_0 r}}{2m_0}.$$

We see that the result is finite for all values of r, including $r=0$. If fact, we can verify directly that $G(0)$ is finite in this case. As we saw before, we have for the dimensionless function the behavior $g(0)\sim N/(\pi L p_m)$ and, since in the case $d=1$ it holds that $G=ag$, it follows that $G(0)\sim 1/(\pi p_m)$, which is also finite. The complete equality of the two results corresponds to the choice $p_m = 2m_0/\pi$ for the lower extreme p_m on the integral used in the approximate calculation of σ^2.

Passing now to the case $d=3$, in this case we have from equation (4.1.3) that

$$G(r) \sim \frac{1}{(2\pi)^3}\int_0^{2\pi} \mathrm{d}\phi \int_{-1}^{1} \mathrm{d}[\cos(\theta)] \int_0^{N\pi/L} \mathrm{d}p\, \frac{p^2}{p^2+m_0^2}\, e^{-\imath p r\cos(\theta)}.$$

We can do immediately the integrals over ϕ e θ, obtaining

$$\begin{aligned} G(r) &\sim \frac{1}{4\pi^2}\int_0^{N\pi/L} \mathrm{d}p\, \frac{p^2}{p^2+m_0^2}\, \frac{e^{-\imath p r}-e^{\imath p r}}{-\imath p r} \\ &= \frac{1}{2\pi^2 r}\int_0^{N\pi/L} \mathrm{d}p\, \frac{p}{p^2+m_0^2}\, \sin(pr). \end{aligned}$$

If we now observe that the integrand is even, we may write this as

$$\begin{aligned} G(r) &\sim \frac{1}{4\pi^2 r}\int_{-N\pi/L}^{N\pi/L} \mathrm{d}p\, \frac{p}{p^2+m_0^2}\, \sin(pr) \\ &= \frac{1}{4\pi^2 r}\int_{-N\pi/L}^{N\pi/L} \mathrm{d}p\, \frac{p}{(p-\imath m_0)(p+\imath m_0)}\, \frac{e^{\imath p r}-e^{-\imath p r}}{2\imath}. \end{aligned}$$

where we again wrote the sine in terms of complex exponentials. Each one of these two integrals can be done in the complex-p plane, in the limit $N\to\infty$, in the same way in which we did the integral in the case $d=1$, closing the circuit in the appropriate way in each case. Doing this we obtain

$d = 1$ and $d = 2$ diverge in the limit $m_0 \to 0$. These are what one refers to as *infrared divergences*, a type of behavior which is characteristic of the lower dimensions, in particular of $d = 1$ and $d = 2$. One can verify that the behavior for $m_0 \to 0$ is also problematic in the case of the calculations of σ^2 which we did before. We will now examine how σ^2 behaves in this limit, in each dimension. From equation (4.1.1) we see that σ^2 always diverges if we make $\alpha_0 \to 0$, even on finite lattices, because the term of the sum involving the mode $\vec{k} = \vec{0}$ diverges in this limit. We may write for σ^2

$$\sigma^2 = \frac{1}{N^d \alpha_0} + \frac{1}{N^d} {\sum_{\vec{k}}}' \frac{1}{\rho^2(\vec{k}) + \alpha_0},$$

where in the sum $\sum'_{\vec{k}}$ the zero mode is omitted. As we mentioned before, the Gaussian model on the torus indeed has a zero mode in the case $\alpha_0 = 0$, which is what is causing us trouble. This is not a physical problem, but only a mathematical problem that reflects the fact that the periodical boundary conditions are not completely realistic from the physical point of view. If we want to deal with models where $\alpha_0 = 0$ on finite lattices, it will be necessary to change slightly the dynamics of the models in order to eliminate the degree of freedom corresponding to the zero mode, as indeed we will do in future volumes, when we discuss non-linear models of scalar fields.

However, it is not necessary to make $\alpha_0 = 0$ on finite lattices in order to study field theories which are massless in the continuum limit. It suffices to recall that α_0 is related to the mass by $\alpha_0 = (m_0 a)^2 = (m_0 L)^2 / N^2$, so that α_0 goes to zero in the limit no matter what value is given to m_0. Since we have

$$m_0^2 = \frac{1}{L^2} \alpha_0 N^2,$$

we can either cause m_0 to have a finite non-vanishing limit, by means of a decrease in α_0 given by $1/N^2$, or cause m_0 to vanish in the limit by means of a decrease in α_0 which is faster than $1/N^2$. Hence, there is a way to represent zero-mass theories by means of infinite sequences of finite lattices in which α_0 is always different from zero, which avoids the divergence of the zero-mode term in the sum that defines σ^2. It remains to be seen how this term behaves in the continuum limit, in each dimension. For finite masses we have that this term is

$$\frac{1}{N^d} \frac{N^2}{(m_0 L)^2} = \frac{1}{(m_0 L)^2 N^{d-2}},$$

so that we see that this term goes to zero for $d \geq 3$, is constant for $d = 2$ and diverges with N for $d = 1$. In all cases these results do not significantly affect the calculations made before for $m_0 \neq 0$. For $d = 1$ the zero-mode term has exactly the same behavior found for the sum, for $d = 2$ it is constant while the sum diverges logarithmically and for $d \geq 3$ it goes to zero, while the sum has a finite non-vanishing limit.

non-vanishing values of r. Since for the cases of interest, with $d \geq 3$, $g(0)$ is also finite and non-vanishing in the limit, it follows that *for* $d \geq 3$ *the two-point function* $g(r)$ *is also zero for* $r \neq 0$. In short, we have the continuum-limit results

$$\mathfrak{f}(r) = \begin{cases} 1 & \text{if} \quad r = 0 \\ 0 & \text{if} \quad r \neq 0 \end{cases},$$

$$g(r) = \begin{cases} \sigma^2 & \text{if} \quad r = 0 \\ 0 & \text{if} \quad r \neq 0 \end{cases}.$$

The meaning of these results is that the fundamental fields of quantum field theory become *completely uncorrelated* in the continuum limit. One can say that when one takes the continuum limit all the structure of the two-point function, including the characteristics of the exponential decay related to the mass, collapse into the origin. The result of the continuum limit looks like utter uncorrelated chaos. This is a surprising result, because the correlation between the fields in Euclidean space is directly related to the propagation of perturbations across space-time in the non-Euclidean version of the theory. Furthermore, the nature of this propagation process is supposedly classifiable according to the value of the physical mass m_0, which can be either zero or not zero.

In order to better understand the significance of these functions in quantum field theory it is essential that we introduce the concept of *block variables*, which we shall examine in detail later on. We will see that these block variables are the mechanism by means of which physical order arises out of the utter chaos of the underlying realm of the fundamental field variables. In this way one can say that quantum field theory is an example of a type of self-organizing structure. We will also see that in quantum field theory the only reasonably simple way to deal with the dynamics of the models is to work with the dimensionfull propagator $G(r)$, which is finite at all points but the origin. Only through an analysis involving block variables we may understand why this function is the one that has most physical relevance, despite its divergence at the origin.

The behavior of $g(r)$ shown above will also be useful in the intuitive discussion of the important phenomenon of the *triviality* of the non-linear models of scalar fields, which we will discuss in future volumes. This triviality means that the models fail to contain physical interactions between particles in the continuum limit, despite their non-linear nature. This is one reason why we must look elsewhere for physically relevant interacting models, and are thus naturally led to the study of gauge theories.

Problems

4.1.1. Consider, in the case $d = 1$, the quantity $\Sigma'^2 = L\sigma'^2/N$ where σ'^2 is defined like σ^2 except for the omission from the sum of the zero-mode $k = 0$. Calculate Σ'^2 in the particular case $m_0 = 0$. Analyze from which extreme of the integral comes the main contribution in this case, and verify that one can approximate $N^2\rho^2(k)$ by $(2\pi k)^2$ for large N. It will be useful to recall the definition of the

4.1.7. Obtain the dimensionfull correlation functions $G(r)$ in position space for the cases $d = 2$, $d = 4$ and $d = 5$, calculating the corresponding integrals over momentum space, as discussed in the text.

4.1.8. Calculate the functions $G(\vec{x}_1 - \vec{x}_2)$ in the continuum, for $d = 1$ and $d = 2$, within finite cubical boxes of side L, using fixed boundary conditions with vanishing fields at the border, starting from the results presented in the text for infinite space. Remember that these functions, besides being the propagators of the quantum models in position space, are also the Green functions (fields of unit point-like external sources) of the corresponding classical models. For simplicity make $\vec{x}_2 = \vec{0}$ and calculate the functions in terms of $\vec{x}_1$. Remember also that the Gaussian models are linear and that a principle of superposition holds for them, which enables one to use a version of the method of images, which is very popular in electrostatics, to solve the problem. Your answers should be written in the form of infinite series. In general these series are not absolutely convergent, but they are Borel-sumable, that is, it is possible to find a specific order of summation for which they converge. See if you can figure out what is the special order for these sums.

4.1.9. Consider $\sigma^2(m_0)$ as defined in equation (4.1.1), where $\alpha_0 = (m_0 L)^2/N^2$. Consider the cases for which $d \geq 3$, in which both σ^2 and m_0 have finite and non-vanishing limits in the continuum limit. Differentiate σ^2 as a function of m_0 and show that the resulting sum goes to zero in the limit, thus showing that σ^2 becomes independent of m_0 in the limit. In order to do this, approximate the sums by integrals over the momenta, as was done in the text for the calculation of σ^2.

4.2 Discontinuity of the Configurations

In this section we will discuss one of the most basic properties of quantum field theory, which characterizes its inner workings in a very fundamental way. This is the fact that the field configurations in configuration space that contribute in a dominant way to the expectation values of the observables of the theory are *discontinuous*, in the continuum limit, as functions of the coordinates that span space-time. This property will have important consequences relating to many aspects of the inner workings of the theory, as we will discuss later, mostly in subsequent volumes of these notes.

Let us cite a few examples, so that the reader can judge the importance of the topic: the discontinuity of the field configurations is the basic phenomenon responsible for the appearance of divergent quantities in the perturbative approach to the theory; it causes different finite-differencing schemes on the lattice, which are equivalent in the classical theory, not to be so in the quantum theory; it changes in

the fields may be examined by first taking the lattice spacing to zero, while ε is kept constant in relation to the correlation length of the theory, and only after that making ε tend to zero within the continuous space that results from the first limit. This might be the more natural way to take the limit in order to establish a notion of continuity for fields defined on a lattice, but it is not the most relevant way in the context of the definition of the theory in terms of functional integrals on the lattice.

A different notion of continuity appears in this context. The quantum theory is defined by the functional integral of the exponential of the action, and it is the behavior of the derivatives that this action contains which is of far more direct interest to us. When the models are defined on the lattice, the discrete representation of the action contains finite differences of the fields at close-neighboring sites. Therefore, in the continuum limits within this formalism the quantity ε is *is always kept equal* to the lattice spacing a. Hence, in this case the limits $\varepsilon \to 0$ and $a \to 0$ are taken *simultaneously*, unlike what happened in the other type of limit. In what follows we will stick to this type of limit, which is the one with greater relevance for the definition of the quantum theory of fields by means of the lattice. However, one can show (problem 4.2.2) that the situation does not change qualitatively when one exchanges one type of limit by the other.

As always, we will use the theory of the free scalar field as an example. In order to have a definite case to examine, we will also adopt periodical boundary conditions, but this does not have any fundamental importance for the results. The calculations we must do are not, in fact, very complex. It suffices to use the result obtained before for the propagator of this model in momentum space, which can be written as

$$\langle \widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}')\rangle_N = \frac{\delta^d(\vec{k},-\vec{k}')}{N^d[\rho^2(\vec{k})+\alpha_0]}.$$

From this result it is simple to show that $\langle[\Delta_\mu\varphi(\vec{n})]^2\rangle_N$ tends to a finite and non-vanishing value when $a \to 0$, that is, when $N \to \infty$. Using the Fourier transforms we may write

$$\begin{aligned}
[\Delta_\mu\varphi(\vec{n})]^2 &= \left[\sum_{\vec{k}} \widetilde{\varphi}(\vec{k})\ \Delta_\mu e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\right]\left[\sum_{\vec{k}'} \widetilde{\varphi}(\vec{k}')\ \Delta_\mu e^{\imath\frac{2\pi}{N}\vec{k}'\cdot\vec{n}}\right] \\
&= \sum_{\vec{k}}\sum_{\vec{k}'} \widetilde{\varphi}(\vec{k})\ \widetilde{\varphi}(\vec{k}')\ \rho_\mu(k_\mu)\ \imath\ e^{\imath\frac{\pi}{N}k_\mu}\ e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\ \rho_\mu(k'_\mu)\ \imath\ e^{\imath\frac{\pi}{N}k'_\mu}\ e^{\imath\frac{2\pi}{N}\vec{k}'\cdot\vec{n}},
\end{aligned}$$

where we used the fact that the complex exponentials are eigenvectors of the finite-difference operator, as discussed in section 2.7. We also used the quantities $\rho_\mu(k_\mu)$ defined in equation (2.7.1). Taking now the expectation value on an N-lattice we obtain

$$\langle[\Delta_\mu\varphi(\vec{n})]^2\rangle_N = -\sum_{\vec{k}}\sum_{\vec{k}'}\langle\widetilde{\varphi}(\vec{k})\widetilde{\varphi}(\vec{k}')\rangle_N\ \rho_\mu(k_\mu)\ \rho_\mu(k'_\mu)\ e^{\imath\frac{\pi}{N}(k_\mu+k'_\mu)}\ e^{\imath\frac{2\pi}{N}(\vec{k}+\vec{k}')\cdot\vec{n}}$$

$$\frac{1}{2d} < \langle [\Delta_\mu \varphi(\vec{n})]^2 \rangle \leq \frac{1}{d}.$$

This result shows that, for any finite dimension of space-time, on average over the ensemble of configurations, *the variation of the field from one site to the next one does not approach zero when the lattice spacing goes to zero.* It follows that, on average, in the continuum limit, the configurations of the dimensionless field are not continuous as functions of position. Observe that this is a very violent type of discontinuity, because we are not talking here of a set of isolated discontinuities in a continuous functions. The field is discontinuous in all directions and *at all the points* where it is defined. Obtaining an exact result for $\langle [\Delta_\mu \varphi(\vec{n})]^2 \rangle$ requires more work. One can show (problem 4.2.4) that in the continuum limit the sum in fact assumes its upper bound, so that we have

$$\langle [\Delta_\mu \varphi(\vec{n})]^2 \rangle = \frac{1}{d}.$$

Having established this important result, we may now examine some of its immediate consequences. If we recall that the dimensionfull field ϕ is related to the dimensionless field by $\phi = a^{(2-d)/2}\varphi$, we can determine how the derivatives of the dimensionfull fields behave in the continuum limit. For a small but non-zero we have

$$\langle [\Delta_\mu \phi(\vec{n})]^2 \rangle \sim \frac{a^{2-d}}{d}.$$

The meaning of this relation depends on the dimension d. For $d = 1$ we have that, in the continuum limit,

$$\langle [\Delta_\mu \phi]^2 \rangle \sim a \to 0,$$

while for the derivative $\partial_\mu \phi = \Delta_\mu \phi / a$ itself we have

$$\langle [\partial_\mu \phi]^2 \rangle \sim \frac{1}{a} \to \infty,$$

which shows that in this case the dimensionfull field is continuous but not differentiable. One can show (problem 3.1.2) without difficulty that the quantum theory of the free scalar field in one dimension is formally identical to the quantum mechanics of the harmonic oscillator, by mapping the quantities that appear in one of these two structures onto corresponding quantities of the other. This result for $d = 1$ reproduces, therefore, the well-known quantum-mechanical fact that the one-dimensional configurations involved in the functional integration are in that case *random walks*, continuous but non-differentiable paths, as those of a Brownian motion. In this case the denomination of the functional integral as a path integral is justified, but this is a characteristic *exclusively of the one-dimensional case.* Already for $d = 2$ we have,

that is, the expectation value of the action diverges as N^d. Note that the action is dimensionless and that this divergence has nothing to do with an increase in the volume of the box within which we are defining the model, the action diverges even if we are within a finite box. This is a property related to the behavior of the high-frequency modes of the theory, which we denominate the *ultraviolet regime*, which has nothing to do with the infrared aspects connected to the volume of the box.

We may also examine the behavior of the mass term S_M of the action S_0, the one that contains the parameter α_0,

$$S_M = \frac{\alpha_0}{2} \sum_s \varphi^2(s),$$

in a way analogous to the analysis of S_K. This is another term that will also appear in other models involving scalar fields, usually as part of a potential involving the fields, which establishes non-linear relations among them. The expectation value of this part of the action may be written as

$$\langle S_M \rangle = \frac{\alpha_0}{2} \sum_s \langle \varphi^2(s) \rangle.$$

As we saw in section 4.1, the expectation value $\sigma^2 = \langle \varphi^2 \rangle$ has a finite and non-vanishing limit for $d \geq 3$, diverging for $d = 1$ and $d = 2$. Besides, σ^2 does not depend on position, and it therefore follow that

$$\langle S_M \rangle = \frac{\alpha_0}{2} N^d \sigma^2.$$

Since $\alpha_0 = (m_0 L)^2/N^2$, we have that for $d \geq 3$ this part of the action also diverges, although in a somewhat slower way than the kinetic part,

$$\langle S_M \rangle = \frac{(m_0 L)^2}{2} N^{d-2} \sigma^2 \to \infty.$$

For $d = 2$ the divergence becomes logarithmic, due to the fact that in this case $\sigma^2 \sim \ln(N)$, while in the case $d = 1$ there is no divergence, because in this case σ^2 diverges with N and cancels the factor of N^{-1}, resulting on a finite action. Once more we see that the case $d = 1$ is significantly different from the others. In the cases of greater interest for us, $d \geq 3$, both $\langle S_K \rangle$ and $\langle S_M \rangle$ diverge in the limit, this second term in a somewhat less violent way than the first. We see therefore that the dynamics defined by S_0 tends to be dominated by the term S_K containing the derivatives.

The most important thing is that we arrive at the inevitable conclusion that S_0 typically diverges and therefore that the statistical weights $\exp(-S_0)$ typically go to zero very fast in the continuum limit. It is necessary to emphasize that this is the *minimum* possible value for these weights, very different from the *maximum* possible value that it assumes for the classical solution, which shows that typically the dominant configurations of the quantum theory are *very distant* from the classical solution, if we use the action as a measure of this distance. This fact may

4.2.2. Calculate, in the case of the quantum theory of the free scalar field, the limit

$$\lim_{\varepsilon\to 0}\left[\lim_{N\to\infty}\left\langle[\varphi(\vec{x}+\varepsilon\hat{x}_\mu)-\varphi(\vec{x})]^2\right\rangle_N\right],$$

in the indicated order, at an arbitrary point $\vec{x}$ and for an arbitrary direction μ, showing that it is finite and not zero. In order to do this expand the square and use the values of $\sigma_0^2 = g(\vec{0})$ and $g(\vec{x}-\vec{x}')$ that were calculated in section 4.1. In this way one shows that the fundamental facts associated to the discontinuity of the fields do not depend on the way in which the limit is defined.

4.2.3. Calculate the d-dimensional sum in momentum space

$$\sum_{k_\mu}\rho_\mu^2(k_\mu), \quad \text{where} \quad \rho_\mu^2(k_\mu) = 4\sin^2(\pi k_\mu/N),$$

decomposing the sine into complex exponentials and using the orthogonality and completeness relations that hold for them.

4.2.4. ($\star$) Find out a more restrictive lower bound for the sum that appears in the calculation of the square of the finite difference of the fields,

$$\frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0},$$

that has the property that its limit is equal to $1/d$ in the continuum limit, hence demonstrating rigorously that

$$\langle[\Delta_\mu\varphi(\vec{n})]^2\rangle \to \frac{1}{d}$$

in the continuum limit[1]. Use for the momentum components the interval of values $[0, N-1]$ and the fact that

$$\rho^2(k_1,k_2,\ldots,k_d) = \rho^2(N-k_1,k_2,\ldots,k_d) = \rho^2(N-k_1,N-k_2,\ldots,k_d), \text{ etc.}$$

The idea is to take off the sum classes of terms that end up not contributing in the limit, in particular the terms with $k_\mu < \sqrt{N}$, in addition to decreasing the sum in other ways that simplify it, until one obtains a sum that can be calculated in the limit and that tends to $1/d$.

4.2.5. Consider the quantum theory of the free scalar field, whose action is S_0. Consider a change of variables from the N^d field variables $\varphi(s)$ to another set of N^d variables, one of which is the action S_0 itself, which varies from 0 to ∞.

[1]This calculation was originally developed in collaboration with Dr. See Kit Foong.

object should have vanishing wavelength and, therefore, consist of "quantums" of infinite energy. We are forced to conclude that, as refined and developed as the measurement apparatus may be, it will always end up measuring the field over some region of space-time with finite and non-vanishing dimensions, however small they may be.

Since we are interested in quantum field theory in the continuum limit from the lattice, we will always end up having an infinite number of points within any finite region, when we take the limit. Therefore any measurement instrument will always, in practice, be measuring the field over an *infinite* number of points, never at a single point. The actual result of the measurement by the apparatus depends not only on the values of the fields at the points involved, but also on the nature of the *superposition rule* for the fields, generating from the values of the field at all the points a single resulting value to be associated to the region as a whole. This rule is not arbitrary, of course, it is related to the way in which the measurement apparatus interacts with the fields. Note that, so far as we are able to define the structure of the theory with our current knowledge, the measurement apparatus is an object which remains external do the structure. Hence, any model intended to represent all possible physical measurements based on fields distributed over a continuous space-time should not only discriminate the number and type of fields involved and define a dynamics for them, but should also discriminate a superposition process to be used for each type of field.

In this way we see that, at the stage of development in which the theory is being built here, the discrimination of the superposition process is an *integral part of the definition of a quantum field theory*, in addition to the discrimination of the fields involved and the definition of their dynamics, by means of an action functional S. It is possible that this will cease to be so in a more complete future theory, in which the notion of the physical measurement is included in the structure of the theory from the start, but for the time being we must be content with this state of affairs.

The introduction of block variables in a given model may be understood as a kind of change of variables in the model. However, such a change from point variables to block variables is not invertible, because it involves loss of information about the behavior of the point variables above a certain energy. One should not, however, get the impression that there will be a smaller number of block variables than of the original point variables, that they will always be a finite or even a discrete set. This is due to the fact that it is not necessary to separate space-time into disjoint and exclusive blocks; quite to the contrary, the blocks may very well overlap each other. In fact, we may associate to each single point of space-time a corresponding block variable $\bar{\varphi}$ which is the result of the superposition of the fields φ inside a region of volume V_r centered at that point. In this way we produce a block field $\bar{\varphi}(\vec{n})$ defined over all of space-time, just like the fundamental field $\varphi(\vec{n})$. These new fields are sometimes denominated *block-renormalized fields* for blocks of volume V_r. Note that this is a specific definition using the term "renormalized", which is used in many different ways, not necessarily clear or even consistent, in the usual formalism.

Given a certain energy limit, we may define the corresponding block-renormalized

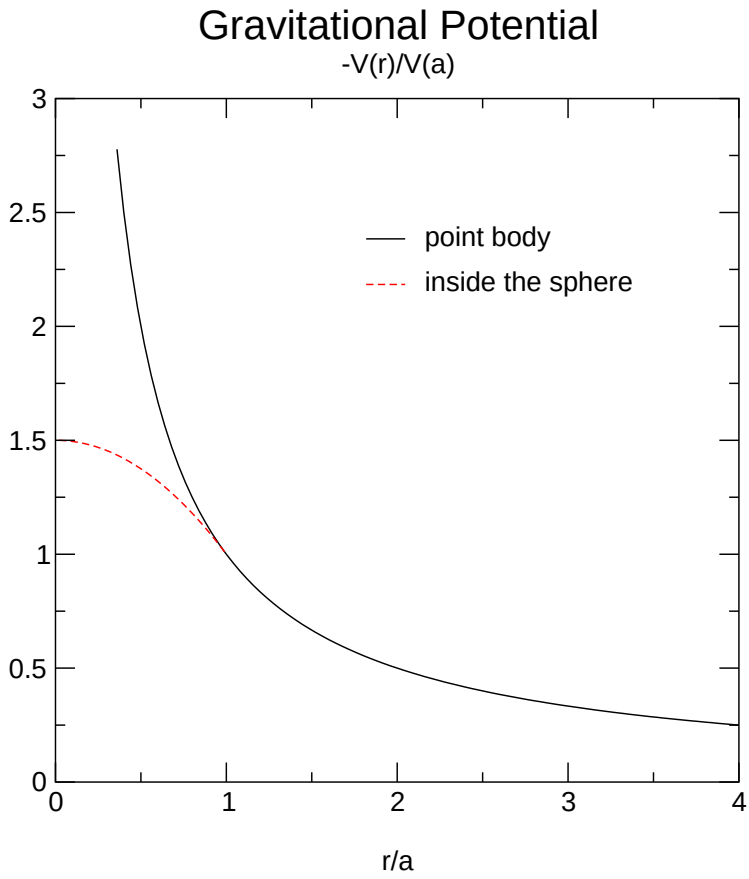


Figure 4.3.2: The gravitational potentials of the point body and of the extended spherical body, showing the smoothing of the singularity.

Newtonian gravitation problem in which one calculates the gravitational potential of a spherical homogeneous body of radius a. In fact, the Newtonian gravitational potential of a point mass is just the Green function of the three-dimensional Laplacian, that is, the Green function of the free theory with $m_0 = 0$ in three dimensions. The geometrical situation is described in figure 4.3.1. Solving this elementary problem of classical mechanics one verifies that, outside the sphere, what is seen is exactly the potential of a point particle located at the origin, with mass equal to the total mass of the body. However, inside the sphere the situation is very different, instead of the singularity of the Green function at the origin, we have a finite and smooth potential over all the interior of the sphere. In figure 4.3.2 a comparison of the two potentials can be found. At distances that are large compared to the radius a of the sphere we have the simple potential of a point mass, while a distances that are small compared to the radius we have a finite field, smoothed out by a mechanism we may call the "smearing" of the point source. This situation is similar to the one we will find for our block variables, with the size of the block playing the role of the volume of the spherical body.

$$\begin{aligned} g_r(\bar{\mathbf{n}}_1, \bar{\mathbf{n}}_2) &= \frac{1}{N_r^{2d}} \sum_{B_1} \sum_{B_2} \langle \varphi(\mathbf{n}_1) \varphi(\mathbf{n}_2) \rangle \\ &= \frac{1}{N_r^{2d}} \sum_{B_1} \sum_{B_2} g(\mathbf{n}_1, \mathbf{n}_2). \end{aligned}$$

We may now write the Green function $g(\mathbf{n}_1, \mathbf{n}_2)$ in terms of the Fourier modes of the lattice as usual,

$$g(\mathbf{n}_1, \mathbf{n}_2) = \sum_{\mathbf{k}} e^{\imath \frac{2\pi}{N} \mathbf{k} \cdot (\mathbf{n}_2 - \mathbf{n}_1)} \widetilde{g}(\mathbf{k}),$$

where it becomes explicit that $g(\mathbf{n}_1, \mathbf{n}_2)$ is a function only of $\mathbf{n}_2 - \mathbf{n}_1$. For the free theory we know that

$$\widetilde{g}(\mathbf{k}) = \frac{1}{N^d} \frac{1}{\rho^2(\mathbf{k}) + \alpha_0},$$

so that we obtain for the block propagator

$$g_r(\bar{\mathbf{n}}_1, \bar{\mathbf{n}}_2) = \frac{1}{N_r^{2d}} \frac{1}{N^d} \sum_{B_1} \sum_{B_2} \sum_{\mathbf{k}} e^{\imath \frac{2\pi}{N} \mathbf{k} \cdot (\mathbf{n}_2 - \mathbf{n}_1)} \frac{1}{\rho^2(\mathbf{k}) + \alpha_0}.$$

If we now define coordinates $\mathbf{n}_1'$ and $\mathbf{n}_2'$ internal to the blocks, which give the position of the sites with respect, respectively, to $\bar{\mathbf{n}}_1$ and $\bar{\mathbf{n}}_2$, then we have for the sites the relations

$$\mathbf{n}_1 = \bar{\mathbf{n}}_1 + \mathbf{n}_1', \ \mathbf{n}_2 = \bar{\mathbf{n}}_2 + \mathbf{n}_2', \quad \text{in addition to} \quad \mathbf{R} = \bar{\mathbf{n}}_2 - \bar{\mathbf{n}}_1,$$

from which it follows that

$$\mathbf{n}_2 - \mathbf{n}_1 = \bar{\mathbf{n}}_2 - \bar{\mathbf{n}}_1 + \mathbf{n}_2' - \mathbf{n}_1' = \mathbf{R} + \mathbf{n}_2' - \mathbf{n}_1', \tag{4.3.1}$$

so that we may write for the block propagator

$$\begin{aligned} g_r(\bar{\mathbf{n}}_1, \bar{\mathbf{n}}_2) &= \frac{1}{N_r^{2d}} \frac{1}{N^d} \sum_{B_1} \sum_{B_2} \sum_{\mathbf{k}} \frac{1}{\rho^2(\mathbf{k}) + \alpha_0} \, e^{\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{R}} \, e^{-\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{n}_1'} \, e^{\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{n}_2'} \\ &= \frac{1}{N^d} \sum_{\mathbf{k}} \frac{e^{-\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{R}}}{\rho^2(\mathbf{k}) + \alpha_0} \left(\frac{1}{N_r^d} \sum_{B_1} e^{-\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{n}_1'} \right) \left(\frac{1}{N_r^d} \sum_{B_2} e^{\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{n}_2'} \right). \end{aligned} \tag{4.3.2}$$

We now see that the block propagator depends only on $\mathbf{R} = \bar{\mathbf{n}}_2 - \bar{\mathbf{n}}_1$. The two sums in parenthesis are now internal sums within each block, they do not depend on the position of the blocks, but only on the momenta. Since the blocks are all equal by hypothesis, these two parenthesis are the complex conjugates of each other. They are in fact a *form factor* $f_r^{(d)}(\mathbf{k})$, in terms of which we may write

$$g_r(\mathbf{R}) = \frac{1}{N^d} \sum_{\mathbf{k}} \frac{e^{\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{R}}}{\rho^2(\mathbf{k}) + \alpha_0} \left| f_r^{(d)}(\mathbf{k}) \right|^2, \tag{4.3.3}$$

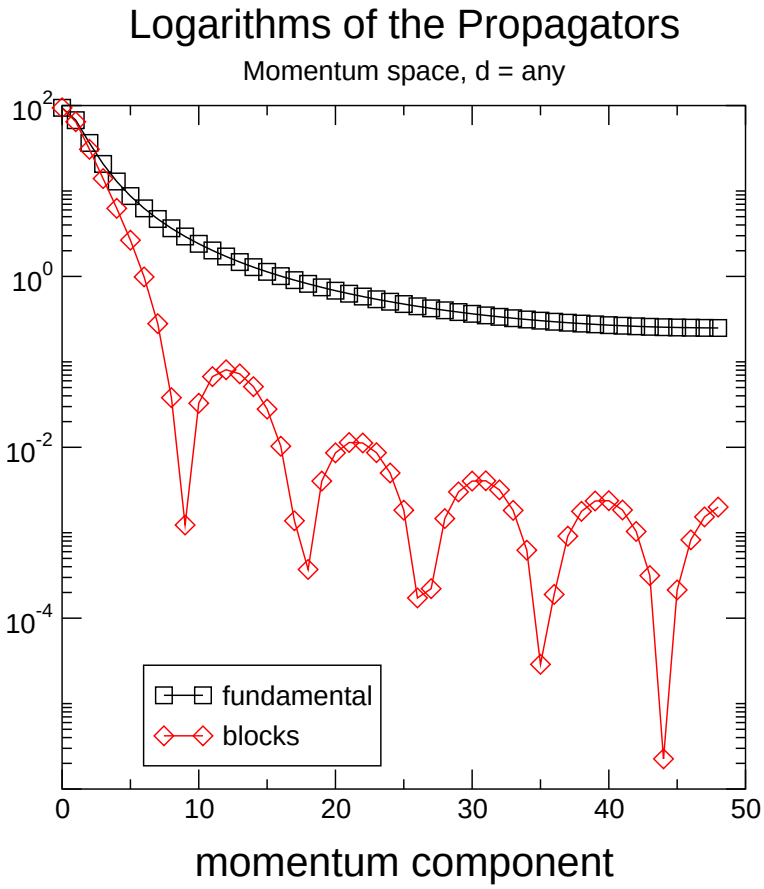


Figure 4.3.4: Logarithms of the fundamental and block propagators in momentum space.

$$= \frac{1}{N_r}\,\frac{\sin\left(\frac{\pi}{N}kN_r\right)}{\sin\left(\frac{\pi}{N}k\right)}$$
$$= \frac{r\sin\left(\frac{k\pi}{r}\right)}{N\sin\left(\frac{k\pi}{N}\right)}.$$

This is true if $k \neq 0$, and if $k = 0$ we have immediately that $f_r(0) = 1$. Finally observe that, for any mode $\mathbf{k}$ of the lattice which coincides with an internal mode of the block, f_r vanishes because the sum that defines it coincides in this case with the sum that appears in the orthogonality and completeness relations of the block itself. We may see from the expression above that this will be true for modes $\mathbf{k}$ such that $k_\mu N_r/N = k_\mu/r$ is an integer for at least one value of μ. In other words, f_r tends to suppress the modes of the lattice whose wavelengths fit an integer number of times within the block, getting, so to say, in resonance with it. If the wavelength does not fit exactly an integer number of times within the block, the mode will be partially suppressed, only a little if the number of times it fits inside is small, more if that number is large. In short, one perceives that f_r tends to suppress preferentially

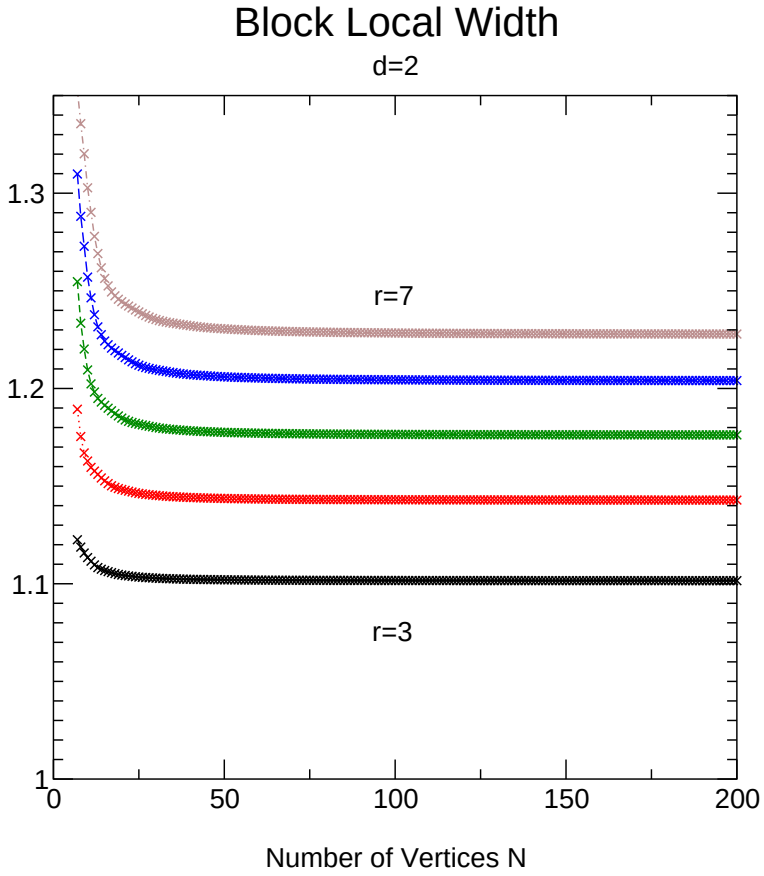


Figure 4.3.6: Behavior of the local block width as a function of N, for $d = 2$.

which is exactly the expression of the propagator of the fundamental dimensionless field in momentum space. We see therefore that for the correlations at large distances, much larger than the size of the blocks, the propagators of the fundamental field and of the blocks do in fact coincide, displaying the same long-range behavior. Examining their expressions in momentum space we see that the two propagators have the same simple pole at the position $-\alpha_0$, characterizing this long-range behavior. In fact, since for $k \to 0$ we have that $f_r \to 1$, we can see that the two propagators have the same behavior for small values of the momentum.

As we saw in section 4.1, the dimensionless propagator of the fundamental field goes to zero away from the origin, hence the same will happen with the dimensionless version of the block propagator. It follows that it is more convenient to use the dimensionfull version of the block propagator which, starting from equation (4.3.3), is given by

$$G_r(\mathbf{R}) = \frac{1}{N^2 L^{d-2}} \sum_{\mathbf{k}} \frac{e^{\imath \frac{2\pi}{N} \mathbf{k}\cdot\mathbf{R}}}{\rho^2(\mathbf{k}) + \alpha_0} \left| f_r^{(d)}(\mathbf{k}) \right|^2 . \tag{4.3.4}$$

As we also saw in section 4.1, the dimensionfull propagator of the fundamental field

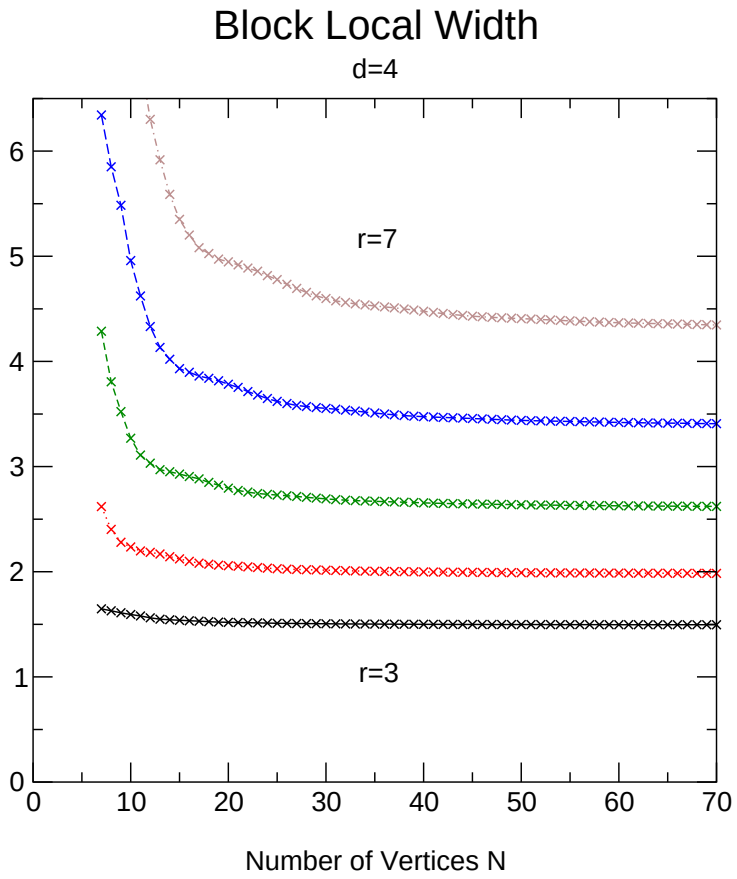


Figure 4.3.8: Behavior of the local block width as a function of N, for $d = 4$.

variables. Note that for $d = 1$ and $d = 2$ the curves seem to tend to eventually accumulate near some finite value as r increases. For $d = 3$ we see that the width σ_r^2 seems to increase linearly with r, while for $d = 4$ and $d = 5$ it seems to increase faster than linearly with r. These facts are related to the fact that, at first sight, $G_r(\mathbf{R})$ seems to go to zero for $d \geq 3$ when we make the size L of the box tend to infinity, due to the factors of L that appear in its definition. Of course, in this case keeping the blocks at a constant size corresponds to making r increase linearly with L, so that the size $L_r = L/r$ of the blocks remains finite. One can verify (problem 4.3.1) that this increase of σ_r^2 with r exactly compensates the factor $1/L^{d-2}$ that appears in the expression for $G_r(\mathbf{R})$, resulting therefore in a finite and non-vanishing block propagator also in the case of the theory in infinite space, that is, in the limit $L \to \infty$.

We see therefore that the dimensionfull block propagator in position space is a finite and non-vanishing function at all points. We may therefore define for the block variables a correlation function like the one we discussed in section 3.2, normalized to be equal to 1 at the origin, which, unlike the corresponding function in the case of the fundamental field, will not be a singular function,

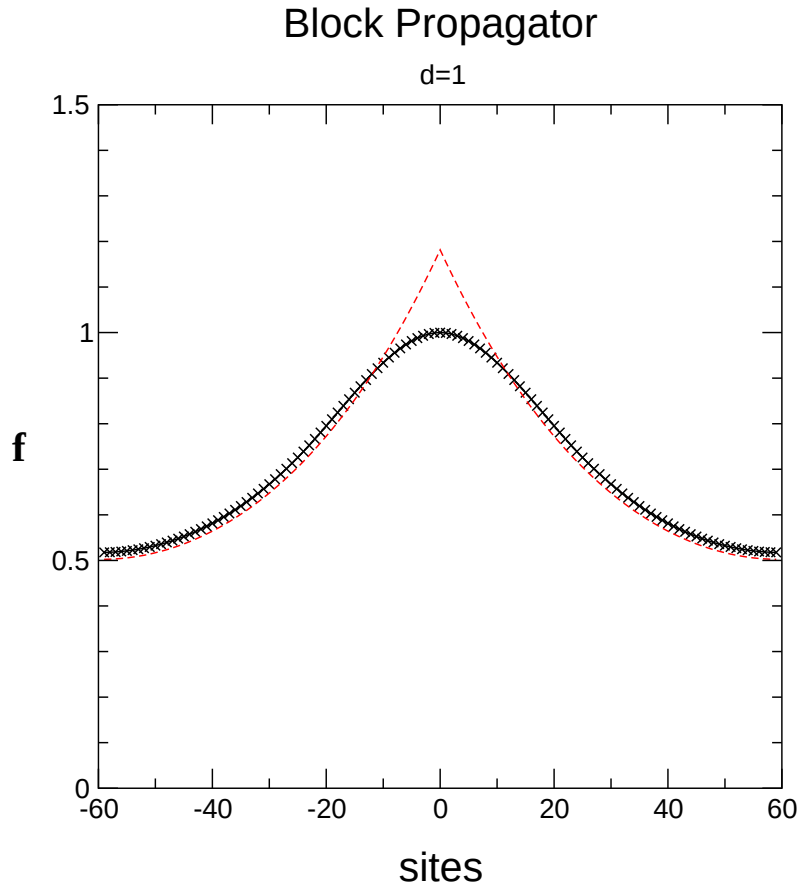


Figure 4.3.10: Block propagator in position space, for $d = 1$.

in a finite and non-vanishing way in the continuum limit of a theory in which the fundamental variables become completely uncorrelated in the same limit. We may see that the mechanism which causes this behavior is in fact very simple, if we examine what happens *during* the process of taking the limit. The fundamental field becomes completely uncorrelated in the limit, but while we are taking the limit there is a very large and ever increasing number of values of the fundamental field which are superposed within each block, with the consequence that a very large number of correlations between the fields inside one of the blocks and the fields inside the other block also superpose. During the limit the increase in the correlation function of the superposition, due to the increase in the number of superposed values, exactly compensates the decrease in the correlation function between each pair of fundamental field values, one in each block. The result is a finite and non-vanishing correlation function between the blocks, despite the complete lack of correlation of the fundamental field in the continuum limit.

It becomes clear, then, how to go about the physical interpretation of the theory. Usually we deal with it in terms of the fundamental field because it is simpler to act in this way, but the physical interpretation must be always in terms of block

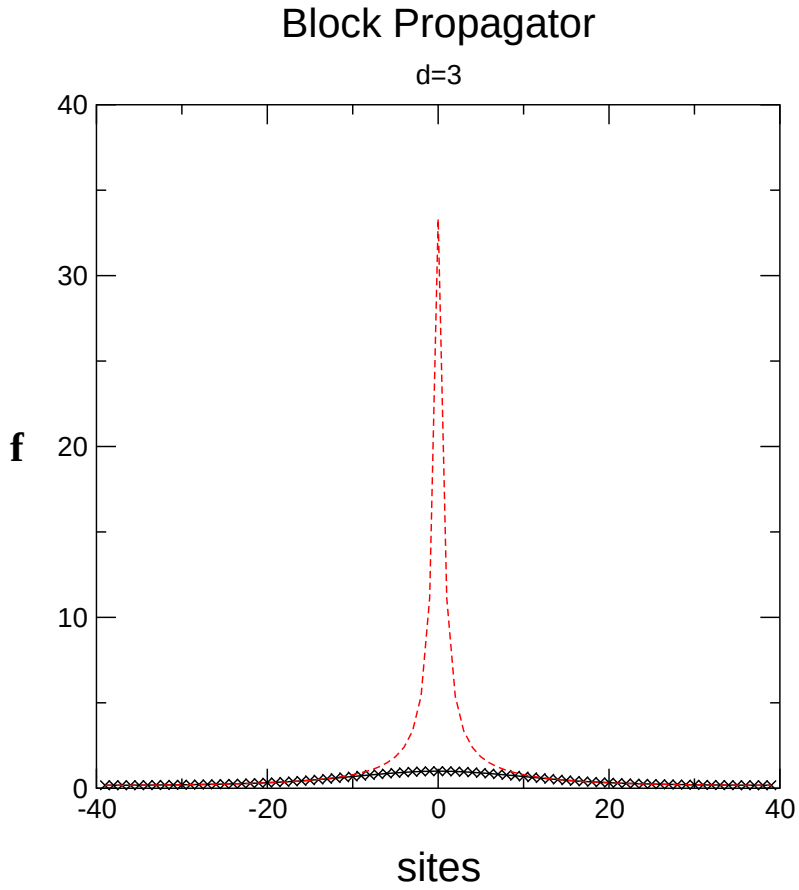


Figure 4.3.12: Block propagator in position space, for $d = 3$.

the momentum space is intrinsically more realistic, from the physical point of view, than that in terms of the position space. This is associated to the fact that the concept of wave is more natural and more elementary than the concept of particle in quantum field theory.

It is interesting to observe that, since the fundamental field becomes completely uncorrelated in the continuum limit, which is a very singular limit, it is *not* really possible to *first* take the limit and only *afterward* extract the physical consequences predicted by the theory. It is only possible to extract these physical consequences by taking the limit from finite lattices directly of the relevant physical quantities, in blocks of appropriate size. Hence, we see that the taking of the continuum limit from the lattice is an integral part of the manipulation of the theory for obtaining physical results.

Problems

4.3.1. (a) Write a program to calculate σ_r^2 in dimensions d from 1 to 5, for a given lattice size N. Use the program to calculate σ_r^2 for the largest fixed value

propagator, calculate its derivative $\partial_{\mathbf{R}} G_r(\mathbf{R})$ and show that it is always negative, indicating that the propagator in a monotonically decreasing function of $\mathbf{R}$.

(b) Calculate also the second derivative and solve the equation $\partial^2_{\mathbf{R}} G_r(\mathbf{R}) = 0$, in order to find the position of the inflection point of $G_r(\mathbf{R})$. Do this numerically if necessary. Find out the physical meaning of your answer.

Chapter 5

The Concept of Energy

One of the most important universal concepts of physics is the concept of energy, which we did not touch up to now in our technical development. In this chapter we will correct this state of affairs, introducing and exploring the concept of energy, thus continuing our probe into the fundamental structure of the theory, and extending it in this important new direction. This will require the redefinition of the theory in the context of the canonical formalism, which we will develop entirely on the Euclidean lattice. We will see that it is possible to do this without any problems, and that the usual familiar results are recovered in the $d = 1$ case of quantum mechanics. However, significant differences with respect to the results of the traditional formalism will be found in the case of quantum field theory, that is, for the cases $d \geq 2$.

At first the exploration of the concept of energy will be limited to the study of the vacuum state of the theory, which has already been defined, but one is quickly led to consider other states, resulting in the definition and exploration of particle states, that is, states with energies and momenta corresponding to multiples of some fundamental quanta. These particle states will be associated to the modes of the d-dimensional cavity containing the physical system, in momentum space, an association which is of great physical importance, since it can be realized experimentally in the non-relativistic limit. The important on-shell condition characterizing the physical states of relativistic particles will appear naturally from the resulting structure when one considers the continuum limit.

We will see that the introduction of the particle states permits a deeper and more direct probe into the structure of the theory, which is closer to the observability aspects of the physical structure. However, some difficulties of a very fundamental nature will also be found, when we try to make closer contact with the traditional formalism involving state-vectors and operators in a Hilbert space. These difficulties do not appear in the definition and calculation of the correlation-function aspects of the structure, but only when one considers the issue of the definition of the energy and of particle states. The results of the last section of this chapter will lead us to depart even further from the traditional approach to the subject.

understood as a site variable related to the link variable $\Delta_0\varphi$ which is associated to the link that starts at that site and points in the positive temporal direction. We may now define a dimensionless Hamiltonian density is a way analogous to the usual definition,

$$\begin{aligned} \mathcal{H} &= \bar{\pi}\Delta_0\varphi - \imath\mathcal{L} \Rightarrow \\ \mathcal{H} &= -\frac{\imath}{2}\left[\bar{\pi}^2 + \sum_i (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right], \end{aligned} \tag{5.1.1}$$

which is the usual definition except for the factor of $\imath$, due to the Euclidean nature of our development, and of the factor -1, chosen by mere convenience. As we shall see later, independently of the choice of sign adopted here there will always exist in the theory states with both positive energy and negative energy, just as in the traditional formalism. We may now add over the spacial part and write dimensionless versions of the Lagrangian and of the Hamiltonian,

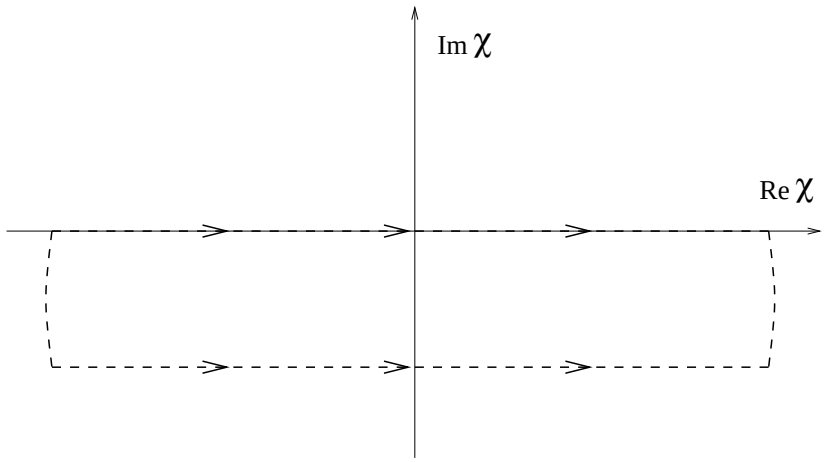
$$\begin{aligned} \mathbf{L} &= \frac{1}{2}\sum_{\mathbf{x}}\left[(\Delta_0\varphi)^2 + \sum_i (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right], \\ \mathbf{H} &= -\frac{\imath}{2}\sum_{\mathbf{x}}\left[\bar{\pi}^2 + \sum_i (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]. \end{aligned}$$

Observe that we wrote $\mathbf{H}$ in terms of $\bar{\pi}$ and $\mathbf{L}$ in terms of $\Delta_0\varphi$, in the usual way. Classically nothing changes if we write $\mathbf{H}$ in terms of $\imath\Delta_0\varphi$, since this and $\bar{\pi}$ are equal. However, as we shall see in what follows, in the quantum theory it is necessary to take seriously the distinction between $\bar{\pi}$ and $\Delta_0\varphi$.

In order to define the quantum theory there are two paths we may follow. On the one hand, we might follow our usual definition and write a dimensionless version of the energy, as well as of any other observable depending on $\bar{\pi}$, assuming that $\bar{\pi} = \imath\Delta_0\varphi$, as the expectation value

$$\begin{aligned} \mathcal{E} &= \frac{\int [\mathbf{d}\varphi]\ \mathbf{H}'\ e^{-S}}{\int [\mathbf{d}\varphi]\ e^{-S}} \\ &= -\frac{\imath}{2}\sum_{\mathbf{x}} \frac{\int [\mathbf{d}\varphi]\left[-(\Delta_0\varphi)^2 + \sum_i (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right] e^{-S}}{\int [\mathbf{d}\varphi]\ e^{-S}}, \end{aligned}$$

where $\mathbf{H}'$ is $\mathbf{H}$ with $\bar{\pi}$ exchanged by its classical value $\imath\Delta_0\varphi$. The dimensionfull version of the energy is given by $E = \mathcal{E}/a = N_T\mathcal{E}/T$, in terms of the lattice spacing a or of the total temporal length T of the box. On the other hand, we might start with a definition of the quantum theory in terms of independent variables $\bar{\pi}$ and



Completing a closed circuit with two small arcs at infinity, at which the integral is zero, we use the residue theorem for the exponential, which has no poles, obtaining

$$\int_{-\infty-\imath\Delta_0\varphi}^{\infty-\imath\Delta_0\varphi}[\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2} = \int_{-\infty}^{\infty}[\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2},$$

which is a convergent integral that gives the usual result, which is already known. However, the important fact here is that these integrals do not depend on φ, which means that in 5.1.4 we succeeded in decoupling the integrals on $\bar{\pi}$ from those on φ. The factor that remains from the completion of the square in 5.1.4,

$$e^{-\frac{1}{2}\sum_s(\Delta_0\varphi)^2},$$

completes in 5.1.3 the expression for the action, so that we have

$$\langle\mathcal{O}\rangle = \frac{\displaystyle\int[\mathrm{d}\varphi]\;\mathcal{O}[\varphi]\; e^{-\frac{1}{2}\sum_s\left[\sum_\mu(\Delta_\mu\varphi)^2+\alpha_0\varphi^2\right]}}{\displaystyle\int[\mathrm{d}\varphi]\; e^{-\frac{1}{2}\sum_s\left[\sum_\mu(\Delta_\mu\varphi)^2+\alpha_0\varphi^2\right]}} = \frac{\displaystyle\int[\mathrm{d}\varphi]\;\mathcal{O}[\varphi]\; e^{-S}}{\displaystyle\int[\mathrm{d}\varphi]\; e^{-S}},$$

that is, we recovered the usual definition. However, if the observable $\mathcal{O}$ depends on $\bar{\pi}$ then the results can only be obtained by means of the canonical definition. If we substitute $\bar{\pi}$ by its classical value $\imath\Delta_0\varphi$ and use the usual definition, the result will be, in general, different from the result obtained by means of the canonical definition.

An interesting exercise to illustrate the calculation of expectation values of observables that depend on $\bar{\pi}$ is the calculation at a given site of the observables $\langle\bar{\pi}(s) - \imath\Delta_0\varphi(s)\rangle$ and $\langle[\bar{\pi}(s) - \imath\Delta_0\varphi(s)]^2\rangle$, by means of which we can examine the nature of the relation between $\bar{\pi}$ and $\imath\Delta_0\varphi$ in the quantum theory. Of course, if we calculate these observables according to the previous, non-canonical definition, we will obtain zero for both. For the calculation of the first of these two observables we start from the canonical definition given in equation (5.1.2), whose numerator can be written as

so that we have

$$\langle \mathbf{H} \rangle = -\frac{\imath}{2} \sum_{\mathbf{x}} \frac{\int [\mathrm{d}\varphi]\; e^{-S} \int [\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2} \left(\chi^2 + 2\imath \chi \Delta_0 \varphi - 2\imath \mathcal{H}' \right)}{\int [\mathrm{d}\varphi]\; e^{-S} \int [\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2}},$$

where $\mathcal{H}'$ is the expression of $\mathcal{H}$ with the variable $\bar{\pi}$ changed to $\imath \Delta_0 \varphi$. The linear integral on χ vanishes by symmetry and we have then

$$\begin{aligned} \langle \mathbf{H} \rangle &= -\frac{\imath}{2} \sum_{\mathbf{x}} \frac{\int [\mathrm{d}\varphi]\; e^{-S} \int [\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2} \left(\chi^2 - 2\imath \mathcal{H}' \right)}{\int [\mathrm{d}\varphi]\; e^{-S} \int [\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2}} \\ &= -\frac{\imath}{2} \sum_{\mathbf{x}} \frac{\int [\mathrm{d}\chi]\; \chi^2 e^{-\frac{1}{2}\sum_s \chi^2}}{\int [\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2}} + \sum_{\mathbf{x}} \frac{\int [\mathrm{d}\varphi]\; \mathcal{H}' e^{-S}}{\int [\mathrm{d}\varphi]\; e^{-S}}. \end{aligned}$$

Doing the Gaussian integrations in the first term we obtain

$$\langle \mathbf{H} \rangle = -\frac{\imath}{2} N_L^{d-1} + \langle \mathbf{H}' \rangle,$$

where $\mathbf{H}'$ is the $\mathbf{H}$ that corresponds to $\mathcal{H}'$. In other words, we see that the expectation values of $\mathbf{H}$ and $\mathbf{H}'$, calculated respectively according to the definition of the observables in the canonical formalism and according to the usual definition of the observables, differ by a quantity which is divergent in the limit $N_L \to \infty$, except in the case $d = 1$ of quantum mechanics. Observe however that this is a constant quantity, in the sense that it does not depend on the parameters and dynamical variables of the model, being therefore of little physical relevance.

We may proceed now to the complete calculation of the energy of the vacuum, by evaluating the second term of the expression above. Writing this term explicitly we have

$$\langle \mathbf{H}' \rangle = -\frac{\imath}{2} \sum_{\mathbf{x}} \frac{\int [\mathrm{d}\varphi]\; e^{-S} \left[-(\Delta_0 \varphi)^2 + \sum_i (\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right]}{\int [\mathrm{d}\varphi]\; e^{-S}}.$$

In order to simplify the calculation, we will use translation invariance along the time direction, which is equivalent to a kind of internal conservation of energy. This invariance exists by construction in the vacuum state of the model we are dealing with. We may define a new observable $\mathbf{H}_b$, related to the energy, through the average of $\mathbf{H}$ over a temporal block, which might be the whole lattice,

$$\mathbf{H}_b = \frac{1}{N_T} \sum_t \mathbf{H}.$$

With this result we can assemble the final expression for the dimensionless energy,

$$\begin{aligned}
\mathcal{E} &= -\frac{\imath}{2N_T} N_L^{d-1} N_T - \frac{\imath}{2N_T} \sum_p \frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \\
&= -\frac{\imath}{2N_T} \sum_p \left(\frac{\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho_0^2 + \sum_i \rho_i^2 + \alpha_0} + \frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho_0^2 + \sum_i \rho_i^2 + \alpha_0} \right) \\
&= -\frac{\imath}{N_T} \sum_p \frac{\sum_i \rho_i^2 + \alpha_0}{\rho_0^2 + \sum_i \rho_i^2 + \alpha_0},
\end{aligned}$$

where we used the facts that $N_L^{d-1} N_T = \sum_p 1$ and that $\rho^2 = \rho_0^2 + \sum_i \rho_i^2$. We may now write the final result for the dimensionfull form $E = \mathcal{E}/a$ of the energy,

$$E = -\frac{\imath}{T} \sum_{k_0} \sum_{k_i} \frac{\left(\sum_i \rho_i^2 + \alpha_0 \right)}{\rho_0^2 + \left(\sum_i \rho_i^2 + \alpha_0 \right)}. \tag{5.1.5}$$

In order to better understand this result it is necessary to examine the behavior of the sums it contains. For this it is useful to examine first the case $d = 1$, which corresponds to the quantum mechanics of a harmonic oscillator with angular frequency ω, in which case we have $\alpha_0 = \omega^2 a^2 = \omega^2 T^2 / N_T^2$ and we may write

$$\begin{aligned}
E &= -\frac{\imath}{T} \sum_{k_0} \frac{\alpha_0}{\rho_0^2 + \alpha_0} \\
&= -\frac{\imath}{T} \sum_{k_0 = -k_m}^{k_M} \frac{\omega^2}{\omega^2 + 4 \left(\frac{N_T}{T} \right)^2 \sin^2 \left(\frac{k_0 \pi}{N_T} \right)},
\end{aligned} \tag{5.1.6}$$

where k_m and k_M are the minimum and maximum values of k_0 on lattices with a given N_T. Note that the term $k_0 = 0$ of this sum, unlike all the others, is simply equal to 1 and does not depend on ω, while all the others go to zero for $\omega \to 0$. It follows that in this limit the sum goes to 1 and we have, therefore, $E = -\imath/T$ for $\omega = 0$. Since $1/T$ is the energy scale associated to the temporal size of our box, we see that this effect is due to the infrared cutoff established by the box. In the limit in which we make the box infinite in the temporal direction this effect disappears and we have $E = 0$ for $\omega = 0$.

In order to determine the exact value of this sum in the opposite case, when instead of $\omega = 0$ we have $\omega \gg 1/T$, it is necessary to make a numerical evaluation.

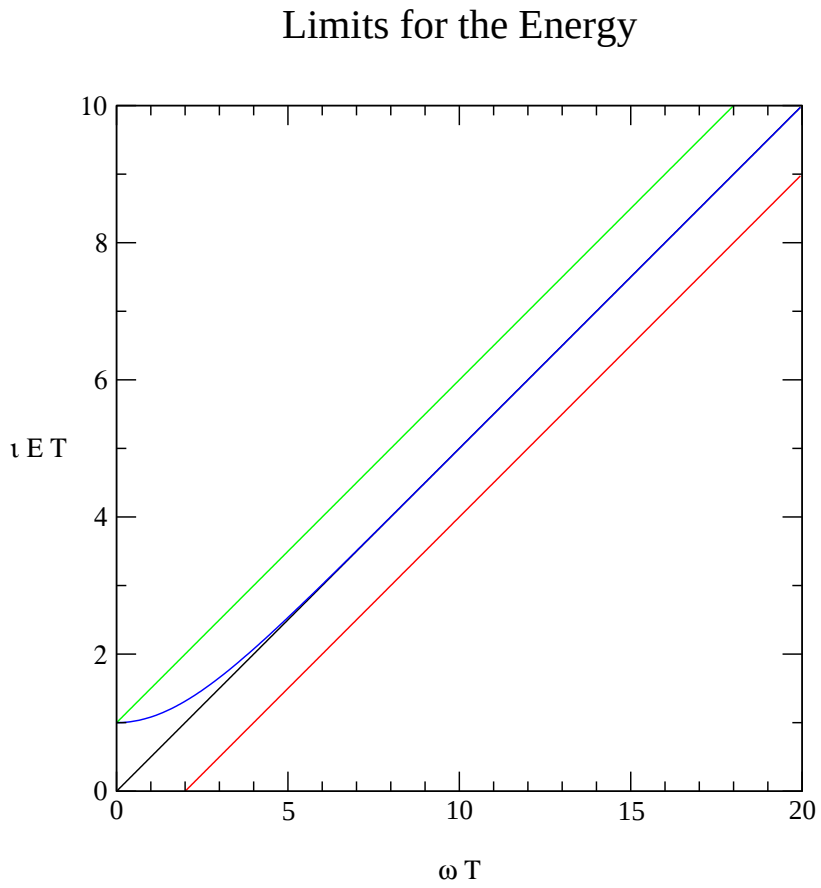


Figure 5.1.1: The energy as a function of the variable ωT. The curved line corresponds to the numerical result for $N_T = 1000$. The central straight line corresponds to the continuum limit in an infinite temporal box. The other straight lines correspond to the upper and lower bounds which are mentioned in the text and proposed as problems to the reader.

$N_T \to \infty$. Note that, for each finite lattice, the lattice result is above the continuum limit for ωT sufficiently small, but falls below it above a certain value of this variable. We are seeing here an ultraviolet effect: if we increase sufficiently the frequency ω, decreasing therefore the corresponding wavelength until it is of the order of the lattice spacing a, we start to see clearly the distortions cause by the discrete character of the lattice. The numerical evidence indicates clearly that $\imath E = \omega/2$ is the exact result for the energy in the continuum limit within an infinite temporal box, but it seems that it is rather difficult to obtain this result analytically.

We may now return to the discussion of the d-dimensional case for $d \geq 2$, whose result for the energy is given in equation (5.1.5), which we may rewrite as

$$E = -\frac{\imath}{T} \sum_{k_i} \left(\sum_{k_0} \frac{A^2}{\rho_0^2 + A^2} \right) , \tag{5.1.7}$$

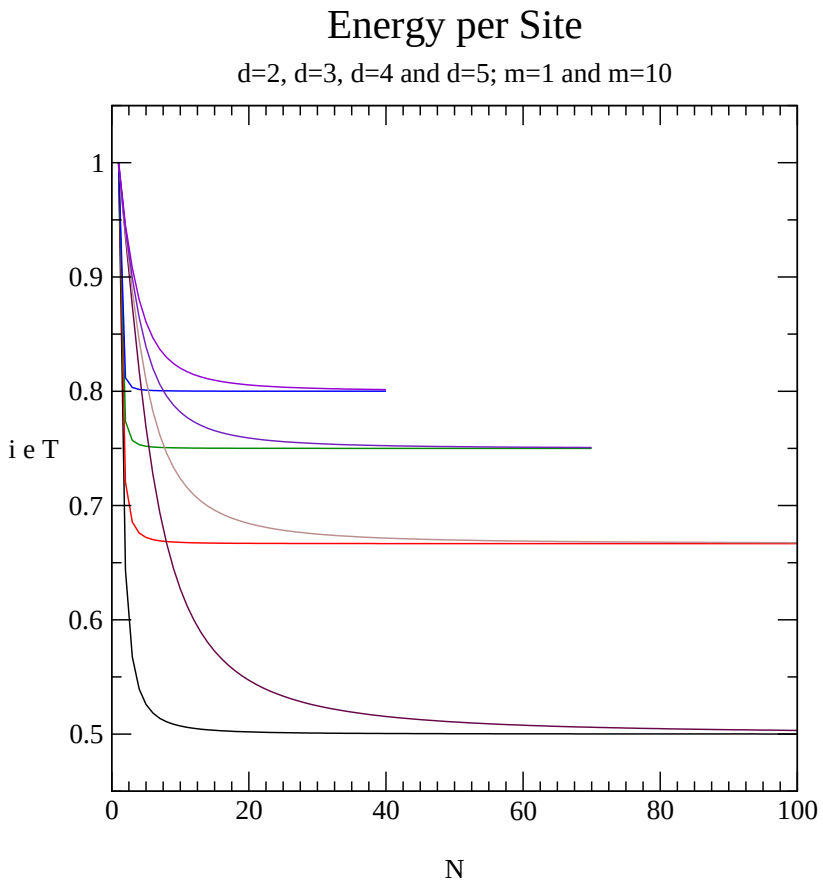


Figure 5.1.3: The energy per site as a function of N in the symmetrical case $N_T = N_L = N$. Each pair of curves corresponds to a different dimension d, converging to the value $(d-1)/d$ in the limit $N \to \infty$. In each pair the curve that converges faster is the one that corresponds to $m_0 = 1$.

in fact as $N_L^{d-1} N_T$. We can verify this fact doing a numerical evaluation of the sums involved (problem 5.1.6). Since the sums diverge, it is more convenient to evaluate the energy per site $e = E/(N_L^{d-1} N_T)$,

$$\imath eT = \frac{1}{N_L^{d-1} N_T} \sum_{k_0} \sum_{k_i} \frac{\sum_i \rho_i^2 + \alpha_0}{\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}, \tag{5.1.8}$$

The graph in figure 5.1.3 shows the result of such a calculation, done in the symmetrical case $N_T = N_L = N$. As one can see, the quantity $\imath eT$ converges quite rapidly to the value $(d-1)/d$, in each dimension, when we make $N \to \infty$, for any value of the mass m_0. In fact, one can demonstrate that this quantity can be written (problem 5.1.7) as

for each Fourier mode existing within a $(d-1)$-dimensional box. This is the sum of the so-called zero-point energies, the energies of the ground states of each one of the N_L^{d-1} uncoupled harmonic oscillators that are associated to each one of these $(d-1)$-dimensional modes.

However, this argument cannot do more than to give us a general but imprecise idea about the relation between the case $d = 1$ and the case $d \geq 2$ since, in order to make the argument rigorous, it would be necessary to first take the limit $N_T \to \infty$, thus reducing the problem to the quantum mechanics of a system with a finite number of degrees of freedom in its $(d-1)$-dimensional section, taking only after that the limit $N_L \to \infty$. However, the fact is that the results of the $d = 1$ case that were used above are not valid if we take the limits over N_T and N_L separately in this order. This is due to the fact that the quantity $A^2 = \sum_i \rho_i^2 + \alpha_0$ which appears in the denominator of the sum over k_0 in equation (5.1.7) behaves in a way that is different from the behavior of the corresponding quantity in the case of quantum mechanics, $\alpha_0 = (wT/N_T)^2$. We should recall that the complete expression of A^2 is

$$A^2 = \alpha_0 + \sum_{i=1}^{d-1} 4 \sin^2\left(\frac{k_i \pi}{N_L}\right),$$

where we have N_L within the argument of the sine function, not N_T. While $N_T^2 \alpha_0$ has a finite limit when we make $N_T \to \infty$, the quantity

$$N_T^2 \sin^2\left(\frac{k_i \pi}{N_L}\right)$$

does not have a finite limit, but instead of that diverges as N_T^2. If we had $N_T = N_L$, that is, the symmetrical limit, then the sine function would go to zero as N_T^{-1}, compensating for this divergence, but it is not possible to take the limit $N_T \to \infty$ while N_L is kept finite and still obtain finite results. In addition to this, in this case we cannot say that $\rho_i N_T/T$ approaches $p_i = 2\pi k_i/T$ as we did above.

As an exercise to illustrate the difference between the results of the two formalisms, starting from the result of the traditional formalism for the energy of the vacuum,

$$\imath E = \frac{1}{2} \sum_{k_i} \sqrt{\mathbf{p}^2 + m_0^2},$$

we may translate it to the lattice, writing a corresponding result for the energy per site, valid for the case $N_T = N_L = N$ in the limit $N \to \infty$,

$$\imath eT = \frac{1}{2N^{d-1}} \sum_{k_i} \sqrt{\sum_i \rho_i^2 + \alpha_0^2},$$

and then calculate numerically, for large values of N, the sum which appears in the resulting expression (problem 5.1.8). One verifies that the result obtained in this

In order to do this you should consider in separate the terms $k_0 = 0$ and $k_0 = N_T/2$ of the sum and observe that all the others can be organized in pairs. In this way, rewrite the sum in terms of a sum of a monotonically decreasing function. After that, compare the sum with the integral of this function taken in an appropriate interval. Making a graph of the function, including the points of the sum and the integral, may help a lot. You will have to look up in a table of integrals the value of the definite integral

$$\int_0^{\pi/2} \frac{1}{1 + A^2 \sin^2 x}.$$

Take the $N_T \to \infty$ limit of these relations and show that

$$\frac{\omega T}{2} - 1 \leq \Sigma \leq \frac{\omega T}{2} + 1.$$

5.1.3. The lower bound derived in problem 5.1.2 can be improved. Re-examine the comparison between the sum and the integral in this case and take into consideration the collection of triangles that can be fitted between the graph of the integral and the graph of the sum. Once more, drawing the graph with some care may help a lot. Calculate exactly the sum of the areas of these triangles and show that sum Σ satisfies the inequality

$$\frac{\omega T}{2} \sqrt{\frac{(2N_T)^2}{(\omega T)^2 + (2N_T)^2}} \leq \Sigma,$$

which is tighter than the previous one. You will have to show that the graph of the monotonically decreasing function that appears inside the sum has its concavity turned upwards along all the domain of the integral. You can do this calculating the second derivative of the function and showing that the first derivative is also a monotonic function, in this case an increasing function. After that take the limit $N_T \to \infty$ and show that

$$\frac{\omega T}{2} \leq \Sigma.$$

Show also that the value obtained for the lower bound of the sum in the limit $N_T \to \infty$ is larger than the value of the lower bound of the sum for finite N_T, that is, show that taking the $N_T \to \infty$ limit tightens the lower bound.

5.1.4. Repeat the analysis made in problems 5.1.2 and 5.1.3 and determine upper and lower bounds for the sum Σ in the case in which N_T is odd, in which the limits of k_0 are $k_m = -(N_T - 1)/2$ and $k_M = (N_T - 1)/2$. Write the corresponding inequalities for $\imath E$ and verify that they are compatible with the inequalities obtained for the case of even N_T.

5.2 Energy and States of Particles

In possession of the concept of energy within the lattice formalism, we will now discuss in considerable more detail the concept of state. This discussion will lead us to the construction within this formalism of states with a given number of particles and, therefore, to the concept of particle itself. This is a central concept within the structure of the theory, which is directly connected with the fundamental issues of the observation of physical phenomena and of the process of measurement.

Up to now we have been defining and developing a formalism that allows us to define and calculate, at least in principle, any observables within any given model of quantum field theory. We have been doing this through the use of a statistical model in which we define a certain statistical distribution of probabilities that applies to each and every one of the possible configurations of the fields. This distribution is the Boltzmann distribution, which can be expressed in terms of the action functional S of a given model as

$$|0\rangle \sim \frac{[\mathrm{d}\varphi]\ e^{-S[\varphi]}}{\int [\mathrm{d}\varphi]\ e^{-S[\varphi]}},$$

or, if we wish to use the canonical formalism, as

$$|0\rangle \sim \frac{[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ e^{\imath \sum_s [\bar{\pi}\Delta_0\varphi - \mathcal{H}(\varphi,\bar{\pi})]}}{\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ e^{\imath \sum_s [\bar{\pi}\Delta_0\varphi - \mathcal{H}(\varphi,\bar{\pi})]}}.$$

The symbolism of Dirac "bras" and "kets" that we use here expresses the fact that our interpretation of the structure that we are building is that this statistical distribution is a representation of the vacuum state of the theory, for this particular model.

It is a difficult task to define a-priori what the vacuum might be. The classical idea that it is a situation in which there is total absence of any physical content is not very useful in the context of the quantum theory, due to the concept of uncertainty that is inherent to such a theory. We will simply say that this state defines completely the physical situation in the region of space-time where it is realized, and accept its introduction as part of the definition of the quantum theory. We will also see that it is a state that contains no particles, that is, no observable amount of energy. This does not mean that there is nothing in it, because there is the field, which fluctuates permanently in a rather violent way. One might say that the vacuum is the state that contains nothing but the minimum mount of uncertainty which is inherent to the quantum theory.

This idea which we introduced above, that physical states are connected with certain statistical distributions, immediately suggest the generalization of its application to other stated besides the vacuum. Strictly speaking this is not necessary for the measurement of observables, since we can measure any observables using only the vacuum state. This is a remarkable characteristic of this structure of ours, it is

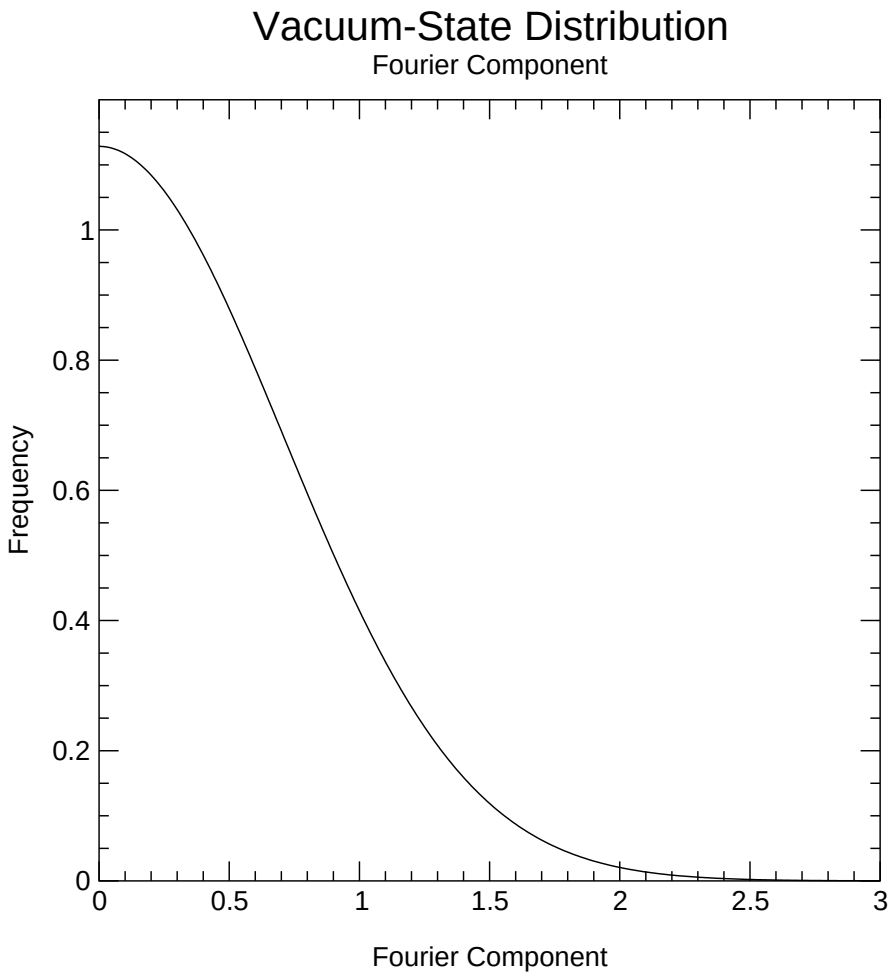


Figure 5.2.1: Qualitative diagram of the probability distribution $\exp(-x^2)$ of the Fourier components of the field in the vacuum state, showing the point of maximum at 0.

Before we begin to examine some properties of this new distribution let us emphasize here that, while we are proposing a relation between states of the quantum theory of fields and statistical distributions of the fields, we are absolutely *not* stating that *any* such statistical distribution is related to a physical state of the theory. There are many distributions that are clearly not related to physical states, such as, for example, any "delta-functional" distribution, that attributes the probability 1 to a certain configuration and the probability 0 to all others, because this would translate into a physical situation in which the fundamental field does not fluctuate at all, which is a classical, not a quantum situation. We will postpone to a future opportunity a more detailed discussion of the conditions that the distributions must satisfy in order to be associated to states, and will limit ourselves here only to the comment that such conditions are related to the principle of uncertainty and to the issues of observation and measurement. Our difficulties with the "ab-initio" definition of the vacuum will have to be resolved in the context of this future discussion, possibly

the configurations that have a larger component of plane wave with momentum $\vec{k}$.

In order to calculate the energy of this new state, we will use the canonical definition and the form of the dimensionless Hamiltonian defined in section 5.1,

$$\mathbf{H} = -\frac{\imath}{2}\sum_{\mathbf{x}}\left[\bar{\pi}^2 + \sum_i (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

With these ingredients we obtain (problem 5.2.1) for the expectation value of the Hamiltonian in the state of one particle with momentum $\vec{k}$,

$$\langle\mathbf{H}\rangle_{1,\vec{k}} = -\frac{\imath}{2}N_L^{d-1} + \frac{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2\mathbf{H}'e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}},$$

where $\mathbf{H}'$ is, as before, the expression of $\mathbf{H}$ with $\bar{\pi}$ substituted by $\imath\Delta_0\varphi$, showing once more that the difference between the canonical definition and the initial definition is just a constant that diverges in the continuum limit. Repeating procedures used before in section 5.1 we may write explicitly for the energy

$$\begin{aligned}\imath E_{1,\vec{k}}T &= \frac{N_T N_L^{d-1}}{2} \\ &\quad + \frac{N_T N_L^{d-1}}{2}\,\frac{\displaystyle\int [\mathrm{d}\widetilde{\varphi}]\ e^{-S[\widetilde{\varphi}]}|\widetilde{\varphi}_{\vec{k}}|^2 \sum_{\vec{q}}\left[-\rho_0^2(\vec{q}) + \sum_i \rho_i^2(\vec{q}) + \alpha_0\right]|\widetilde{\varphi}_{\vec{q}}|^2}{\displaystyle\int [\mathrm{d}\widetilde{\varphi}]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\widetilde{\varphi}]}},\end{aligned}$$

where we recall that we have for $S[\widetilde{\varphi}]$ written in momentum space

$$S[\widetilde{\varphi}] = \frac{N_T N_L^{d-1}}{2}\sum_{\vec{k}}(\rho_{\vec{k}}^2 + \alpha_0)|\widetilde{\varphi}_{\vec{k}}|^2,$$

with

$$\rho_{\vec{k}}^2 = 4\sin^2\left(\frac{k_0\pi}{N_T}\right) + \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right).$$

For the terms of the sum over the momenta $\vec{q}$ such that $\vec{q} \neq \pm\vec{k}$ the calculation proceeds as in the case of the calculation of the energy of the vacuum, but for $\vec{q} = \pm\vec{k}$ there are differences, because in this case we have the expectation value of a larger power of the Fourier component $\widetilde{\varphi}_{\vec{k}}$ of the fields. Taking into account the symmetries by exchange of the sign of $\vec{q}$ in the sum, we may write

$$\begin{aligned}\imath E_{1,\vec{k}}T &= \frac{N_T N_L^{d-1}}{2} + \frac{1}{2}\sum_{\vec{q}\neq\pm\vec{k}}\frac{-\rho_0^2(\vec{q}) + \sum_i \rho_i^2(\vec{q}) + \alpha_0}{\rho_{\vec{q}}^2 + \alpha_0} \\ &\quad + N_T N_L^{d-1}\left[-\rho_0^2(\vec{k}) + \sum_i \rho_i^2(\vec{k}) + \alpha_0\right]\frac{\langle|\widetilde{\varphi}_{\vec{k}}|^4\rangle_0}{\langle|\widetilde{\varphi}_{\vec{k}}|^2\rangle_0},\end{aligned}$$

As we will see later on, we may extend the definition of our states to arbitrary numbers of particles but, before we do that, let us discuss the physical meaning of the expression we obtained for the energy in the continuum limit. Our definition of the one-particle state is in fact the definition of a collection of states, one for each d-dimensional mode $\vec{k}$ existing on the lattice, each one of them having its energy given in terms of $\vec{k}$ by the expression in equation (5.2.1). If we write the version of this result in Minkowski space, thus *de-Euclideanizing* the result, we obtain

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{\rho_0^2(\vec{k}) + \sum_i \rho_i^2(\vec{k}) + \alpha_0}{-\rho_0^2(\vec{k}) + \sum_i \rho_i^2(\vec{k}) + \alpha_0}.$$

There are, in fact, two limits to discuss here, the continuum limit in which we make $N \to \infty$, and the $T \to \infty$ limit in which we make the box infinite in the temporal direction. We will discuss the first limit in the symmetrical case, making $N_T = N_L = N \to \infty$ while we keep T finite, leaving for later on the discussion of other ways to take this limit. In this case we may multiply both the denominator and the numerator by N^2/L^2, take the limit and write the result as

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{p_0^2(\vec{k}) + \mathbf{p}^2(\vec{k}) + m_0^2}{-p_0^2(\vec{k}) + \mathbf{p}^2(\vec{k}) + m_0^2},$$

where $m_0^2 = \alpha_0 N^2/L^2$ and the $(d-1)$-dimensional momentum $\mathbf{p}$ is defined by

$$\mathbf{p}_{\vec{k}}^2 = \lim_{N\to\infty} \frac{N^2}{L^2} \sum_i \rho_i^2(\vec{k}) = \lim_{N\to\infty} \frac{4N^2}{L^2} \sum_i \sin^2\left(\frac{k_i\pi}{N}\right) = \sum_i \left(\frac{2\pi k_i}{L}\right)^2.$$

Let us consider now the limit $T \to \infty$, with L either kept fixed or not. Since T appears in the denominator, our expression for the energy of a particle goes to zero, unless the momentum-dependent expression in the denominator vanishes in the limit. This takes us to the *on-shell condition*, that selects a subset of all possible d-dimensional modes. In order to see this we may rewrite the expression as

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{p_0^2(\vec{k}) + \mathbf{p}_{\vec{k}}^2 + m_0^2}{\left[-p_0(\vec{k}) + \sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}\right]\left[p_0(\vec{k}) + \sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}\right]}.$$

Observe that we can obtain a finite and non-vanishing limit only so long as in the limit one of these two relations holds,

$$p_0(\vec{k}) = \sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2} \quad \text{or} \quad p_0(\vec{k}) = -\sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}.$$

We thus obtain the on-shell condition that relates the energy, the momentum and the rest mass of a relativistic particle. We see also that we may have some limits in which the energy is positive as well as other limits in which it is negative, as mentioned in section 5.1. Besides the two possibilities presented by the two factors in the denominator, in each case it is possible to take the limit in which p_0 approaches

We see therefore that, in order for the expectation value of the energy to coincide numerically with the temporal component of the vector $\vec{k}$, we should impose that the $T \to \infty$ limit be such that $A = -1$. Note that this arbitrariness in the value of A is equivalent to the arbitrariness in the choice of units for the energy.

It is interesting to discuss here the case $d = 1$ and thus verify that we obtain the correct results for the harmonic oscillator in quantum mechanics. In this case the on-shell condition within a finite temporal box reduces, already making $A = -1$, to

$$p_0 = \frac{1}{T} + m_0,$$

that is, except for the infrared effects due to the finite size of the temporal box, the energy parameter p_0 reduces to the mass parameter m_0. Since in this case we do not have the components p_i, this relation determines completely p_0 and, therefore, k_0. If we recall that we have $\alpha_0 = m_0^2 a^2$ and that this same parameter α_0 relates to the angular frequency ω of the harmonic oscillator by $\alpha_0 = \omega^2 a^2$, we see that we have $m_0 = \omega$, so that we may write

$$p_0 = \omega + \frac{1}{T} = \omega \left(1 + \frac{1}{\omega T}\right).$$

We may now substitute this value for p_0 in the expression of the expectation value of the Hamiltonian, obtaining, after some manipulation and keeping only the first-order corrections in $1/T$, in the limit of very large T,

$$\Delta E_1 = \omega \left(1 + \frac{1}{2\omega T}\right),$$

showing that this quantity also suffers infrared deviations, is a way similar to p_0. With a slightly different choice for A, making $A = -1+1/(2\omega T)$ rather than $A = -1$, we can make p_0 and ΔE_1 approach their limits in exactly the same way. In any case, in the $T \to \infty$ limit we have the result

$$\Delta E_1 = \omega,$$

which is the correct result for the difference between the energies of the first excited state and of the fundamental state of a one-dimensional harmonic oscillator in quantum mechanics.

We may now extend our definition of particle states to arbitrary numbers of identical particles. The state of n particles with momentum $\vec{k}$ can be defined by means of the distribution

$$|n, \vec{k}\rangle \sim \frac{[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{-S[\varphi]}},$$

or, in terms of the canonical formalism,

$$\langle S\rangle_0 = \frac{N_T N_L^{d-1}}{2}.$$

One might interpret this result as one half the number of degrees of freedom of the d-dimensional lattice, but this is of no direct physical importance. What is most interesting to us is the calculation of the expectation value of S on the state of one particle with momentum $\vec{k}$, which can easily be done (problem 5.2.3), resulting in

$$\langle S\rangle_{1,\vec{k}} = \frac{N_T N_L^{d-1}}{2} + 1,$$

and, in general, on a state of n particles with momentum $\vec{k}$

$$\langle S\rangle_{n,\vec{k}} = \frac{N_T N_L^{d-1}}{2} + n,$$

Hence, the observable

$$\mathcal{N} = S - \langle S\rangle_0$$

gives us the number of particles of a given state. This can be extended to states for arbitrary numbers of particles with various different momenta, in which case it gives us the total number of particles (problem 5.2.4). Note that this observable is not sensitive to whether or not the particles correspond to modes that satisfy the on-shell condition.

It is interesting to note here that the definition of this observable is quite general and does not depend on any particularity of our simple model here. In fact, it is possible to verify numerically that the observable $\mathcal{N}$ gives us the number of particles even in non-linear models such as, for example, the $\lambda\varphi^4$ model. Not only one verifies that the expectation value of this observable is always proportional to the number n of particles, whatever the values of the parameters of the model may be, but one also verifies that the value of the increment $\Delta\langle\mathcal{N}\rangle$ between the states of n and $n+1$ particles approaches the value 1 in the immediacy of the critical region in the space of parameters of the model, indicating that this increment tends to 1 in the continuum limit. The existing numerical results, still of a somewhat limited quality due to the limitations of the available resources, can be found in [3].

In a linear model such as our standard example here it is possible to define, additionally, observables that function like projection operators, returning the number of particles with a given momentum $\vec{k}$ that exist on the state. The definition of these observables is simple,

$$\mathcal{N}_{\vec{k}} = \frac{1}{2}\left[N_T N_L^{d-1}\left(\rho_{\vec{k}}^2 + \alpha_0\right)|\widetilde{\varphi}_{\vec{k}}|^2 - 1\right].$$

It is easy to verify (problem 5.2.6) that we have for this observable

5.2.5. Calculate the expectation value of the Hamiltonian $\Delta\mathbf{H}$ on the state having n_1 particles with momentum $\vec{k}_1$ and n_2 particles with momentum $\vec{k}_2$ considered in problem 5.2.4. Show in this way that the energy is additive, that is, that the total energy of the state is the sum of the energies of the particles that it contains.

5.2.6. Calculate the expectation value of the observable $\mathcal{N}_{\vec{k}}$ on a state having n particles with momentum $\vec{q}$. Consider in separate the cases in which $\vec{q} \neq \pm\vec{k}$ and the case in which $\vec{q} = \vec{k}$.

5.3 Relation with Hilbert Spaces

In possession of the concept of energy and having constructed the states of particles within the structure of our theory, we will now examine another concept which is of central importance in the traditional formalism, the concept of the eigenstates of an observable. In the traditional formalism the observables are represented by Hermitian operators in a Hilbert space and the physical states are represented by vectors in this space. In that formalism the eigenstates of an observable are the eigenvectors of the corresponding operator. Our first problem here is to determine how to characterize the property of a state being or not being an eigenstate of an observable.

In order to build this characterization of the concept of eigenstate in our formalism, it is necessary to think in terms of expectation values, as it is in terms of the direct definition of these values that our formalism is built. Let us start by recalling that, if a state $|e\rangle$ is an eigenstate of an observable $\mathcal{O}$ with eigenvalue ω, then we have in the traditional formalism

$$\mathcal{O}_{\text{op}}|e\rangle = \omega|e\rangle,$$

where $\mathcal{O}_{\text{op}}$ is an operator and ω a number. In terms of expectation values we can write this in the form

$$\langle e|\mathcal{O}_{\text{op}}|e\rangle = \omega,$$

where we used the fact that the states are normalized, $\langle e|e\rangle = 1$. As a consequence of the relations above we also have

$$\mathcal{O}^2_{\text{op}}|e\rangle = \mathcal{O}_{\text{op}}\omega|e\rangle = \omega\mathcal{O}_{\text{op}}|e\rangle = \omega^2|e\rangle,$$

so that we may write a relation between expectation values,

$$\langle e|\mathcal{O}^2_{\text{op}}|e\rangle = \omega^2\langle e|e\rangle = \omega^2,$$

or, in other words,

for any state in which we may be measuring the dispersion. This is a general fact which is important for us: the addition of a constant to an observable, be it finite or divergent in the limit, does not change the dispersion of the observable. In order to calculate the dispersion of S on the vacuum, we first obtain (problem 5.3.2) the results

$$\langle S\rangle_0 = \frac{N_T N_L^{d-1}}{2},$$

and

$$\langle S^2\rangle_0 = \left(\frac{N_T N_L^{d-1}}{2}\right)^2 + \frac{N_T N_L^{d-1}}{2},$$

so that we have for the dispersion

$$\langle S^2\rangle_0 - \langle S\rangle_0^2 = \frac{N_T N_L^{d-1}}{2},$$

that is, we have

$$\sigma_{\mathcal{N}} = \sigma_S = \sqrt{\frac{N_T N_L^{d-1}}{2}},$$

which, instead of vanishing in the continuum limit, diverges, thus showing that the vacuum is *not* an eigenstate of the observable number-of-particles. Note that this dispersion is small by comparison with the value of $\langle S\rangle_0 = N_T N_L^{d-1}/2$, so that we have

$$\frac{\sqrt{\langle S^2\rangle_0 - \langle S\rangle_0^2}}{\langle S\rangle_0} = \sqrt{\frac{2}{N_T N_L^{d-1}}} \longrightarrow 0,$$

that is, the relative dispersion goes to zero in the continuum limit, but the dispersion itself is not small by comparison to the finite value of $\langle \mathcal{N}\rangle_0$. Hence, the observable $\mathcal{N}$ gives us the correct number of particles in each state, including the value 0 for the vacuum, but the vacuum is not an eigenstate of this observable.

With a little more work we can repeat these calculations for the states of n particles with momentum $\vec{k}$ which we introduced in section 5.2 (problem 5.3.3). In this case we obtain the preliminary results

$$\langle S\rangle_{n,\vec{k}} = \frac{N_T N_L^{d-1}}{2} + n,$$

and

$$\langle S^2\rangle_{n,\vec{k}} = \left(\frac{N_T N_L^{d-1}}{2}\right)^2 + N_T N_L^{d-1}\left(n+\frac{1}{2}\right) + \left(n+\frac{1}{2}\right)^2 - \frac{1}{4},$$

We can calculate the expectation values of $\mathbf{H}^2$ and $(\Delta\mathbf{H})^2$ both by the canonical definition and by the usual definition. Since these observables depend on $\bar{\pi}$ the results of these two calculations will be different. In any case, since $\Delta\mathbf{H}$ and $\mathbf{H}$ are related by the addition of a constant quantity, we know beforehand that both will have the same dispersion. Because of this, we may calculate directly the dispersion of $\mathbf{H}$. Besides the question of using the canonical definition or the usual definition, it is also necessary to consider in detail the question of the temporal average, which we used before to facilitate the calculations. To take this average is equivalent to defining an average Hamiltonian over a temporal block, which we denote as

$$\mathbf{H}_b = \frac{1}{N_T}\sum_t \mathbf{H}.$$

As we observed before, the invariance of the lattice model by discrete temporal translation implies that $\mathbf{H}_b$ and $\mathbf{H}$ have the same expectation value, but these are two conceptually different observables. The observable $\mathbf{H}$ corresponds to the measurement of the energy at a perfectly well-defined instant of time, while the observable $\mathbf{H}_b$ constitutes a type of block variable and we should expect that its fluctuations will be smaller than those of $\mathbf{H}$, due to the average over the temporal block. Since the dispersions of the observables are a measure of the average magnitude of the fluctuations that they undergo, the dispersions will be different. We may, in fact, predict that the dispersion of $\mathbf{H}_b$ will be smaller than that of $\mathbf{H}$, as it is characteristic for block variables.

We see therefore that we have several calculations to do, including two possibilities for the definition of the observable and two possibilities for the definition of the averages. We will present here the calculation of the dispersion of $\mathbf{H}_b$, which is simpler and sufficient for our purposes, leaving the case of $\mathbf{H}$ for the problems of this section (problems 5.3.5, 5.3.6 and 5.3.7). Besides, we will start with the canonical definition of the averages, showing, first of all, the relation of the result obtained by means of this definition with that obtained by means of the usual definition. Let us recall that the Hamiltonian density is given by

$$\mathcal{H} = -\frac{\imath}{2}\left[\bar{\pi}^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right],$$

where summation over i is implicit, so that we have the Hamiltonian

$$\mathbf{H} = \sum_{\mathbf{x}}\mathcal{H} = -\frac{\imath}{2}\sum_{\mathbf{x}}\left[\bar{\pi}^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

Calculating the temporal average of this quantity we obtain the blocked Hamiltonian

$$\mathbf{H}_b = \frac{1}{N_T}\sum_t \mathbf{H} = \frac{1}{N_T}\sum_{\vec{x}}\mathcal{H} = -\frac{\imath}{2N_T}\sum_{\vec{x}}\left[\bar{\pi}^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

We will now calculate the dispersion of $\mathbf{H}_b$, which involves the calculation of the expectation values of $\langle\mathbf{H}_b\rangle$ and $\langle\mathbf{H}_b^2\rangle$. We will do the calculation starting by the

we make the shift

$$\chi = \bar{\pi} - \imath\Delta_0\varphi \Longrightarrow \bar{\pi}^2 - 2\imath\bar{\pi}\Delta_0\varphi = \chi^2 + (\Delta_0\varphi)^2,$$

so that we may write, reconstituting the complete form of the action in the exponent,

$$\begin{aligned}\langle \mathbf{H}_b^2 \rangle &= -\frac{1}{4N_T^2 Z}\sum_{\vec{x}}\sum_{\vec{y}}\int [\mathrm{d}\varphi][\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2}\; e^{-S} \\ &\times \Big\{(\chi+\imath\Delta_0\varphi)^2_{\vec{x}}(\chi+\imath\Delta_0\varphi)^2_{\vec{y}} + 2(\chi+\imath\Delta_0\varphi)^2_{\vec{x}}\left[(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]_{\vec{y}} \\ &\qquad + \left[(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]_{\vec{x}}\left[(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]_{\vec{y}}\Big\},\end{aligned}$$

where S is the action and

$$Z = \int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\; e^{\imath\sum_s(\bar{\pi}\Delta_0\varphi - \mathcal{H})} = \int [\mathrm{d}\varphi][\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s\chi^2}\; e^{-S}$$

is the denominator that normalizes the expectation values. We may now expand the terms inside the brackets, collecting powers of χ, making exchanges of $\vec{x}$ and $\vec{y}$, and recalling that terms with odd powers of χ at a given site vanish due to the symmetry of the integration, in order to arrive at the expression

$$\begin{aligned}\langle \mathbf{H}_b^2 \rangle &= -\frac{1}{4N_T^2 Z}\sum_{\vec{x}}\sum_{\vec{y}}\int [\mathrm{d}\varphi][\mathrm{d}\chi]\; e^{-S}\; e^{-\frac{1}{2}\sum_s\chi^2} \\ &\times \left[\chi^2_{\vec{x}}\chi^2_{\vec{y}} + 4\imath\chi^2_{\vec{x}}\mathcal{H}'_{\vec{y}} - 4\delta^d_{\vec{x},\vec{y}}\chi^2_{\vec{x}}(\Delta_0\varphi)^2_{\vec{x}} - 4\mathcal{H}'_{\vec{x}}\mathcal{H}'_{\vec{y}}\right],\end{aligned}$$

where

$$\mathcal{H}' = -\frac{\imath}{2}\left[-(\Delta_0\varphi)^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]$$

is, as usual, the Hamiltonian density with $\bar{\pi}$ substituted by $\imath\Delta_0\varphi$. We may now use the known results

$$\frac{\int d\chi\; \chi^2\; e^{-\frac{1}{2}\chi^2}}{\int d\chi\; e^{-\frac{1}{2}\chi^2}} = 1 \qquad \text{and} \qquad \frac{\int d\chi\; \chi^4\; e^{-\frac{1}{2}\chi^2}}{\int d\chi\; e^{-\frac{1}{2}\chi^2}} = 3,$$

as well as the result, which can be easily obtained,

$$\sum_{\vec{x}}\langle(\Delta_0\varphi)^2\rangle = \sum_{\vec{k}}\frac{\rho_0^2}{\rho^2+\alpha_0},$$

in order to do the integrations and write

$$\langle \mathbf{H}_b^2\rangle = -\frac{1}{4}N_L^{2(d-1)} - \frac{1}{2}\frac{N_L^{d-1}}{N_T} - \imath N_L^{d-1}\langle \mathbf{H}'_b\rangle + \frac{1}{N_T^2}\sum_{\vec{k}}\frac{\rho_0^2}{\rho^2+\alpha_0} + \langle \mathbf{H}'^2_b\rangle,$$

In order to calculate the indicated expectation values it is necessary to consider in detail and separately the cases in which $\vec{k} = \pm\vec{q}$ and the cases in which $\vec{k} \neq \pm\vec{q}$. In addition to this it is necessary to recall that the expectation values of products of four fields have different behaviors when the Fourier components are real, in comparison to the case in which they have non-vanishing imaginary parts. For simplicity of the argument, let us consider explicitly the case in which N is odd, in which the only real Fourier component is the zero mode, $\vec{k} = \vec{0}$. As usual in this type of calculation, once the answer is obtained in terms of complete sums over the modes in momentum space, we may lift the restriction that N be odd without affecting the validity of the answer. Under these conditions we have the following four mutually exclusive possibilities:

$$\vec{k} = \vec{q} = \vec{0}, \qquad \vec{k} = \vec{q} \neq \vec{0}, \qquad \vec{k} = -\vec{q} \neq \vec{0}, \qquad \vec{k} \neq \pm\vec{q}.$$

Each pair $(\vec{k}, \vec{q})$ which is possible is exclusively in one of these four categories, while the union of the four exhausts all the possibilities for the pairs. With this we can write for our expectation value

$$\begin{aligned}\langle {\mathbf{H}'_b}^2 \rangle &= -\frac{N_L^{2(d-1)}}{4}\left[\alpha_0^2\langle|\widetilde{\varphi}_{\vec{k}=\vec{0}}|^4\rangle + 2\sum_{\vec{k}\neq\vec{0}}(-\rho_0^2+\rho_i^2+\alpha_0)^2\langle|\widetilde{\varphi}|^4\rangle\right. \\ &\qquad \left. + \sum_{\vec{k}\neq\pm\vec{q}}(-\rho_0^2+\rho_i^2+\alpha_0)_{\vec{k}}(-\rho_0^2+\rho_i^2+\alpha_0)_{\vec{q}}\langle|\widetilde{\varphi}_{\vec{k}}|^2|\widetilde{\varphi}_{\vec{q}}|^2\rangle\right].\end{aligned}$$

The expectation values involving different momenta can be factored and, in addition to this, we can use the known results

$$\begin{aligned}\langle|\widetilde{\varphi}_{\vec{k}=\vec{0}}|^4\rangle &= 3\langle|\widetilde{\varphi}_{\vec{k}=\vec{0}}|^2\rangle, \\ \langle|\widetilde{\varphi}_{\vec{k}\neq\vec{0}}|^4\rangle &= 2\langle|\widetilde{\varphi}_{\vec{k}\neq\vec{0}}|^2\rangle, \\ \langle|\widetilde{\varphi}_{\vec{k}}|^2\rangle &= \frac{1}{N_L^{d-1}N_T}\,\frac{1}{\rho^2+\alpha_0},\end{aligned}$$

to write

$$\begin{aligned}\langle {\mathbf{H}'_b}^2 \rangle &= -\frac{1}{4N_T^2}\left[3 + 4\sum_{\vec{k}\neq\vec{0}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)^2\right. \\ &\qquad \left. + \sum_{\vec{k}\neq\pm\vec{q}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)_{\vec{k}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)_{\vec{q}}\right].\end{aligned}$$

One of the three units in the first term and two of the four units in the second term may now be joined with the third term in order to complete the sum that appears in this last one, resulting in

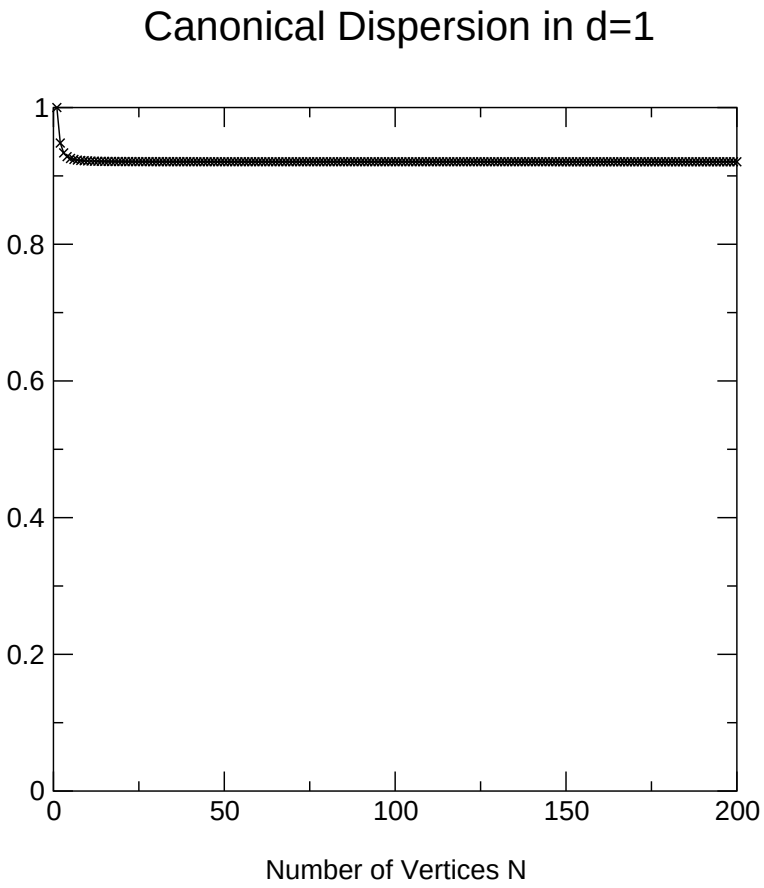


Figure 5.3.1: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, in the case $d = 1$.

that the positive terms predominate in the only factor which is not manifestly positive, the second factor in the numerator of the sum. This is due to the fact that there is an implicit sum over i in ρ_i^2, so that we have $d-1$ positive terms and only 1 negative term in the sum of the ρ's. Since the possible values for each ρ_i and for each ρ_0 are the same, we arrive at the conclusion that the sums are predominantly positive for sufficiently large dimensions d. The only case which raises some doubt, if we recall that $\alpha_0 \to 0$ in the continuum limit, is the case $d = 2$, but in this case it is possible to rewrite the sum in a manifestly positive form (problem 5.3.8).

The issue now is to determine how these sums behave in the continuum limit. Since the term that is being added is homogeneous of order zero on the ρ's, and therefore typically of the order of 1, it is to be expected that the sums behave as $N_L^{d-1} N_T$ or, in the symmetrical limit, as N^d, which is the number of terms in the sum. One exception should be the case $d = 1$, in which all the ρ_i's disappear and the situation changes qualitatively. We can easily evaluate these sums numerically in the symmetrical case, obtaining what is seen in the figures from 5.3.1 to 5.3.5. In

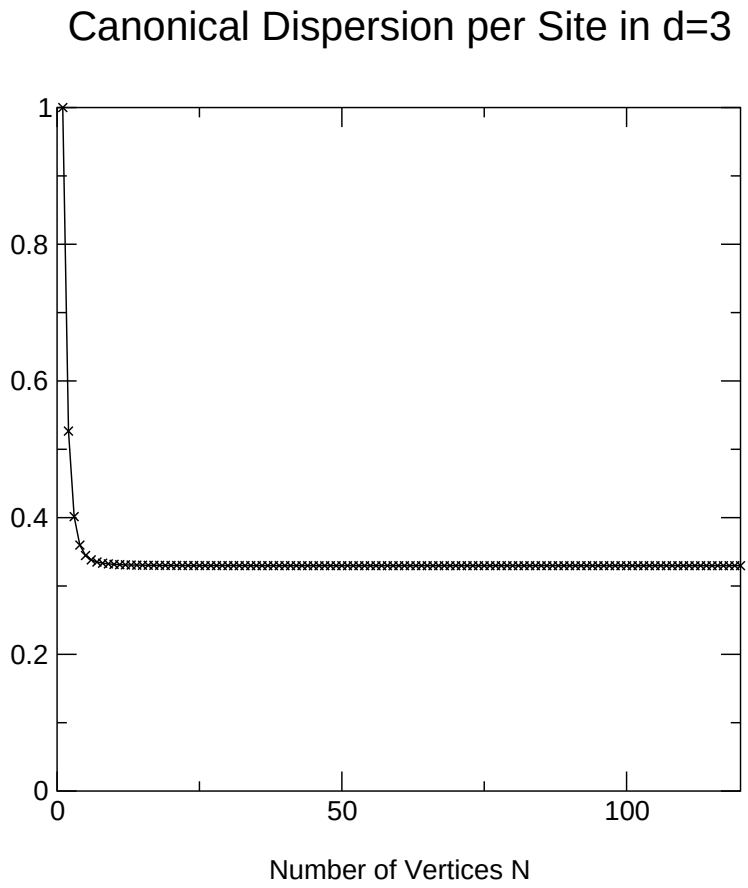


Figure 5.3.3: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 3$.

this particular case we can verify that this result is still obtained if we use the non-blocked Hamiltonian H instead of H_b, but is a much weaker form, since we are forced to adopt a particular way to take the limits for the dispersion to vanish in the limit (problem 5.3.9).

To complete the discussion we may also examine the corresponding results for $\mathbf{H}'_b$, that is, calculated according to the usual definition of the expectation values, instead of the canonical definition. In this case the result can be written as

$$\sigma^2_{\mathbf{H}'_b} = \frac{1}{N_T^2}\mathcal{S}_{\mathbf{H}'_b},$$

where the sum is defined by

$$\mathcal{S}_{\mathbf{H}'_b} = \frac{1}{2}\sum_{\vec{k}}\left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0}\right)^2.$$

The results of the numerical evaluation of the sums $\mathcal{S}_{\mathbf{H}'_b}$, in the case of the symmetrical limit, can be seen in the figures from 5.3.6 to 5.3.10. The only case in which

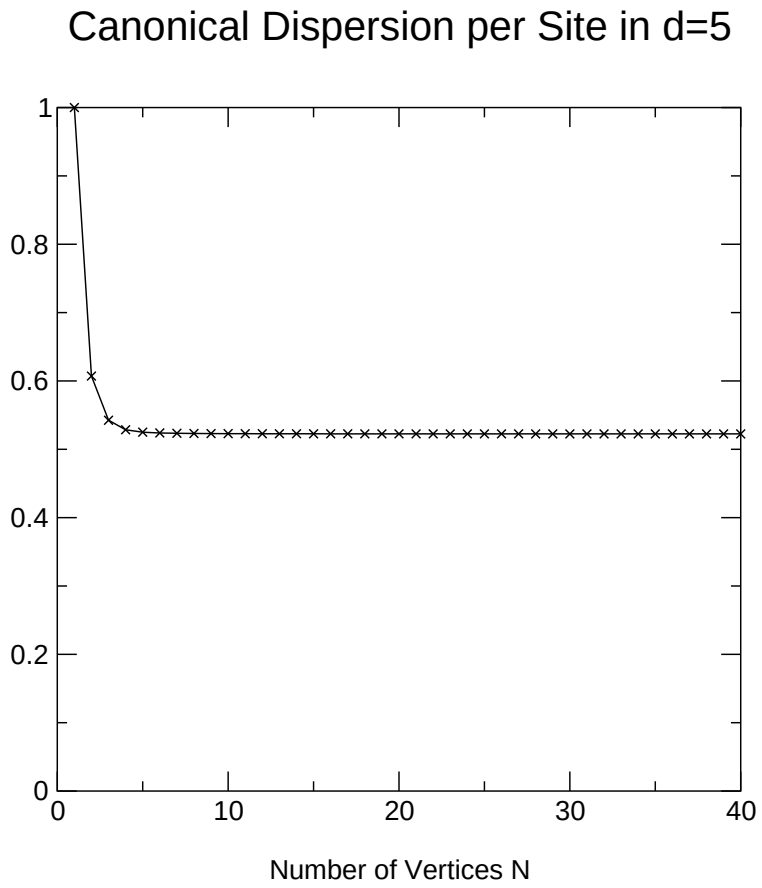


Figure 5.3.5: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 5$.

forced to use if we try to employ the non-blocked Hamiltonian H with the canonical definition of the expectation values (problem 5.3.9). Limits of this type will be discussed in detail in a little while, for the case of the quantum theory of fields. On the other hand, if we try to use the non-blocked Hamiltonian H and the non-canonical definition of the expectation values, then we verify that it is not possible to make the dispersion go to zero in the limit even in the case of quantum mechanics (problem 5.3.10).

In order to discuss in a more direct way the physical significance of these results, it is necessary to first translate these dimensionless results in terms of the dimensionfull physical energy, as we did above for the case of quantum mechanics. We will use in this discussion the results obtained according to the canonical definition of the expectation values. The dispersion $\Sigma^2_{\mathbf{H}_b} = \sigma^2_{\mathbf{H}_b}/a^2$ of the dimensionfull energy is given by

$$\Sigma^2_{\mathbf{H}_b} = \frac{1}{T^2}\mathcal{S}_{\mathbf{H}_b},$$

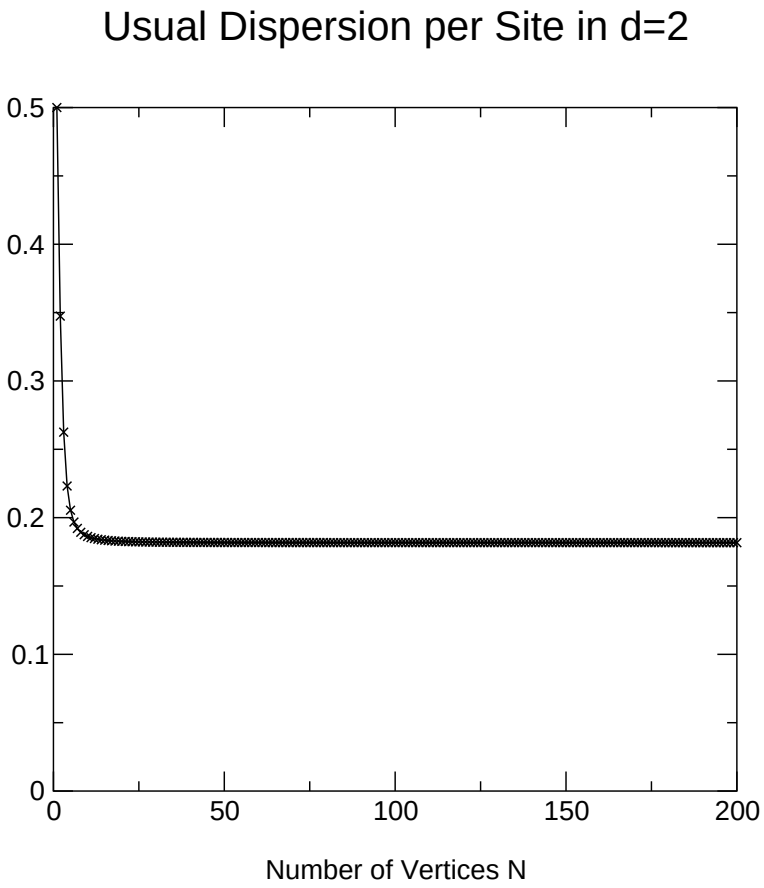


Figure 5.3.7: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 2$.

$$\Sigma^2_{\mathbf{H}_b} \sim \frac{1}{a^2}.$$

For larger dimensions the situation gets progressively worse. So long as we limit ourselves to taking the continuum limit in the symmetrical way, the situation seems to be that the concept of eigenstate and, ultimately, the concept of Hilbert space, only apply to the case of quantum mechanics, and not to the case of the quantum theory of fields.

We will therefore examine what happens if we take the continuum limit in a non-symmetrical way, which obviously only makes sense for $d \geq 2$. The most extreme case in this context is to take first the limit $N_T \to \infty$ with fixed N_L, as in the case of quantum mechanics, and only after that take the limit $N_L \to \infty$. The effect of this procedure is to first reduce the system to the quantum mechanics of an arbitrary but finite number of degrees of freedom, and only after that make the number of degrees of freedom increase without limit. In this case all the sums $\mathcal{S}_{\mathbf{H}_b}$ and $\mathcal{S}_{\mathbf{H}'_b}$

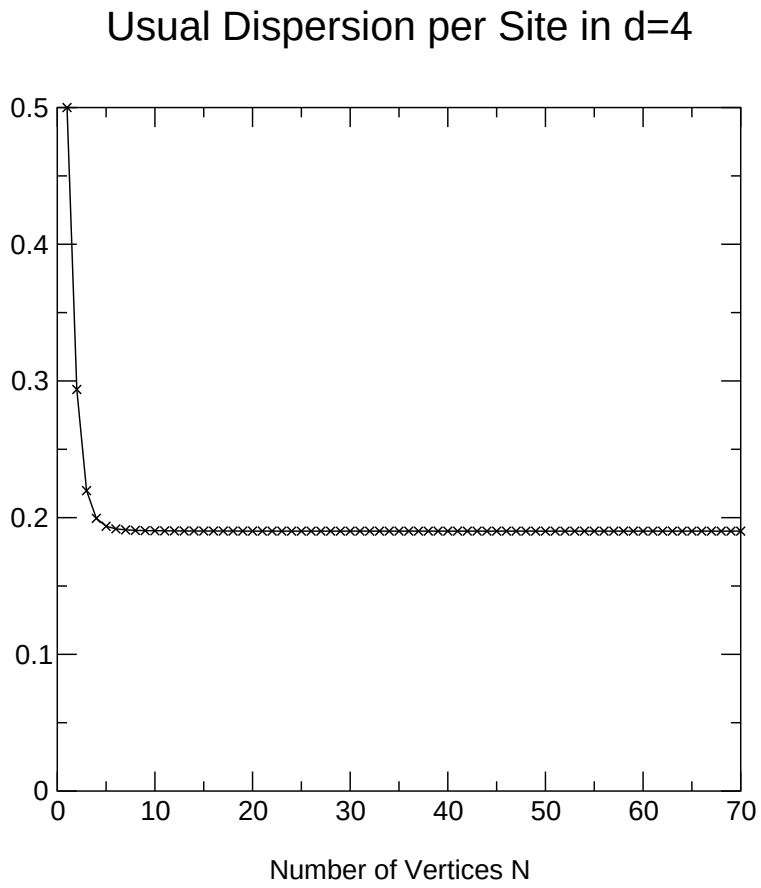


Figure 5.3.9: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 4$.

$$t(\vec{k}) \longrightarrow \left[\frac{-(2\pi k_0)^2 + N_T^2 \sum_i 4 \sin^2\left(\frac{k_i \pi}{N_L}\right) + (N_T/N_L)^2 m_0^2 L^2}{(2\pi k_0)^2 + N_T^2 \sum_i 4 \sin^2\left(\frac{k_i \pi}{N_L}\right) + (N_T/N_L)^2 m_0^2 L^2} \right]^2 .$$

Now, since $1/N_L$ does not go to zero, the sine function that appears in the second terms in the numerator and in the denominator does not become small, so that these terms diverge like N_T^2, as do the third terms. Hence, the only difference between the numerator and the denominator, which is the sign of the first term, tends to disappear, so that we obtain, in the limit $N_T \to \infty$ with fixed N_L and finite T,

$$\mathcal{S}_{\mathbf{H}'_b} \longrightarrow \sum_{\vec{k}} 1 = N_L^{d-1} N_T .$$

The same is true if we make $T \to \infty$ together with $N_T \to \infty$, since T has to increase slower than N_T in order to guarantee that $a \to 0$, that is, that we have in fact a

the sums behave as

$$\mathcal{S}_{\mathbf{H}_b}, \mathcal{S}_{\mathbf{H}'_b} \longrightarrow C(d) N_L^{d-1} N_T,$$

with, in each dimension, some positive constant $C(d)$, smaller than and of the order of 1. However, in order to check these facts beyond any doubt, it is necessary to evaluate numerically these sums in this type of asymmetrical limit (problem 5.3.15).

Let us observe that in this type of limit we have for the dimensionfull dispersions, both for $\Sigma_{\mathbf{H}_b}$ and for $\Sigma_{\mathbf{H}'_b}$, in dimensions $d \geq 2$, the behavior

$$\Sigma^2_{\mathbf{H}_b} \sim N_L^{d-1} \frac{N_T}{T^2}.$$

This allows us to make the dispersion vanish in the limit, it suffices to make T go to infinity sufficiently fast as a function of N_T, in order to compensate the increase of N_T. We can do this by relating T to some finite temporal length $\mathcal{T}$ (something like a mean life) by means of

$$T = N_T^p \mathcal{T}.$$

There are limits for the possible values of the power p. In order for T to go to infinity in the limit, we must have $p > 0$. On the other hand, we must remember that $T = N_T a$ and that there is also the need to make a go to zero in the limit, so that it be in fact a continuum limit. Combining this condition with the equation above we obtain

$$T = N_T a = N_T^p \mathcal{T} \Longrightarrow \mathcal{T} = N_T^{1-p} a,$$

so that in order that we have $\mathcal{T}$ finite with $a \to 0$ it is necessary that $1 - p > 0$, that is, that $p < 1$. Joining these two conditions we see that p must be inside the open interval $(0, 1)$. Writing now the dispersion $\Sigma_{\mathbf{H}_b}$ in this type of limit we obtain

$$\Sigma^2_{\mathbf{H}_b} \sim N_L^{d-1} \frac{N_T}{\mathcal{T}^2 N_T^{2p}} = \frac{N_L^{d-1}}{\mathcal{T}^2} N_T^{1-2p}.$$

In order for this to vanish in the limit we must have $1 - 2p < 0$, that is, $p > 1/2$. This set of conditions over p can be satisfied by values of p in the open interval $(1/2, 1)$, for example $p = 3/4$.

As another way to define asymmetrical limits, we can also generalize the symmetrical limits to the case in which both N_L and N_T increase in the limit, but with N_T increasing faster than N_L, thus establishing an asymmetry. We will call this type of limit the "simultaneous asymmetrical limits". It suffices to establish between these two quantities a relation of the type

$$N_L = N_T^q.$$

In order for N_L to increase slower than N_T, but so that both still increase simultaneously, we must have $0 < q < 1$. Observe that the terms of the sums still have

$$\Delta E_{1,\vec{k}} = \frac{-1}{T} \frac{4\sin^2\left(\frac{k_0\pi}{N_T}\right) + \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right) + \alpha_0}{-4\sin^2\left(\frac{k_0\pi}{N_T}\right) + \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right) + \alpha_0}.$$

We may now multiply the numerator and the denominator by N_T^2 and take the limit $N_T \to \infty$ with $N_L = N_T^q$ and $q > 0$. Note that, since in this case the momentum $\vec{k}$ is fixed and finite, we can approximate all the sine functions by their arguments without introducing any imprecision of thought. When we do this we obtain

$$\Delta E_{1,\vec{k}} \sim \frac{-1}{T} \frac{(2\pi k_0)^2 + N_T^{2(1-q)} \sum_i (2\pi k_i)^2 + N_T^{2(1-q)} m_0^2 L^2}{-(2\pi k_0)^2 + N_T^{2(1-q)} \sum_i (2\pi k_i)^2 + N_T^{2(1-q)} m_0^2 L^2}.$$

Since k_0, k_i and m_0 are finite and $q \neq 1$, in the limit in which $N_T \to \infty$ with $T \to \infty$ the first term becomes negligible by comparison with the other two, both in the numerator and in the denominator, so that we are left with the relation

$$\Delta E_{1,\vec{k}} = \lim_{T\to\infty} \frac{1}{T},$$

which goes to zero. Since the energy of the corresponding state of n particles is n times this result, we see that the energies of all the particle states collapse to zero in this type of limit. In other words, none of the states has energy different from the energy of the vacuum state in the continuum limit, whatever the momentum-space mode it is related to. Another way to say this is that, in this type of limit, there are no physical states left except the vacuum, once the limit is taken. One is left with an empty theory.

The fundamental reason causing this behavior can be identified as the underlying relativistic invariance of the theory. It is this invariance that implies the form of the action and therefore the form of the terms in the results for the energy, with the sum of ρ_0^2 and of the ρ_i^2, all with coefficients 1. The terms $(\Delta_0\varphi)^2$, $(\Delta_i\varphi)^2$ and $\alpha_0\varphi^2$ in the action lead directly to the terms ρ_0^2, ρ_i^2 and α_0 contained in our results. In the ultimate analysis, the relativistic invariance requires that the continuum limit be taken in a symmetrical way.

Note that this does not mean that the box inside which we are defining our model has to be exactly cubical. We may have a fixed proportionality relation between N_T and N_L, such as $N_T = CN_L$ with some constant C, meaning that the temporal size T and the spacial size L of the box may not be the same. However, it is necessary that the continuum limit be taken in a symmetrical way, that is, that N_T and N_L increase with the same speed in the limit. So long as the lattice spacing a remains the same in all the directions of the lattice there is no change in the form of the action and therefore no change in our results here. In other words, the requirement of symmetry in the continuum limit is a characteristic related to the ultraviolet regime, not to the infrared regime of the theory.

quantum-mechanical system of coupled harmonic oscillators with finite couplings, which is to make $\beta_0 \to 0$, also implies that $\nu \to 0$, that is, leads to the total absence of wave propagation in the continuum limit in Minkowski space.

Note that recovering the balance between the three terms of the sums in our results for the energy, which leads to the on-shell condition, also implies making $\beta_0 \to 0$ in this asymmetrical limit. This analysis can be extended to the case of the simultaneous asymmetrical limits, with the same basic results. Any trial at recovering the on-shell condition in these limits implies the absence of wave propagation in the continuous limit in Minkowski space. With the introduction of β_0 the numerator and the denominator that appear in our results acquire the form

$$\pm 4 \sin^2\left(\frac{k_0\pi}{N_T}\right) + \beta_0 \sum_i 4 \sin^2\left(\frac{k_i\pi}{N_L}\right) + \alpha_0,$$

so that in order to compensate the factor $(N_T/N_L)^{2(1-q)}$ that appears in the second terms when we multiply both the numerator and the denominator by N_T^2 we must make $\beta_0 \to 0$ in the limit, which is equivalent, from the point of view of quantum mechanics, to making finite the couplings between sites and, from the point of view of quantum field theory, to the absence of wave propagation in the continuum limit in Minkowski space.

We end this section with the interesting historical observation that this is not the first time that the existence of a useful Hilbert space for quantum field theory is submitted for discussion. In a very interesting (but difficult to find) little book titled "Lectures on Quantum Field Theory" [4] no lesser a figure than Dirac gave us his views about the state of the subject. In this book one finds the following two statements, that we take the liberty of quoting here:

> The interactions that are physically important in quantum field theory are so violent that they will knock any Schrödinger state vector out of Hilbert space in the shortest possible time interval.
>
> [The Schrödinger picture] is thrown out by the interactions which physicists are interested in being so violent in the high frequencies, and it doesn't seem to be possible to get interactions satisfying relativity which do not have this violent behaviour in the high frequencies.

These statements are by no means exactly the same that we are led by our results to make here, since Dirac is talking about interactions between fields and the Schrödinger picture of quantum mechanics, but the reference to the lack of usefulness of the Hilbert space, because the dynamics of the theory does not allow it to permanently contain the states, and the reference to relativistic invariance as being in conflict with the usual Hilbert space structure, are both, at the very least, extremely interesting and suggestive.

Problems

5.3.6. Calculate, according to the usual (non-canonical) definition of the expectation values, using the Fourier components of the fields, the dimensionless dispersion $\sigma^2_{H'} = \langle \mathbf{H}' \rangle^2 - \langle \mathbf{H}'^2 \rangle$, of the non-blocked Hamiltonian, obtaining

$$\begin{aligned}\sigma^2_{H'} &= \frac{1}{2N_T^2} + \frac{1}{N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 \\ &+ \frac{1}{2N_T^2} \sum_{\mathbf{k}} \sum_{k_0} \sum_{q_0} \frac{\left| -e^{-\imath\pi \frac{k_0 - q_0}{N_T}} \rho_0(k_0)\rho_0(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0 \right|^2}{[\rho_0^2(k_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0]\,[\rho_0^2(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0]}.\end{aligned}$$

5.3.7. Combine the results of problems 5.3.5 and 5.3.6 and calculate completely the dispersion $\sigma^2_H = \langle \mathbf{H} \rangle^2 - \langle \mathbf{H}^2 \rangle$, obtaining

$$\begin{aligned}\sigma^2_H &= \frac{1}{2N_T^2} + \frac{1}{2N_T} \sum_{\vec{k}} \frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} + \frac{1}{N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 \\ &+ \frac{1}{2N_T^2} \sum_{\mathbf{k}} \sum_{k_0} \sum_{q_0} \frac{\left| -e^{-\imath\pi \frac{k_0 - q_0}{N_T}} \rho_0(k_0)\rho_0(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0 \right|^2}{[\rho_0^2(k_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0]\,[\rho_0^2(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0]}.\end{aligned}$$

Compare your result with the dispersion of the blocked Hamiltonian $\mathbf{H}_b$ and show that $\sigma^2_H > \sigma^2_{H_b}$, as expected.

5.3.8. Show that the sum $\mathcal{S}^2_{H_b}$ in dimension $d = 2$,

$$\mathcal{S}_{H_b} = \sum_{\vec{k}} \frac{(\rho_1^2 + \alpha_0)(-\rho_0^2 + \rho_1^2 + \alpha_0)}{(\rho_0^2 + \rho_1^2 + \alpha_0)^2},$$

can be written as a manifestly positive quantity in the case of the symmetrical limit, in which $N_L = N_T = N$. Use the possibility of interchanging, in this symmetrical case, the variables k_0 and k_1 within the sum.

5.3.9. Write the dispersion σ_H of the non-blocked Hamiltonian in the $d = 1$ case of quantum mechanics. Evaluate the behavior in the $N_T \to \infty$ limit of the sums that appear in this result. In order to do this, consider the expressions in the limit $\alpha_0 \to 0$, which is the most relevant for us because α_0 in fact vanishes in the continuum limit. Note that in this limit you must treat separately the terms with $k_0 = 0$ and/or $q_0 = 0$. Use your results to show that the corresponding dimensionfull dispersion behaves in the limit as

$$\Sigma^2_H \sim \frac{-N_T}{T^2}.$$

Find out how to define limits in which $N_T \to \infty$ and $T \to \infty$ simultaneously so as to guarantee that this dimensionfull dispersion vanishes in the limit.

Chapter 6

Conclusions and Outlook

In this last chapter we discuss what conclusions can be drawn from the work done so far and presented in this book, describe some things that will be discussed in the next volume of the series, and finally talk about the future possibilities for research in the context of the ideas presented here. In the first section we present a fairly complete analysis of the final situation we are faced with after the development presented in the previous chapters. In the second section we propose a basic idea about one of the main problems that remains open within the theoretical structure we are building; it should be noted here that the material found in that section is of a rather speculative character. We will close this book with a short description of some other things that have been done, of some of the open problems and of some possibilities for further research in the area.

6.1 Analysis of the Situation

Let us consider what has been successfully obtained within the formalism presented in the previous chapters. First of all, in chapter 2 we obtained a complete and correct realization of the classical theory of fields using the lattice and the continuum limit from it. In addition to this, as was shown along chapters from 3 to 5, the same formalism in the quantum case for dimension $d = 1$ succeeded in producing a complete and correct realization of non-relativistic quantum mechanics. In the case of dimensions $d \geq 2$ we can go so far as to say that the formalism can be used to produce a fairly complete and constructive mathematical definition of the quantum theory of fields.

The definition of the Gaussian model on the Euclidean lattice results in the correct set of correlation functions for that simple model. A closer examination of the structure of the two-point function, which is the only non-trivial function of the model, revealed some rather surprising aspects of its behavior, but these issues were completely resolved by the introduction of block variables, leading to a completely satisfactory physical interpretation of the correlation functions of the theory. While it is a widely accepted position that all the observables in quantum field theory must be averages over spacial regions or blocks, the same does not seem to be so clear with

in momentum space than in position space. Elementary particles are therefore extended objects, not point-like objects. From a conceptual point of view the particles should really be identified with exchanges of packets of energy between external sources and the quantum field within the cavity. These exchanges do not happen in a sharply localized way, but over the whole extent of the cavity. In the non-relativistic limit, in which one makes $T \to \infty$ while keeping L finite, this association of relativistic particles with the d-dimensional cavity is mapped onto a corresponding association of the physical particles with the modes of the $(d-1)$-dimensional cavity that is left after the limit. This is a direct consequence of the non-relativistic limit of the on-shell condition, which establishes the expected values for the energy of the particles in terms of the momenta of the modes of the $(d-1)$-dimensional cavity.

We see, therefore, that the construction of the theory on the lattice is successful in many respects. There remains, however, one main issue to be dealt with, because we arrived at the unexpected result that neither the vacuum state nor any of the particle states are eigenstates of the blocked Hamiltonian observable, which is in sharp contrast with the situation in the case of non-relativistic quantum mechanics, in which we do find that the vacuum is an eigenstate of the blocked Hamiltonian. Due to this the construction does not lead to the usual structure of states and operators in a Hilbert space, as one might have expected it would do. Since there is a well-known formalism due to Osterwalder and Schrader [6] dealing precisely with the construction of a Hilbert space structure starting from the lattice structure, we must now compare our results with those of that formalism.

It is the examination of the asymmetrical continuum limits discussed in section 5.3, which first reduce the structure of the theory to the quantum mechanics of a finite number of coupled degrees of freedom, and only after that may let the number of degrees of freedom tend to infinity, that leads us to make contact with the Osterwalder-Schrader formalism. In this formalism the authors establish necessary and sufficient conditions for the construction of a positive-norm Hilbert space from the discrete structure defined on a lattice. When one examines the development of the argument in that formalism, one observes that it implicitly assumes that $N_T = \infty$ from the very beginning, so that the applicability of its conclusions to lattice systems such as the ones discussed in this book is limited to those that result from the asymmetrical limits.

Although the condition that $N_T = \infty$ is not explicit within the hypothesis of the formalism, it is implied by the operations that are performed during the development of the argument. One of the basic hypothesis of that formalism, which is given explicitly, is that the lattice must be separable into two disjoint sets by means of the definition of a $(d-1)$-dimensional boundary surface, which defines a moment in time. This eliminates the possibility of the use of periodical boundary conditions in the temporal direction of the lattice, as we have done regularly in this book. In addition to this, during the development one requires the possibility of performing temporal translations under which the system should be invariant. Without periodical boundary conditions this is only possible if the lattice is infinite in the temporal

the electromagnetic field, are excitations of the modes of oscillation of the electromagnetic field within the cavity. The photons are clearly identified with packets of energy that are exchanged between an external source, in this case the atom, and the modes of oscillation of the field within the cavity.

The only way in which it seems possible to keep the symmetry between the temporal and spacial directions and still be within the hypothesis of the Osterwalder-Schrader formalism is to start with lattices that are infinite in all directions. Starting with both N_T and N_L infinite would be compatible with the aforementioned hypothesis of that formalism, but is equivalent to giving up the constructive definition of the theory by a limiting process from finite and discrete mathematical systems. We regard this as philosophically unacceptable, since adopting such a definition would rule out any truly constructive analysis of the structure of the theory. Note that it would also rule out any type of finite computational simulation as a calculational tool for the theory.

It seems to us that there is no reasonable way out of this situation, and that we must accept the fact that the traditional Hilbert-space formalism is not an appropriate tool for the description of relativistic quantum theory at the most fundamental level. A constructive definition which could include such a formalism at the fundamental level is, it would seem, still to be exhibited. As we will see in our continued explorations in the next volume, the usual perturbative theory can be formulated entirely on the lattice, without any reference to Hilbert spaces, and hence all the calculations that can be made in that formalism can also be performed within the lattice formalism, possibly with some quantitative differences, so that not much is lost in the perturbative front. In fact, something is gained, due to a much clearer and more solid insight into the mathematical structure of the theory.

Note that the loss of the usual Hilbert-space formalism is not really a physical loss, but rather a mathematical one. The fundamental physical principle underlying the quantum theory, the principle of uncertainty, is not lost. In fact, one can say that the exact opposite is true, and that quantum field theory contains a higher degree of uncertainty than non-relativistic quantum mechanics, as was argued by Landau and Peierls a long time ago [8]. This is reflected in the violent fluctuations undergone by the fundamental field, leading to its being typically a completely discontinuous function, and also causing the Hilbert-space formalism to cease to be an appropriate tool for the description of the structure of the theory. It is possible, however, that the Hilbert-space structure can be recovered as an approximation, under certain conditions. For example, this is certainly to be expected in the non-relativistic limit of the theory.

One situation in which one would expect that an approximate Hilbert-space structure can be implemented would be for an effective theory using block variables and an energy cutoff. This is made reasonable due to the fact that the behavior we see in quantum field theory is clearly related to the large fluctuations of the fields, and these become much smaller for the block variables. As we saw in section 4.3, the larger the blocks, the smaller the fluctuations undergone by the block variables, so that large blocks are associated to the classical limit of the theory. If in some specific

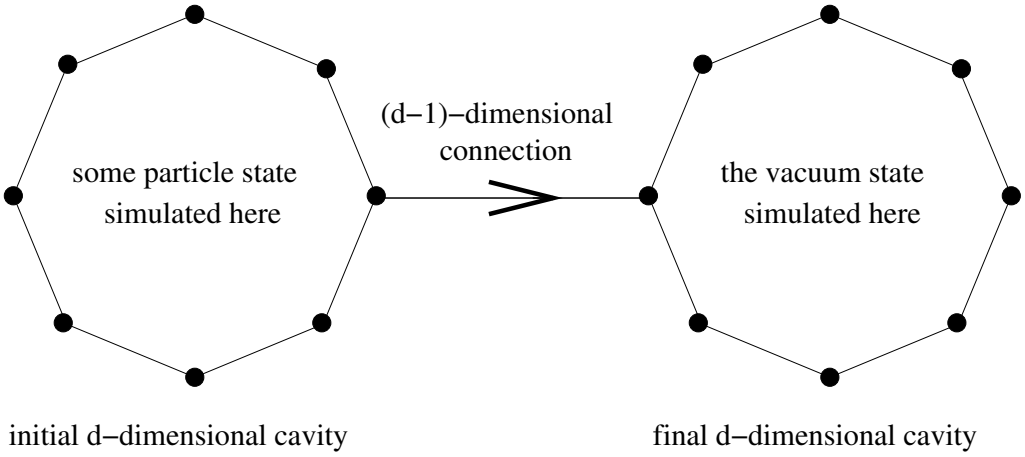


Figure 6.2.1: The lattice model proposed as a representation of the temporal evolution of blocked quantities.

boundary conditions we will adopt periodical boundary conditions for each lattice. Note that there is no problem involved with the use of the periodical boundary condition in the temporal direction within each box, because this internal temporal variable does not represent temporal evolution. The middle arrow represents the interface between the two lattices, connecting a $(d-1)$-dimensional spacial section of the left lattice with a corresponding spacial section of the right one.

The $(d-1)$-dimensional surface interfacing the two boxes will become an arrow of time, establishing a temporal ordering between the two boxes, in the following way: the initial box will contain a full realization of some state of particles, that is, a stochastic simulation of the corresponding statistical distribution; one then takes the field that results from this distribution, on the chosen $(d-1)$-dimensional space-like surface perpendicular to the temporal variable of that box, and copies it dynamically into a corresponding space-like surface of the final box; within the second box one builds a direct stochastic realization of the statistical distribution of another physical state, typically the vacuum state, at all sites except for this $(d-1)$-dimensional space-like surface, which will function as a dynamical boundary condition for the rest of the lattice within the second box.

If the state in the first box is, say, a one-particle state with momentum $\vec{k}$, then the second box will be subject to the effect of a $(d-1)$-dimensional surface containing a section of that first ensemble. This will affect the distribution within the second box, which will no longer be simply the vacuum. In this way the physical situation within the first box can propagate into the second box, along what we may call Monte-Carlo time, in a type of diffusion process, leading eventually to an equilibrium situation which represents the physical propagation of the state. The physical propagation is expressed as the difference between what we implemented directly in the second box (the vacuum state) and what eventually turns up within it as a consequence of the influence of the first box (in this example, possibly a one-particle state). Note that the cause-and-effect relationship is only from the first box to the second box,

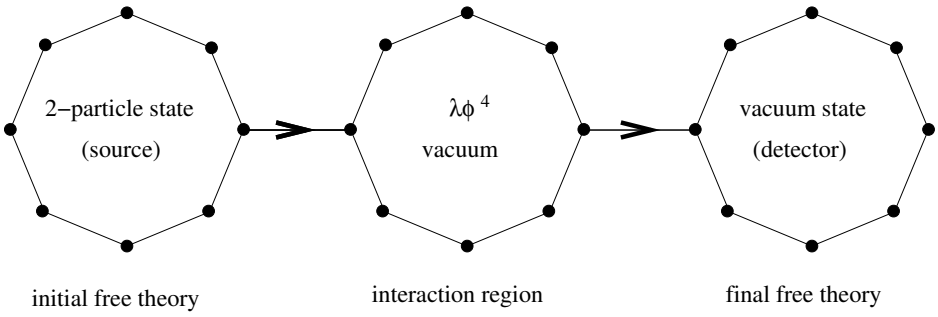


Figure 6.2.2: The lattice model proposed as a representation of a scattering process.

vectors pointing more directly through the $(d-1)$-dimensional interface. However, definite answers to any of the many questions one could ask about this idea will have to wait for the results of further research, probably involving some large-scale stochastic simulations of the proposed system.

If this idea turns out to work, then one can readily imagine other uses for it, for example the direct representation of scattering processes, as illustrated in figure 6.2.2. Here we have three consecutive boxes, the initial one holding an initial state of two particles, say with momenta $\vec{k}_1$ and $\vec{k}_2$. The middle box is an interaction region, where an interaction such as one finds in the $\lambda\phi^4$ polynomial model is turned on, and the parameters of the model are tuned so that the physical mass of its particles is equal to the physical mass of the incoming free particles. The third box contains the free vacuum and is a detection region, where one will look to find out what particles with which momenta show up. This would be a discrete realization of the scattering structure which is usually represented by asymptotic "in" and "out" fields and states in the traditional approach to the subject.

One can go further on with ideas like this, for example proposing the definition of thermal states, by starting with a state containing some set of many particles, and propagating it through a large number of consecutive interaction regions, until the set of particles finds a true thermal equilibrium distribution, that is, a distribution of particles that no longer changes when it passes through an interaction region. For practical reasons one could adopt the following alternative approach: instead of a long series of interaction regions, use only one interaction region and add to the system a feedback mechanism from the third box to the first box, that modifies the initial distribution of particles so that it converges to the final distribution of particles which is detected in the third box. In any case, one can see that there is plenty of field for exploration and further research in this subject.

6.3 Problems and Possibilities

The facts about the theory found in the explorations described in this book have some important consequences on the treatment of some other models, namely the non-linear models of scalar fields usually referred to as the polynomial models and

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