important work on it still lies ahead. These volumes are being written and published freely through the Internet in the hope that they may be useful for physicists involved with this difficult subject. Students and researchers troubled by the deficiencies of the usual approach to the subject may find here some food for thought.

All the source code of the programs used to produce the data and results presented in this book will be made available through the network. At a time when progress in science is so dependent on computer work, sometimes on massive amounts of it, it is a question of scientific integrity and of intellectual honesty that the source code used in science be made openly available to all those that may be interested in it. It is important that the source code be made available, not only in order to allow for its free and open criticism, but also to allow it to be used and improved by others, thus promoting cooperation in this most crucially important human activity.

Considering that the historical development of science, and consequently of the technology that springs from it, has given us the means to promote very easily and cheaply the publication of truly massive amounts of information, as well as the tools needed to retrieve very fast whatever part of this information we find relevant, it is only appropriate that we use this new technology for the dissemination and development of scientific ideas, and hence for the furthering of science.

We would like to acknowledge here the contribution to parts of the material contained within this book by former students and collaborators who were active in this subject in the past. The work on the discontinuity of the fields was done in collaboration with Dr. Timothy Edward Gallivan and Dr. See Kit Foong. Some of the work on states of particles was done in cooperation with Dr. Silvana Perez. Some contributions to specific things were made by Mr. Arnaldo Gomes de Oliveira Filho. When appropriate, due credit will be given in footnotes along the text. We would also like to thank those that helped by reading and correcting the manuscript at various stages of its production.

The world of bits, on the other hand, is better described, perhaps, as the world of information. The concept of information is much harder to define than the concept of energy, perhaps because it is a rather new concept, while the concept of energy has a long story behind it. However, it is rather easy to recall a few familiar examples, such as the contents of a book, the contents stored within a digital computer, and the contents of the nuclear DNA of the cells of a living being. Energy and information are very different concepts. While the most fundamental property of energy is its conservation, that is, the fact that it may be transformed into many different forms while its total amount remains constant in all physical processes, information can be easily destroyed, and can also be created, usually with some difficulty, as those involved in research activities know well.

The two concepts are of course related, and one may even go so far as to further classify information according to the nature of this relation. For example, one may consider active and passive forms of information, the active form being one that interacts more closely with some object capable of information processing, enabling it to do things it would not be otherwise capable of doing, while the passive form consists of stacks of data that may or may not be used by this information-processing enabled object. Examples of active information in the case of a digital computer are the programs that can run on it, while passive information consists of stacks of data that can be used by such programs. In the case of the human mind one can say that the acquisition of skills, such as playing the piano or performing differentiations and integrations in mathematical calculus, is as example of the existence of active information within the mind, while the memorization of lists of things and facts may be understood as the acquisition by the mind of passive information.

Our universal duality becomes then the duality of energy and information. What we must point out here is that physical theory exists in the interface between these two worlds. If, on the one hand, it must contain a representation of objective physical reality, its structure must also allow for reasonably easy manipulation by the human mind, which is an object living in the world of information. Note that just as one can think of the hardware and software aspects of a computer, so one can think of the brain as a hardware aspect belonging to the world of energy, and of the mind as a software aspect belonging to the world of information. It is the mind that matters here.

One very fundamental example of an object that deals with the interface between these two worlds is the concept of a physical measurement, which is one of the fundamental concepts of quantum mechanics. A physical measurement can be described as a process taking place in the world of energy that has as its end-result the production of a certain amount of information. It is therefore a process that starts in the world of energy and ends up in the world of information. We see therefore that both the experimental or measurement aspect and the theoretical aspect of physics exist in the same realm.

Since physical theory exists in the interface of the worlds of energy and information, it may be argued that its structure must cater as much to the facts of objective physical reality as to the characteristics and limitations of the mind it is built to

structures. What we mean here is that the structures involved in the construction of the limits be not only discrete, but actually finite as well, in terms of the number of elements involved.

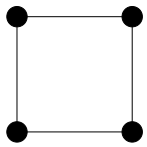
A simple and familiar object defined by a limiting procedure of this kind is the Riemann integral, which is defined as a limit from a set of finite sums, that is, sums with a finite number of terms. Note that there is no veto here to the existence of some other definition, equivalent to the original one, which may be formulated exclusively in terms of continuum quantities. What we impose here is a veto against continuum mathematical structures that *cannot* be formulated as limits from strictly finite mathematical structures. We will also regard the definition by such a limiting procedure as the most fundamental one, and choose it over any others in case any doubts arise regarding the equivalences among them.

This philosophical attitude, which some may regard as a preconception or prejudice, can be motivated by the fact that, ultimately, the set of all possible physical measurements and experiments that can be actually carried out by us within any possibly large but certainly finite amount of time is certainly a finite set. It is therefore not natural to think that the results of all these measurements and experiments can only be systematized and encoded within a mathematical structure which is intrinsically undefinable in terms of finite mathematical structures. One may also formulate this philosophical concept in terms of the number of particles of either matter or radiation that can be ever detected by us, which is also necessarily a finite number.

The next subject to be discussed is that of the definition of observables within the theory. As explained before, we do not expect the theory to consist only of observable quantities. Even non-relativistic quantum mechanics contains elements that, although playing important roles within the theory, are not themselves observable, such as the wave function. We expect the theory to contain elements that are there for the convenience of the mind, not because they are observables. One such object in quantum field theory is the fundamental field itself, because the value of the field at a given point of space-time is not an observable of the theory.

What is required of the theory regarding the physical observables is that they be clearly and concisely identified as such. The definition of the theory must include a clear and concise discrimination of the parts or aspects of the structure which are physical observables. The requirement of conciseness is included because it will not do to have a definition which has to be revised or modified each time a new quantity comes into consideration. There must be a global and fixed set of criteria that can be used to identify the quantities which correspond to physical observables.

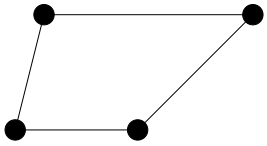
Note that this leaves open the possibility that one may use a computer, or some other computational means, to perform mathematical probes into the structure of the theory, which may not necessarily correspond to physically realizable observations. This "inner look" into the mathematical structure of the theory may be useful for establishing a better understanding of the inner workings of the theory, which may have consequences for our understanding of the realm of physical observables, even if only in an indirect way. In the subsequent chapters we will be using this



Lattices have the property that the number of links connected to each site is constant, the same for all sites. This number will always be even and equal to $2d$, where d is the dimension of the lattice. In this second example we have $d = 1$, the lattice has dimension 1, and it is said to be one-dimensional. The lattice in the previous example is also one-dimensional, but in that case there are two links that are connected to only one site. We say that the lattice in the first example, unlike the one in the second example, has a *boundary*.

The existence or not of a boundary will have, later on, an important role to play in the development of the theory, relating to the different types of *boundary conditions* that may or may not be adopted under various circumstances. Since the second example can be obtained from the first, by the interconnection of the two links with loose ends, resulting in a cyclic structure, we say that the second example adopts *periodic boundary conditions*.

Observe that, for the time being, there is no additional structure in this object, besides the connectivity of sites and links. In particular, there is no geometric structure or notion of distance. Our second example could be represented as



without any change in the structure of the object as defined so far. We will usually employ symmetrical pictorial representations of the lattices, for simplicity of the drawings, but it is important to keep in mind that there are no predetermined notions regarding the geometry of the lattice or the length of the links.

Also for simplicity of the drawings that we will use to illustrate the ideas, we will usually use as examples lattices of dimension 1 or 2. However, our fundamental interest will be in lattices of dimension 3 and 4. Occasionally we may make use of lattices with $d = 5$, but never with dimensions larger than this. The case $d = 1$ is very different from the others, within the scope of the quantum theory to be developed, and will be used as counterpoint, in order to contrast its results with the corresponding results of the lattices with larger dimensions. The case $d = 2$ is also significantly different from the others, and will be used only for illustration. A typical two-dimensional lattice could be represented as shown in figure 1.2.1.

In the case of the adoption of periodical boundary conditions the links identified in this drawing with the same numbers or letters would be interconnected. Since it is unpractical to draw the toroidal structure of a lattice of dimension 2 or larger with periodical boundary conditions, sometimes we may simply state that such boundary conditions have been adopted and represent the lattice as shown in figure 1.2.2,

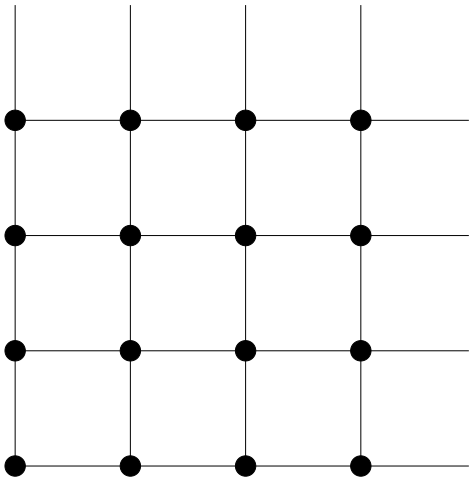


Figure 1.2.2: A simpler representation of a two-dimensional lattice with periodical boundary conditions.

questions of the theory, and it is from it that arise all the fundamental difficulties we will find during the development of the theory.

Still for simplicity, we will usually consider only *hypercubical* lattices, with a symmetrical structure containing the same number N of sites in all the d directions, as in the examples given in figures 1.2.1 and 1.2.2. When it becomes necessary, for the discussion of some point of foundation of the theory, as will happen later on, we will lift this restriction. Also, we will usually employ periodical boundary conditions, in all directions of the lattice, except when we come to the specific discussion of the issue of the choice of boundary conditions.

It is clear that the structure of the lattices can be generalized and made more complex in many different ways. We are taking here a small subset of the set of all possible lattices, which is particularly simple and symmetrical. Our strategy here is to focus attention only on the simplest cases, until some fundamental reason appears to lead us to more complex and sophisticated representations of the structure of the physical models we are dealing with.

Finally, let us note once more that the limit $N \to \infty$ by itself means nothing in terms of the physical geometry of the lattice. In particular, nothing happens to the physical lengths of the links in this limit, since there is as yet no notion of physical length established within the structure we are building. Later on, when the notion of metric distance appears, it will be discussed in detail in regard to its nature, origin and role in the structure and in the physical interpretation of the quantum theory.

Note that all such fields are scalars, not vectors. In further parts of the development one would see that vector fields in space-time are associated to the links and not to the sites of the lattice. The vectors drawn above are vectors in the internal space of the fields, not in space-time. These internal spaces are simple vector spaces in which act symmetry transformations among the fields. Usually these are continuous objects even in finite lattices, while space-time is represented in a discrete form by the lattice. In this book we will not discuss such possibilities any further, and will limit ourselves to scalar fields with a single real component. However, many of the results we will arrive at will apply to multi-component fields as well.

In part of what follows we will be interested in single configurations, or particular possibilities for the field function φ, specially when we discuss the so-called *classical* version of the theory. However, our greater objective is the exploration of what we will refer to as the *quantum* theory, for which we will be interested, not in particular cases for the function φ, but rather in the *set of all possible functions* φ, a set which we will call the *space of configurations* of φ. On finite lattices this usually is a continuous space with a large but finite dimension. For example, for a single-component real field in a lattice with N^d sites the space of configurations is $\mathbb{R}^{(N^d)}$. Only in the limit $N \to \infty$ we will have an infinite-dimension space as part of our structure.

We have, then, the structure of the lattice and the fields defined over it, which are the basic elements for the construction of the theory. The theory will be about *functionals* of the fields, that is, functions that associate a real value to each one of the possible configurations φ of the field. We will be interested in several functionals of this type. A very simple example of such a functional is one which associates to each configuration φ the value that it assumes at a given site s_0, namely the value $\varphi(s_0)$. Usually we will be interested in more complex functionals than these, which involve sums over all the sites of the lattice. An example of such a functional, still quite simple, would be the one which associates to φ the sum of its values at all the sites,

$$F_0[\varphi] = \sum_s \varphi(s),$$

where the dependence of the functional on the configuration will always be denoted by square brackets and the sum symbolized by the subscript s extends over all the sites of the lattice. If we describe the lattice by a set of integer variables n_μ, $\mu = 1, \ldots d$, where each one of the d components n_μ of the vector $\vec{n}$ is an integer which numbers the sites along one of the directions of the lattice, we may write this sum explicitly as

$$\sum_s \equiv \sum_{\vec{n}} \equiv \sum_{n_1=1}^{N} \cdots \sum_{n_d=1}^{N}.$$

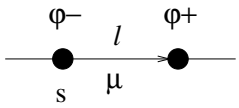
Hence, we may denote $\varphi(s)$, equivalently, by $\varphi(\vec{n})$, the first notation being more conceptual while the second makes more explicit reference to the system of integer coordinates. In the two-dimensional case, for example, we will usually employ

kind of action, which depends only on the fields at individual sites, and which we may call *ultra-local*, is too simple to be of much interest to us. For the theory of quantum fields it is essential that the action depend also on products of the fields at neighboring sites. This is what happens when we include in the action, in the continuum limit, dependencies on the *derivatives* of the fields. In finite lattices we define as the objects that play the role of derivatives certain finite differences between values of the fields.

If φ_+ and φ_- are the two values of a real field φ on the sites at the two ends of a link in the direction μ, φ_+ being on the positive side of the link and φ_- on the negative side, according to the orientation defined by a given system of integer coordinates, the finite derivative of the field is defined as

$$\Delta_\ell \varphi = \Delta_\mu \varphi(s) = \varphi_+ - \varphi_-.$$

The positive and negative orientations of the direction μ which are mentioned here are those in which the integer coordinate n_μ associated to that direction is, respectively, increasing and decreasing in magnitude. The notations $\Delta_\ell \varphi$ and $\Delta_\mu \varphi(s)$ are equivalent because, given a site s and a positive direction of μ starting from it, a certain link ℓ is uniquely determined,



We see that the finite derivative is a variable naturally associated to an oriented link, not to sites. In this way, we may now define a new action functional as

$$S[\varphi] = \sum_\ell (\Delta_\ell \varphi)^2 + \sum_s \varphi^2(s),$$

which also satisfies the two fundamental conditions. The first sum, as symbolized by the subscript ℓ, extends over all the links of the lattice, that is, it is an abbreviation for a double sum, over all sites and all the directions of the lattice. We may write explicitly that

$$\sum_\ell \equiv \sum_\mu \sum_s \equiv \sum_{\mu=1}^{d} \sum_{n_1=1}^{N} \cdots \sum_{n_d=1}^{N}.$$

Clearly, we may generalize this expression for the action, without any violation of the two conditions, if we multiply each one of the two terms by any positive coefficients. We will be specially interested in the particular form of this action given by

$$S_0[\varphi] = \frac{1}{2} \sum_\ell (\Delta_\ell \varphi)^2 + \frac{\alpha_0}{2} \sum_s \varphi^2(s), \tag{1.3.1}$$

motion but rather on the action functional as the object defining the physical models. This classical topic may not be our fundamental objective but it is useful to illustrate the role of each element of the structure and also to help to orient the reader, comparing the elements that appear here with with the corresponding elements as seen in the traditional approach to the subject, usually in graduate courses.

In order to establish this relation it will be necessary to take the limit $N \to \infty$ in our theory. Before this, however, there are two other things we must do. First, we must define what we will call a *finite classical field theory*, on each finite lattice. In addition to this, it will be necessary to introduce one more basic element into the structure, to wit, an *external dimensional scale*.

In order to define the classical theory on finite lattices we consider the action $S_N[\varphi]$ of a given model, on a given lattice of size N. We say that a *classical solution* of the model is a configuration φ_0 which minimizes $S_N[\varphi]$ locally, that is, at which the action has a local minimum. The stability condition that we imposed on $S_N[\varphi]$ implies that there is at least one local minimum of the action, the one located at the position of the global minimum guaranteed by that condition. For the action S_0 of the free theory we see immediately that the classical solution is simply the identically null configuration, $\varphi \equiv 0$, for all N. Note that, in principle, S_N may have more than one local minimum and that, when this happens, we will have more than one classical solution. This is not the case for S_0, but it is possible to construct actions with this property, as we may see in a future opportunity.

Let us also recall that we are assuming the use of periodical boundary conditions. In general the nature of the classical solutions depends on the boundary conditions. With the introduction of other elements into the structure, such as other types of boundary conditions or other terms in the action, the classical solutions may be much less trivial than the simple example we gave here. In particular, later on we will discuss the concept of *external sources*, which is very important for the physical interpretation of the theory and in the presence of which the classical solutions will change in significant and important ways.

Having defined what we mean by the classical solution of the theory on each finite lattice, we turn to the limit $N \to \infty$. We must now introduce into the theory a dimensional scale, that is, a notion of distance in our structure. We assume that, in a certain given system of physical units, external to our model and to be added to our lattice structure, the length of a side of the lattice, which is formed by N consecutive sites and links in a given direction, has the value L, a quantity with dimensions of length in that external system of units. In what follows we will make some choices as to the type of limit we will consider here. Both here and in the quantum theory it is possible to take the limit $N \to \infty$ of the models in several different ways, depending on what is done with the parameters of the model during the limiting process.

Let us imagine that L remains fixed and finite during the limit, which means that we are taking the limit in such as way that our lattice remains perfectly fitted within a cubic box with periodical boundary conditions and volume $V = L^d$. We will also make the parameter α_0 go to zero in the limit, in a certain well-defined

$$S_0[\phi] = \frac{1}{2}\int_V \mathrm{d}^d x \sum_\mu [\partial_\mu \phi(\vec{x})]^2 + \frac{m_0^2}{2}\int_V \mathrm{d}^d x\ \phi^2(\vec{x}).$$

We will refer to this limit as the *continuum limit* of the classical theory, because in it the lattice spacing a goes to zero while the lattice acquires an increasing number of points and tends to occupy densely the volume V of the interior of the box. The object that results from this process is the usual classical theory of the free scalar field within a box with periodical boundary conditions. In the limit the dimensionfull coordinates $0 \leq x_\mu \leq L$ describe the continuous interior of the box and, on finite lattices, they relate to the dimensionless coordinates n_μ by $x_\mu = n_\mu a$.

The functional $S_0[\phi]$ above is the usual action that defines the classical dynamics of the free scalar field within a box. Note that, for the dimensionfull mass parameter m_0 that appears in the second term to be finite in the limit, it is necessary that the dimensionless parameter α_0 go to zero as $1/N^2$, for any value of the mass in the limit. This type of behavior for the dimensionless parameters of the theory is very general. Usually there is a particular set of values of the parameters of the theory that they must approach in any continuum limit which is to be of physical interest. We refer to these special values as *critical*, for reasons that will become clearer later. In our case here the value 0 is a *critical point* of the parameter α_0.

In this continuum limit the classical solution of the model is given by the Euler-Lagrange equation, which in this case is no more than a generalization of the d-dimensional Laplace equation, including the mass term. We can derive this equation by means of the direct application of the principle of minimum action. In order to do this we make a generic variation $\delta\phi(\vec{x})$ of the fields, which is infinitesimal but may be different in each point, and then determine the condition that the field must satisfy so that the action does not change to first order, as a consequence of this variation. Calculating the variation δS_0 to first order in $\delta\phi$ we obtain

$$\delta S_0[\phi] = \int_V \mathrm{d}^d x \left\{ \sum_\mu [\partial_\mu \phi(\vec{x})]\delta[\partial_\mu \phi(\vec{x})] + m_0^2 \phi(\vec{x})\delta\phi(\vec{x}) \right\}.$$

Using now the easily verifiable fact that $\delta[\partial_\mu \phi(\vec{x})] = \partial_\mu[\delta\phi(\vec{x})]$ we obtain

$$\delta S_0[\phi] = \int_V \mathrm{d}^d x \left\{ \sum_\mu [\partial_\mu \phi(\vec{x})]\partial_\mu[\delta\phi(\vec{x})] + m_0^2 \phi(\vec{x})\delta\phi(\vec{x}) \right\}.$$

We may now integrate the first term by parts. There is no surface term, due to the periodical boundary conditions, and we therefore have

$$\begin{aligned} \delta S_0[\phi] &= \int_V \mathrm{d}^d x \left\{ -\sum_\mu [\partial_\mu^2 \phi(\vec{x})]\delta\phi(\vec{x}) + m_0^2 \phi(\vec{x})\delta\phi(\vec{x}) \right\} \\ &= \int_V \mathrm{d}^d x\ \delta\phi(\vec{x}) \left\{ -\sum_\mu \partial_\mu^2 \phi(\vec{x}) + m_0^2 \phi(\vec{x}) \right\}. \end{aligned}$$

With this we have on finite lattices the equation of movement which determines the classical solution, whose derivation will be left to the reader (problem 2.1.1),

$$-\Delta^2\varphi + \alpha_0\varphi = 0. \tag{2.1.3}$$

In three dimensions and in the continuum limit the zero-mass version of our equation of movement reduces to the Laplacian on the torus, since we are using here periodical boundary conditions. This is a rather familiar situation, since it is just the electrostatics of a torus without internal charges. Something analogous to this happens in the case of four dimensions, in which we obtain an Euclidean version of the wave equation for the scalar potential, which is also a part of classical electrodynamics. If we write equation (2.1.1) explicitly in four dimensions we obtain

$$-\partial_x^2\phi - \partial_y^2\phi - \partial_z^2\phi - \partial_t^2\phi + m_0^2\phi = 0,$$

where x, y and z are the three spacial Cartesian coordinates and t corresponds to the time. The process of passing from Euclidean space to Minkowski space can be effected by the exchange of t for $\imath t$ in this expression, which takes us to

$$-\vec{\nabla}^2\phi + \partial_t^2\phi + m_0^2\phi = 0.$$

where $\vec{\nabla}^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ is the three-dimensional Laplacian. In the case $m_0 = 0$ this is the usual wave equation. In general, the passage to Minkowski space is effected identifying within the answers obtained in Euclidean space the metrical tensor $g_{\mu\nu} = \delta_{\mu\nu}$ of this space and changing the sign of its diagonal term which corresponds to the temporal coordinate. In the example above we may write the equation in Euclidean space as

$$-\sum_{\mu,\nu} g_{\mu\nu}\partial_\mu\partial_\nu\phi + m_0^2\phi = 0$$

and making the transformation to Minkowski space by transforming the metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

This process of de-Euclideanization may always be realized in this fashion, either in position space or in momentum space.

Problems

2.1.1. Derive the equation of movement (2.1.3) on finite lattices, applying the principle of minimum action to the action of the free theory given in equation (1.3.1).

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repeating the derivation made previously for the periodical boundary conditions, in $d = 1$,

$$\begin{aligned}
\sum_l (\Delta_\ell \varphi)^2 &= \left(\Delta_{\ell_{b-}}\varphi\right)^2 + \ldots + (\Delta_\ell\varphi)^2 + \ldots + \left(\Delta_{\ell_{b+}}\varphi\right)^2 \\
&= (\varphi_0 - \varphi_1)^2 + (\varphi_1 - \varphi_2)^2 + \ldots \\
&\quad + \ldots + (\varphi_{n-1} - \varphi_n)^2 + (\varphi_n - \varphi_{n+1})^2 + \ldots \\
&\quad + \ldots + (\varphi_{N-1} - \varphi_N)^2 + (\varphi_N - \varphi_{N+1})^2 \\
&= \varphi_0^2 - 2\varphi_0\varphi_1 + \varphi_1^2 + \varphi_1^2 - 2\varphi_1\varphi_2 + \varphi_2^2 + \ldots \\
&\quad + \ldots - \varphi_n(\varphi_{n-1} - 2\varphi_n + \varphi_{n+1}) + \ldots \\
&\quad + \ldots + \varphi_{N-1}^2 - 2\varphi_{N-1}\varphi_N + \varphi_N^2 + \varphi_N^2 - 2\varphi_N\varphi_{N+1} + \varphi_{N+1}^2 \\
&= \varphi_0^2 - \varphi_0\varphi_1 - \varphi_0\varphi_1 + 2\varphi_1^2 - \varphi_1\varphi_2 + \ldots \\
&\quad + \ldots - \varphi_{n-1}\varphi_n - 2\varphi_n^2 + \varphi_n\varphi_{n+1} + \ldots \\
&\quad + \ldots - \varphi_{N-1}\varphi_N + 2\varphi_N^2 - \varphi_N\varphi_{N+1} - \varphi_N\varphi_{N+1} + \varphi_{N+1}^2 \\
&= -\varphi_0(\varphi_1 - \varphi_0) - \varphi_1(\varphi_0 - 2\varphi_1 + \varphi_2) + \ldots \\
&\quad + \ldots - \varphi_n(\varphi_{n-1} - 2\varphi_n + \varphi_{n+1}) + \ldots \\
&\quad + \ldots - \varphi_N(\varphi_{N-1} - 2\varphi_N + \varphi_{N+1}) + \varphi_{N+1}(\varphi_{N+1} - \varphi_N) \\
&= -\varphi_0(\varphi_1 - \varphi_0) - \sum_{n=1}^{N} \varphi_n(\varphi_{n-1} - 2\varphi_n + \varphi_{n+1}) + \varphi_{N+1}(\varphi_{N+1} - \varphi_N),
\end{aligned}$$

where φ_0 and φ_{N+1} are the fields at the external border, $\varphi_1 \ldots \varphi_N$ are the fields in the interior, $\Delta_{\ell_{b\pm}}$ are the derivatives at the two opposite borders and we have detailed what happens at each one of the two ends. This time it results that the final form relating a sum over links with a sum over sites is

$$\sum_l (\Delta_\ell \varphi)^2 = -\varphi_0 \Delta_{\ell_{b-}}\varphi - \sum_{n=1}^{N} \varphi(n)\Delta^2\varphi(n) + \varphi_{N+1}\Delta_{\ell_{b+}}\varphi, \tag{2.2.1}$$

where we now have, unlike the previous case, surface terms to consider.

In order to derive the equation of motion it is more convenient to start from the initial form of the action given in equation (1.3.1), which we now write separating explicitly the internal links ℓ_i and the links to the border $\ell_{b\pm}$, still in one dimension, for simplicity,

$$S_0[\varphi] = \frac{1}{2}(\Delta_{\ell_{b-}}\varphi)^2 + \frac{1}{2}\sum_{\ell_i}(\Delta_{\ell_i}\varphi)^2 + \frac{1}{2}(\Delta_{\ell_{b+}}\varphi)^2 + \frac{\alpha_0}{2}\sum_{n=1}^{N}\varphi^2(n).$$

In order to find the configuration that minimizes the action we use the usual techniques of the calculus of variations, making variations $\delta\varphi$ of the field on all the internal sites. On the border sites the field remains fixed at the values given by the boundary conditions. We impose then that the variation of the action be zero for *any* $\delta\varphi(n)$. This variation of the action is given by

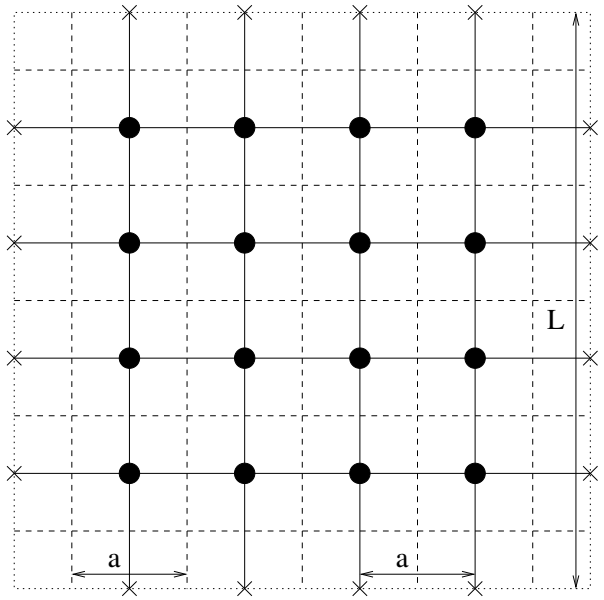

Figure 2.2.2: The geometrical elements of a two-dimensional lattice with a fixed boundary.

reduces to the three-dimensional Laplacian and in this case we indeed have the theory of electrostatics, φ being the electric potential within a cubic box of volume $V = L^3$ that contains no charges. However, this time the solution is not necessarily trivial, because there may be charges on the surfaces that are the borders of the box in the continuum limit, causing the potential not to be zero at these surfaces. In this case the solution of the equation will not be simply $\varphi \equiv 0$ within the box, but will have, instead of this, a value that will depend on the fixed values at the borders. This is the typical example of electrostatic problem that may be solved numerically, for example, by the relaxation method associated to the Laplacian (problems 2.2.2 and 2.2.3).

Observe that the sum over links in equation (2.2.1) may be written, in terms of the dimensional variables, generalizing again to d dimensions, as

$$\sum_{\vec{n}} a^d \sum_{\mu} \frac{\left[\Delta_\mu \phi(\vec{n})\right]^2}{a^2} = \sum_{\vec{n}_b} a^{d-1} \phi_b \frac{\Delta_{\ell_{be}} \phi}{a} - \sum_{\vec{n}} a^d \phi(\vec{n}) \frac{\Delta^2 \phi(\vec{n})}{a^2},$$

where $\sum_{\vec{n}_b}$ is a sum over the external border, ϕ_b is the field at the border and $\Delta_{\ell_{be}} \phi$ is the finite external normal derivative of the field at the border. We have now the integral $\sum_{\vec{n}} a^d$ over the volume and the integral $\sum_{\vec{n}_b} a^{d-1}$ over the oriented external surface, so that in the continuum limit we obtain

$$\int_V \mathrm{d}^d x \sum_{\mu} \left[\partial_\mu \phi(\vec{x})\right]^2 = \int_{S=\partial V} \mathrm{d}^{d-1} x \; \phi(\vec{x}) \partial_\perp \phi(\vec{x}) - \int_V \mathrm{d}^d x \; \phi(\vec{x}) \partial^2 \phi(\vec{x}),$$

where $S = \partial V$ is the surface which is the border of the volume V and $\partial_\perp$ is the external normal derivative to this surface. If we assume that in the continuum limit

lattices for the corresponding objects in the continuum limit, which are differential operators. In order to define the action functionals to be used in the quantum theory it is useful to first study the relation between the discrete and continuum objects in the scope of the classical theory. We will then, in this section, imagine that we are starting from the continuum objects and trying to model them, approximating them by discrete objects. It is clear that this is not our main point of view, but there is no harm in adopting it temporarily to illustrate the discussion of the nature of the relation between these mathematical objects.

Let us recall, then, that we are only talking about the classical theory of fields, described on finite lattices, with the intention of taking the classical continuum limit. It is therefore implicitly understood in all this discussion the existence of an external dimensional scale L and of the corresponding lattice spacing a. For ease of presentation, we will use in this section the dimensional coordinates $\vec{x}$ and the corresponding versors $\hat{x}_\mu$, for each one of the $\mu = 1, \ldots, d$ direction of the space. Let us consider now in more detail the definition on the lattice of the finite difference operator Δ_μ. Considered as an approximation of the differential operator "partial derivative" it may be represented in several different ways, for example as the *forward difference operator* $\Delta_\mu^{(+)}$, which when applied to a function $f(\vec{x})$ on the lattice produces

$$\Delta_\mu^{(+)} f(\vec{x}) = f(\vec{x} + a\hat{x}_\mu) - f(\vec{x}),$$

or as the *backward difference operator* $\Delta_\mu^{(-)}$, which is defined by

$$\Delta_\mu^{(-)} f(\vec{x}) = f(\vec{x}) - f(\vec{x} - a\hat{x}_\mu),$$

or even as the *symmetrical difference operator* or *central difference operator* $\Delta_\mu^{(\mathrm{c})}$, which is given by

$$\Delta_\mu^{(\mathrm{c})} f(\vec{x}) = \frac{1}{2}[f(\vec{x} + a\hat{x}_\mu) - f(\vec{x} - a\hat{x}_\mu)].$$

The reason for the existence of all these different representations is that the finite difference operator is in fact an operator with its arguments on sites and its values on links, and there is no unique or natural way to represent it only on sites. Note the absence of factors of a in the denominator in these definitions. In the continuum limit the partial differentiation operator ∂_μ may be identified with Δ_μ / a in any of the forms given above,

$$\partial_\mu = \lim_{a \to 0} \frac{\Delta_\mu^{(+)}}{a} = \lim_{a \to 0} \frac{\Delta_\mu^{(-)}}{a} = \lim_{a \to 0} \frac{\Delta_\mu^{(\mathrm{c})}}{a}.$$

It is clear that the operator ∂_μ can only be applied to differentiable functions in the continuum limit, unlike the realizations of Δ_μ on the lattice, which can be applied to any functions defined on the lattice.

way, with different realizations of the finite-difference operator Δ_μ for each factor involved, for example as $(\Delta_\mu^{(c)}\varphi)(\Delta_\mu^{(+)}\varphi)$, integration by parts is just an application of the Stokes theorem and it therefore a simplicial operation which is *exact* on the lattice. The form above for the action is *exactly* equal to the previous ones, with the use of any consistent realization of Δ_μ. With the use of $\Delta_\mu^{(\pm)}$ the Laplacian operator Δ^2 that appears above may be defined through its action on lattice functions as

$$\Delta^2 f(\vec{x}) = \sum_\mu \Delta_\mu^2 f(\vec{x}),$$

where the definition of the action on the functions of the "second difference" Δ_μ^2 in the direction μ is given by (no sum over μ here)

$$\Delta_\mu^2 f(\vec{x}) = f(\vec{x} + a\hat{x}_\mu) - 2f(\vec{x}) + f(\vec{x} - a\hat{x}_\mu),$$

resulting therefore in

$$\Delta^2 f(\vec{x}) = \sum_\mu [f(\vec{x} + a\hat{x}_\mu) - 2f(\vec{x}) + f(\vec{x} - a\hat{x}_\mu)].$$

Note that these operators are naturally defined with values on sites, as is necessary for the expression of the action in terms of the Laplacian. The second derivative maps values of the function f at the points $\vec{x}$, $\vec{x} + a\hat{x}_\mu$ and $\vec{x} - a\hat{x}_\mu$ to a resulting value to be associated to the point $\vec{x}$. One can show (problems 2.3.2 and 2.3.3) that the second-derivative operator is obtained by the iterated application of $\Delta_\mu^{(+)}$ (which maps $\vec{x} + a\hat{x}_\mu$ and $\vec{x}$ on $\vec{x}$) and $\Delta_\mu^{(-)}$ (which maps $\vec{x} - a\hat{x}_\mu$ and $\vec{x}$ on $\vec{x}$).

It is necessary to emphasize at this point that the iteration of $\Delta_\mu^{(c)}$ does *not* produce the operator Δ^2 defined above but, instead of that, results in a different realization of it, $\Delta^2_{(c)}$, related to the differences of second order given by

$$\Delta^2_{(c)} f(\vec{x}) = \frac{1}{4} \sum_\mu [f(\vec{x} + 2a\hat{x}_\mu) - 2f(\vec{x}) + f(\vec{x} - 2a\hat{x}_\mu)].$$

In the context of the classical theory this is related to a higher-order approximation $\Delta^2_{(c)}$ to the continuum operator Δ^2. Note that, with its use, the action S_0 would involve more than couplings between next neighbors. It is clear that our point here is not to obtain better approximations to the solutions of the classical theory and we will never use these higher-order realizations of the finite-difference operator. For us the important realizations are those that appear in the various forms of the action that we have already seen, which may be obtained by the direct application of the realization on the links, be it in the form $\Delta_\mu^{(+)}$ or in the form $\Delta_\mu^{(-)}$.

Of course we could consider the definition of the theory with the finite-difference operator $\Delta_\mu^{(c)}$ defined on sites and the higher-order realization Δ^2 given above. The interesting thing is that the theory would still be the same in any case, and that we would be simply rescaling the continuum limit by a factor of two. In fact one can

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

2.3.2. Show that one can obtain the second-difference operator Δ_μ^2 by the iteration of the forward-difference operator $\Delta_\mu^{(+)}$ and the backward-difference operator $\Delta_\mu^{(-)}$, in any order, that is, show that

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

Remember that $\Delta_\mu^{(+)}$ maps $\vec{x} + a\hat{x}_\mu$ and $\vec{x}$ to $\vec{x}$ and that $\Delta_\mu^{(-)}$ maps $\vec{x} - a\hat{x}_\mu$ and $\vec{x}$ to $\vec{x}$, and consider in detail the action of these operators over lattice functions, calculating for example $\Delta_\mu^{(+)}[\Delta_\mu^{(-)} f(\vec{x})]$ and $\Delta_\mu^{(-)}[\Delta_\mu^{(+)} f(\vec{x})]$.

2.3.3. Show that the twice-repeated iteration of either $\Delta_\mu^{(+)}$ or $\Delta_\mu^{(-)}$ does not reproduce the second-difference operator as defined in the text, that it, show that

$$\Delta_\mu^{(+)}\Delta_\mu^{(+)} \neq \Delta_\mu^2 \neq \Delta_\mu^{(-)}\Delta_\mu^{(-)}.$$

Verify in each case that, with respect to the definition given in the text, there is a displacement of the point to which the value of the operator should be associated, and examine the consequences of this displacement in the case of fixed boundary conditions, and in the case of periodical boundary conditions.

2.3.4. Consider the action $S_0[\varphi]$ of the free scalar field written on a lattice with $N = 2N'$ sites in one dimension, with the use of the central finite-difference operator $\Delta_{(c)}$. Let s_o run over the N' sites with odd integer coordinates and s_e over those with even integer coordinates. Show that it is possible to write the action as

$$S_0[\varphi] = S_o[\varphi] + S_e[\varphi],$$

where $S_o[\varphi]$ depends only on the fields $\varphi(s_o)$ at the odd sites and $S_e[\varphi]$ only on the fields $\varphi(s_e)$ at the even sites. In this way one sees that the classical dynamics of the system separates in two independent parts.

2.3.5. Apply the Euler-Lagrange equation or the principle of minimum action to the actions $S_o[\varphi]$ and $S_e[\varphi]$ of problem 2.3.4 and show that the equations of motion relative to each one of the two sets of sites do not involve at all the variables at the sites of the other set. In this way one sees that the classical dynamics of the system decouples into independent dynamics for each one of the two sets of sites.

Is is not difficult to verify that the Laplacian operator is represented by the following matrix in this space formed by the vectors containing the values of the fields at the sites,

$$\Delta^2 = \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & -2 \end{bmatrix}. \tag{2.4.1}$$

Note that almost all elements are zero, thus indicating the absence of long-range couplings on the lattice. The only non-zero elements are the three central diagonals indicated and the two elements at the corners along the anti-diagonal. These two elements are the ones that establish the periodical boundary conditions. It suffices to apply this matrix to the vector that represents the field to verify that it reproduces the definition of the Laplacian on finite lattices given in (2.1.2).

The same procedure can be realized on lattices with dimensions larger than 1, however in this case there is a slight complication because if the lattice is not one-dimensional then it does not establish a natural order for the sites. We will establish here a standard order for writing the components of vectors and matrices in the space of field configurations, which will also be very useful for computer simulations. Starting with a two-dimensional lattice with integer coordinates $\vec{n} = (n_1, n_2)$, where $n_1, n_2 = 1, \ldots, N$, consider the integer ι defined by

$$\iota = 1 + (n_1 - 1) + (n_2 - 1)N.$$

Observe that ι varies from 1 to N^2 when n_1 and n_2 assume all the possible values, from 1 to N. The interesting thing is that this operation is invertible, that is, given a certain value of ι between 1 and N^2 it is possible to determine uniquely the values of n_1 and n_2 that correspond to it. Hence, ι enumerates all the sites in a definite way. This operation, which we call the *indexing* of the lattice by the *index* ι, is similar to the operation of writing integers in the base N. The inversion of the operation is realized by means of integer division. One can show (problem 2.4.1) that

$$n_2 = 1 + \frac{\iota - 1}{N},$$

where the division is integer division, that is, there is truncation of the result as is usual in the integer arithmetic of digital computers. Note that due to this the order of operations is important here. Once n_2 is obtained, we have for n_1

$$n_1 = \iota - (n_2 - 1)N.$$

As one can see, the relation between the index ι and the integer coordinates is in fact a bijection because, besides defining ι from a set of integer coordinates n_μ, given a value for ι we may also solve for all the coordinates n_μ, dividing $\iota - 1$ successively by $N^{d-1}, N^{d-2}, \ldots, N^1, N^0$, so as to recover each one of the n_μ as the complements of the remainders of the successive divisions. This is, therefore, an unequivocal way to pile up all the sites of a d-dimensional lattice into a single vector of size $n = N^d$. The same ordering procedure can and should be used for the elements of the matrices acting on these vectors.

The linear operators that act on this space are representable, of course, by $n \times n$ matrices, as we saw before for the Laplacian in one dimension, with periodical boundary conditions. One can verify that the determinant of that matrix is zero (problem 2.4.3), which is a consequence of the fact that the operator Δ^2 has a null eigenvector, or a *zero mode*, on the torus. The matrix form of the operator has a global character, including in its structure the boundary conditions which are adopted. For example, the Laplacian in one dimension with fixed boundary conditions, where each integer coordinate varies from 0 to $N+1$ and we have a total of $n' = (N+2)^d$ sites, is represented by the $n' \times n'$ matrix

$$\Delta^2 = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \end{bmatrix} . \tag{2.4.2}$$

In this case the operator is, in fact, an operator that acts on a space of dimension n' with values in a sub-space of dimension $n = N^d$, since it does not make sense to calculate the Laplacian at the sites of the fixed border, at which we defined it to act as the identity, in order to complete the square matrix above. On the other hand, one can verify (problem 2.4.4) that the determinant of this matrix is not zero, but $(n'-1)(-1)^{n'}$ instead, reflecting the fact that there is no zero-mode for fixed boundary conditions.

Back to the case of periodical boundary conditions, the Euclidean Klein-Gordon operator $-\Delta^2 + m^2$ is represented in this case by the matrix

$$-\Delta^2 + m^2 = \begin{bmatrix} 2+m^2 & -1 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 2+m^2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2+m^2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2+m^2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2+m^2 & -1 \\ -1 & 0 & 0 & \cdots & 0 & -1 & 2+m^2 \end{bmatrix} ,$$

2.4.1. Show that, if the index ι for a two-dimensional lattice is defined as $\iota = 1 + (n_1 - 1) + (n_2 - 1)N$, then one can recover from it the integer coordinates n_1 and n_2 by means of the operations

$$n_2 = 1 + \frac{\iota - 1}{N} \quad \text{and} \quad n_1 = \iota - (n_2 - 1)N,$$

in the indicated order, where the division is an integer division, that is, there is truncation of the result as is usually the case in the integer arithmetic of digital computers.

2.4.2. Repeat the demonstration described in problem 2.4.1 for the case of three dimensions, in which the index is defined as $\iota = 1 + (n_1 - 1) + (n_2 - 1)N + (n_3 - 1)N^2$ and the inversion operations are, in order,

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

2.4.3. Show, in the case $d = 1$ on a lattice with periodical boundary conditions, that the determinant of the Laplacian given in equation (2.4.1) is zero, for any value of N.

2.4.4. Show, in the case $d = 1$ on a lattice with fixed boundary conditions, that the determinant of the Laplacian given in equation (2.4.2) has its value given by $(n' - 1)(-1)^{n'}$, where $n' = (N + 2)^d$.

2.4.5. Show, in the one-dimensional case, executing explicitly the matrix products, that the iteration of $\Delta^{(+)}$ and $\Delta^{(-)}$, in any order, has Δ^2 as the result,

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

2.4.6. Write explicitly the matrix of the Laplacian operator on a lattice with $N = 4$, in two dimensions, with periodical boundary conditions.

2.4.7. Write the operations for the inversion of the index for a lattice in $d = 4$, with periodical boundary conditions.

2.4.8. This one is just for fun: write explicitly the matrix of the Laplacian operator on a one-dimensional lattice with $N = 2$ and periodical boundary conditions.

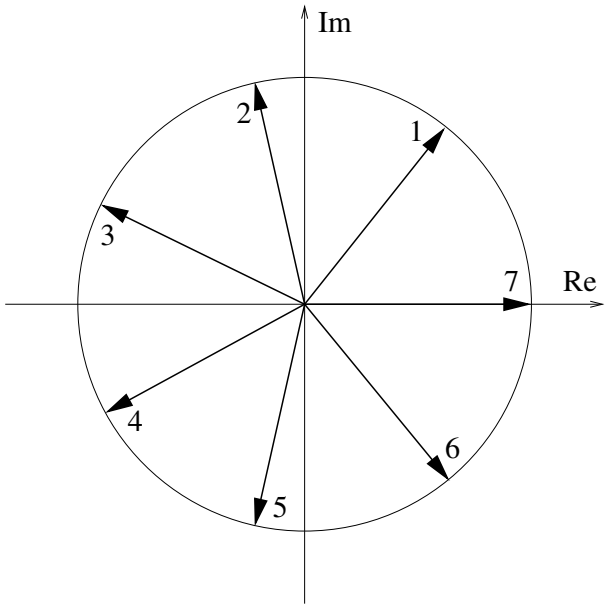

Figure 2.5.2: Example of a complex unit circle for $N = 7$.

Note that, since the sum of the complex numbers is equivalent to the sum of the two-dimensional vectors shown in the figure, its symmetry implies that

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

Note that this argument does not depend on the parity of N, but only on the fact that the vectors are equally spaced along the circle. In figure 2.5.2 we show an example with $N = 7$.

We will now consider the slightly more complicated case in which we multiply the argument of the exponential by another integer $0 \leq k \leq N - 1$, obtaining the function

$$e^{\imath 2\pi kn/N}.$$

In this case, as n varies from 1 to N the function goes around the circle exactly k times. In the case $k \neq 0$ we will still be defining in this way sets of points equally spaced along it. For example, for $k = 2$ we have, for the two values of N used before, the phases shown in figures 2.5.3 and 2.5.4.

As one can see, in the case $N = 7$ all the possible phases end up occupied a single time, as before, but in a different order. In the case $N = 8$ only one half of the possible phases ends up occupied, each one of them twice. Hence, in this latter case, in which N is divisible by k, the set of phases ends up reduced to the set of the case $N' = N/k = 4$, repeated k times. From the symmetry of the resulting sets of phases in either case, we see that it is still true that the sum of all these phases is zero,

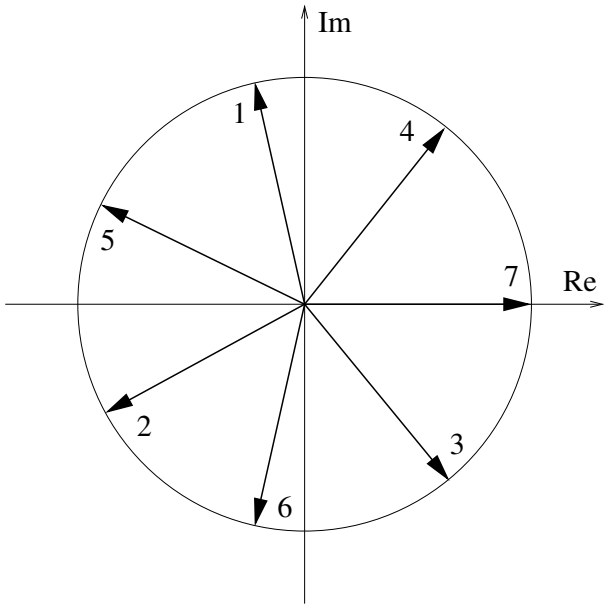

Figure 2.5.4: A double lap on the complex unit circle with $N = 7$.

For the case $k = 0$ and $q = 1$ the formula cannot be used due to the zero in denominator, but in this case the result is obvious because all the elements of the sum are equal. In the problems a different approach to this question is proposed, equally rigorous and more complicated and detailed (problems 2.5.5, 2.5.6 and 2.5.7).

Observe that we may use integer coordinates for the sites with values in the interval $[0, N-1]$, or any other interval containing N consecutive integers, as well as in the interval $[1, N]$, as we have been doing. In addition to this, the exponential that appears in the sum above is symmetrical by the exchange of n e k, so that it is equally true that

$$\sum_{k=0}^{N-1} e^{i2\pi kn/N} = N\delta(n, N).$$

One can also see that the modes $k = 0$ e $k = N$ are in reality the same mode, in fact k and $k+N$ always represent the same mode (problem 2.5.2). Thus, in the case of the k coordinates we may also choose the extremes of the interval of variation arbitrarily, so long as we always take N consecutive values. For reasons associated to the physical interpretation of these modes, it will be convenient that we take the intervals of variation of k in a way as symmetrical as possible around 0. For this reason we will adopt the following standard intervals, one for odd N,

$$k = -\frac{N-1}{2}, \ldots, 0, \ldots, \frac{N-1}{2},$$

and another for even N,

$$k = -\left(\frac{N}{2} - 1\right), \ldots, 0, \ldots, \left(\frac{N}{2} - 1\right), \frac{N}{2}.$$

2.5.4. Show that any function $f(\vec{n})$ on the torus can be written as a linear combination of the collection of N^d functions $\exp(\imath 2\pi \vec{k} \cdot \vec{n}/N)$ and give explicitly the coefficients of the expansion.

2.5.5. In this problem, for simplicity, we will number the sites from 0 to $N-1$. Given a certain N in $d=1$ and a certain value of k, show that the set of phases defined by

$$\left\{ e^{\imath \frac{2\pi}{N} nk} \;\middle/\; n = 0, \ldots, N-1 \right\}$$

is contained within the set of phases given by

$$\left\{ e^{\imath \frac{2\pi}{N} m} \;\middle/\; m = 0, \ldots, N-1 \right\}$$

where the integer m is given in terms of n by

$$m = nk - pN$$

where p is some integer. We say that n is equal to m module N. In this way we succeed to map the phases generated by any given k back to the interval described by an integer from 0 to $N-1$.

2.5.6. Show that if N is not divisible by k in problem 2.5.5 then the two sets of phases are identical, that is, the relation between them is a bijection or one-to-one. Use this fact to establish that the sum of the phases for $k \neq 0$ is zero in this case. Hint: show that, if n_1 is mapped to m_1 and n_2 to m_2, then $m_1 = m_2 \Rightarrow n_1 = n_2$.

2.5.7. If N is divisible by k in problem 2.5.5, that is, if $N = N'k$ for some N', then show that only the phases corresponding to the lattice of size N' appear in the first set. Show that each one of them appears exactly k times. Use these facts to establish that the sum of the phases for $k \neq 0$ is zero in this case, effectively reducing the problem of the N-lattice to the problem of the N'-lattice.

2.5.8. Write a program to verify the orthogonality relation of the momentum-space mode-functions in $d=1$, for a given fixed N and any given k.

associated to $\vec{p}$ are still discrete, of course, so that the inverse is given by an infinite series rather than a finite sum, but not by an integral,

$$\varphi(\vec{x}) = \sum_{\vec{p}}^{\infty} e^{-\imath\vec{p}\cdot\vec{x}}\widetilde{\varphi}(\vec{p}).$$

Note that the factor of $1/L^d$ in the transform guarantees that φ and $\widetilde{\varphi}$ still have the same dimensions. These relations are valid for both the dimensionless field φ and the dimensionfull field ϕ, because they are homogeneous on the fields, and therefore we may write

$$\begin{aligned}\widetilde{\phi}(\vec{p}) &= \frac{1}{V}\int_V \mathrm{d}^d x\, e^{\imath\vec{p}\cdot\vec{x}}\phi(\vec{x}),\\ \phi(\vec{x}) &= \sum_{\vec{p}}^{\infty} e^{-\imath\vec{p}\cdot\vec{x}}\widetilde{\phi}(\vec{p}).\end{aligned}$$

The orthogonality and completeness relations may now be written in the form

$$\begin{aligned}\frac{1}{V}\int_V \mathrm{d}^d x\, e^{\imath\vec{x}\cdot(\vec{p}-\vec{p}')} &= \delta^d(\vec{p},\vec{p}'),\\ \sum_{\vec{p}}^{\infty} e^{\imath\vec{p}\cdot(\vec{x}-\vec{x}')} &= V\delta^d\left(\vec{x}-\vec{x}'\right),\end{aligned}$$

where, in the limit, the product $N^d\delta^d(\vec{n},\vec{n}')$ transforms into the product of the volume by the Dirac delta function $\delta^d\left(\vec{x}-\vec{x}'\right)$ (problem 2.6.2). We have here the usual relations for the case of the Fourier transform within a continuous finite box, that is, for the Fourier series.

Next we may think about taking the limit $L\to\infty$, increasing the box until it takes all space, which will lead us to the usual Fourier transforms in infinite space. Since the moment of the lowest non-zero mode in the box has magnitude $(2\pi/L)$, and since they are equally spaced, the volume occupied by each mode in momentum space is given by $(2\pi/L)^d$, which goes to zero as $L\to\infty$, so that in this case the form of the inverse transformation will also approach an integral. Taking a large but still finite box, the transform and its inverse can be written approximately as

$$\begin{aligned}\widetilde{\phi}(\vec{p}) &= \frac{1}{V}\int_V \mathrm{d}^d x\, e^{\imath\vec{p}\cdot\vec{x}}\phi(\vec{x}),\\ \phi(\vec{x}) &= V\int \frac{\mathrm{d}^d p}{(2\pi)^d}\, e^{-\imath\vec{p}\cdot\vec{x}}\widetilde{\phi}(\vec{p}),\end{aligned}$$

where, strictly speaking, we cannot yet take the limits because of the divergent factors of V. The orthogonality and completeness relations may now be written as

$$\begin{aligned}\frac{1}{V}\int_V \mathrm{d}^d x\, e^{\imath\vec{x}\cdot(\vec{p}-\vec{p}')} &= \frac{1}{V}\delta^d\left(\vec{p}-\vec{p}'\right),\\ V\int \frac{\mathrm{d}^d p}{(2\pi)^d}\, e^{\imath\vec{p}\cdot(\vec{x}-\vec{x}')} &= V\delta^d\left(\vec{x}-\vec{x}'\right),\end{aligned}$$

2.6.3. Calculate the finite Fourier transform of the field defined, on a one-dimensional periodical lattice with an even number $N = 2M$ of sites, by $\varphi(n) = (-1)^n$.

2.6.4. Show that, for a real field φ, $\widetilde{\varphi}(-\vec{k}) = \widetilde{\varphi}^*(\vec{k})$. In particular, show that $\widetilde{\varphi}(\vec{0})$ is real. In addition to this, in case we have even N in dimension $d = 1$, show that $\widetilde{\varphi}(N/2)$ is real.

2.7 Eigenvalues and Eigenvectors of the Laplacian

Having discussed before the relevant realizations of the finite-difference operators Δ_μ and Δ^2, we are now in a position to study their eigenvalues and eigenvectors. For simplicity, it is more convenient to start the discussion by the eigenvalues of the symmetrical realization $\Delta_\mu^{(\mathrm{c})}$, but it is also interesting to compare the results for the various realizations, as we shall do.

The eigenvectors of the finite-difference operators with periodical boundary conditions are the exponential functions $\exp(\imath 2\pi \vec{k} \cdot \vec{n}/N)$ that appear in the Fourier transformations. We will also refer to these eigenvectors as *eigenfunctions*. We have, for example, by the direct application of the definition of eigenvector followed by a simple calculation (problem 2.7.1), that

$$\Delta_\mu^{(\mathrm{c})} e^{\imath \frac{2\pi}{N} \vec{k} \cdot \vec{n}} = \imath \sin\left(\frac{2\pi}{N} \vec{k} \cdot \hat{n}_\mu\right) e^{\imath \frac{2\pi}{N} \vec{k} \cdot \vec{n}},$$

where $\hat{n}_\mu = \hat{x}_\mu$ is the versor in the direction μ. Observe that the eigenvalue is complex and that, therefore, the operator is not Hermitian. We may define the quantity

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

that plays a role similar to that of the linear momentum in the case of the continuum formalism. For the realization $\Delta_\mu^{(+)}$, with values on links, we have

$$\Delta_\mu^{(+)} e^{\imath \frac{2\pi}{N} \vec{k} \cdot \vec{n}} = \left(e^{\imath \frac{2\pi}{N} \vec{k} \cdot \hat{n}_\mu} - 1\right) e^{\imath \frac{2\pi}{N} \vec{k} \cdot \vec{n}}.$$

For $\Delta_\mu^{(-)}$ we have a similar relation. Note that, as in the case of $\Delta_\mu^{(c)}$, the eigenvalue of $\Delta_\mu^{(+)}$ is also complex. We may write this eigenvalue as

$$2\imath e^{\imath \frac{\pi}{N} \vec{k} \cdot \hat{n}_\mu} \sin\left(\frac{\pi}{N} \vec{k} \cdot \hat{n}_\mu\right),$$

or, defining a new version of the quantity $\rho_\mu(k_\mu)$, that plays the role of the linear momentum, by

thus showing that the equation is solved by modes for which $\rho^2 = -\alpha_0$. Since the parameter α_0 is positive, this can only be satisfied in the non-Euclidean version of the theory, in which the sum $\rho^2 = \sum_\mu \rho_\mu^2$, which is here manifestly positive, changes so as to have a negative element,

$$\rho^2 = -\rho_0^2 + \sum_{i=1}^{d-1} \rho_i^2.$$

It is clear that, on finite lattices and depending on the value of α_0, there might be no mode such that $\rho^2 = -\alpha_0$, which just shows the discrete nature of the solutions within a finite box, even in the non-Euclidean case. However, if we take the so-called infra-red limit, making the size L of the box tend to infinity, the separations between consecutive square momenta ρ^2 of the modes become infinitesimal and in this case it is always possible to find a mode with ρ^2 arbitrarily close to any given positive value of α_0. The relation $\rho^2 + \alpha_0 = 0$ is referred to as the *on-shell condition* and is a characteristic of the plane waves that constitute the relativistically invariant classical solutions of the theory in non-Euclidean space.

Problems

2.7.1. Show, using directly the definition of the finite-difference operators, that the functions $f_{\vec{k}}(\vec{n}) = \exp(\imath 2\pi \vec{k} \cdot \vec{n}/N)$ are eigenfunctions of these operators. In order to do this apply to these functions the definition of the operators at an arbitrary internal site and remember that the boundary conditions are periodical.

2.7.2. Show, using the definition of the Laplacian that follows from the definitions of the finite-difference operators $\Delta_\mu^\pm$, that the functions $f_{\vec{k}}(\vec{n}) = \exp(\imath 2\pi \vec{k} \cdot \vec{n}/N)$ are eigenfunctions of the finite-difference Laplacian. In order to do this apply to these functions the definition of the Laplacian at an arbitrary internal site and remember that the boundary conditions are periodical.

2.8 Eigenvectors for Fixed Boundary Conditions

We examined in sections 2.5, 2.6 and 2.7 the case in which periodical boundary conditions are adopted and, in that case, the transformations that take us from position space to momentum space are given by the finite Fourier transforms. When other types of boundary conditions are adopted in position space we will still have a momentum space, as well as transformations between it and position space, but these will no longer be the Fourier transforms, but other type of transform involving complete sets of orthogonal functions.

implies that there is no zero mode, because the fixed boundary conditions would force the corresponding eigenfunction to be identically zero, over the complete extension of the lattice. In other words, with these boundary conditions the Laplacian has no normalizable (non-null) eigenvector with a zero eigenvalue.

The eigenfunctions $f^N_{\vec{k}}(\vec{n})$ on finite lattices satisfy the orthogonality and completeness relations

$$\sum_{\vec{n}} f^N_{\vec{k}}(\vec{n}) f^N_{\vec{k}'}(\vec{n}) = (N+1)^d \delta^d(\vec{k}, \vec{k}'), \tag{2.8.2}$$

$$\sum_{\vec{k}} f^N_{\vec{k}}(\vec{n}) f^N_{\vec{k}}(\vec{n}') = (N+1)^d \delta^d(\vec{n}, \vec{n}'). \tag{2.8.3}$$

where in this case the Kronecker delta functions and sums are defined by

$$\begin{aligned}
\sum_{\vec{n}} &= \sum_{n_1=1}^{N} \cdots \sum_{n_d=1}^{N}, \\
\sum_{\vec{k}} &= \sum_{k_1=1}^{N} \cdots \sum_{k_d=1}^{N}, \\
\delta^d(\vec{k}, \vec{k}') &= \delta(k_1, k_1') \ldots \delta(k_d, k_d'), \\
\delta^d(\vec{n}, \vec{n}') &= \delta(n_1, n_1') \ldots \delta(n_d, n_d').
\end{aligned}$$

It is not difficult to demonstrate these orthogonality and completeness relations (problem 2.8.4) by writing the eigenfunctions in terms of complex exponentials, with the use of

$$\sin\left(\frac{\pi k_\mu n_\mu}{N+1}\right) = \frac{1}{2\imath}\left[e^{\imath \frac{\pi k_\mu n_\mu}{N+1}} - e^{-\imath \frac{\pi k_\mu n_\mu}{N+1}}\right],$$

where there is no sum over μ, and then using the formula for the sum of a geometrical progression, generalized to the complex context, as we already did in section 2.5. Note that, since the sine functions are zero for $n = 0$, $n = N+1$, $k = 0$ and $k = N+1$, it is possible to extend the sums, both those over $\vec{n}$ and those over $\vec{k}$, from the interval $[1, \ldots, N]$ to the interval $[0, \ldots, N{+}1]$. It is important to emphasize that, just as in the case of periodical boundary conditions, these orthogonality and completeness relations are *exact* on each finite lattice.

For fixed null boundary conditions the transformation of the field from position space to momentum space and its inverse are written as

$$\begin{aligned}
\widetilde{\varphi}(\vec{k}) &= \frac{1}{(N+1)^d} \sum_{\vec{n}} f^N_{\vec{k}}(\vec{n}) \varphi(\vec{n}), \\
\varphi(\vec{n}) &= \sum_{\vec{k}} f^N_{\vec{k}}(\vec{n}) \widetilde{\varphi}(\vec{k}).
\end{aligned}$$

Since the role played by the transformations to momentum space is always the same and they are always associated to decompositions of the functions of position in some basis of orthogonal functions, we often will, for simplicity of exposition, commit the abuse of language of referring to the transformation to momentum space as Fourier transforms, whatever the boundary conditions in use may actually be.

Problems

2.8.1. Show that, with fixed boundary conditions in which the field is zero at the border, the functions $f^N_{\vec{k}}(\vec{n})$ given in equation (2.8.1) are eigenfunctions of the finite-difference Laplacian. Derive also the expression for the corresponding eigenvalues ρ^2_f.

2.8.2. Show that the exponential functions $\exp[\imath 2\pi(\vec{k}\cdot\vec{n})/N]$, that we used in the case of periodic boundary conditions, are *not* eigenfunctions of the Laplacian with fixed boundary conditions where the field is zero at the border. In order to see this, examine in detail the situation at the sites next to the border.

2.8.3. Show that, with fixed boundary conditions where the field is zero at the border, the functions $f^N_{\vec{k}}(\vec{n})$ given in equation (2.8.1) are *not* eigenfunctions of the finite-difference operator Δ_μ. Examine in detail the situation at the sites next to the border.

2.8.4. Demonstrate the orthogonality and completeness relations for fixed boundary conditions given in equation (2.8.2), decomposing the sine functions that appear in the eigenfunctions $f^N_{\vec{k}}(\vec{n})$ into complex exponentials and using the formula for the sum of a geometrical progression, which can be generalized to the complex context, as we already saw in section 2.5.

2.8.5. Show that in the continuum limit inside a finite box the eigenfunctions of the Laplacian are given by the functions $f_{\vec{k}}(\vec{x})$ defined in equation (2.8.5). Starting from the orthogonality and completeness relations on finite lattices given in equation (2.8.2) demonstrate that the corresponding relations in the continuum limit are those given in equation (2.8.6). Show also that in this limit the eigenvalues of the Laplacian are those given in equation (2.8.8).

2.8.6. Show that the functions defined on a one-dimensional lattice with N sites and fixed boundary conditions, given by

$$f_\kappa(n) = \begin{cases} \kappa = 0: & 1, \\ \kappa = 1,\ldots,N: & \cos\left(\frac{2\pi n k}{N+1}\right), \quad \text{where} \quad k = 1,\ldots,N, \\ \kappa = N+1,\ldots,2N: & \sin\left(\frac{2\pi n k}{N+1}\right), \quad \text{where} \quad k = 1,\ldots,N, \end{cases}$$

where $n = 0,\ldots,N+1$ and $\kappa = 0,\ldots,2N$, are all orthogonal to one another, so long as the sums over position space are defined by

$$\widetilde{\varphi}_\kappa = \sum_{\iota=1}^{N^d} F_{\kappa\iota}\varphi_\iota = F_{\kappa\iota}\varphi_\iota,$$

where we will usually omit the explicit sum as we did here, hence adopting the summation convention for the matrix products. The equation above represents the matrix product of the matrix $\mathbb{F}$ of components $F_{\kappa\iota}$ by the vector φ of components φ_ι, resulting in another vector $\widetilde{\varphi}$ of components $\widetilde{\varphi}_\kappa$. In this language the Fourier transform of the field φ_ι is an N^d-vector $\widetilde{\varphi}_\kappa$ that may be written in matrix notation as $\widetilde{\varphi} = \mathbb{F}\varphi$.

From the point of view of configuration space, Fourier transformation is a simple change of basis in a vector space. We may consider the set of N^d vectors $\widehat{\varphi}_\iota$, which are equal to 1 at a particular site in position space and to 0 at all the others, as a basis of the space of configurations, since any configuration φ may be written as a linear combination of these basis versors. In the same way, the set of N^d vectors $\widehat{\widetilde{\varphi}}_\kappa$, which are equal to 1 at a particular mode in momentum space and to 0 at all the others, also form a basis of the same space. This is so because, since the Fourier transformation exists for any configuration, is linear and invertible, any configuration may also be written as a linear combination of this other set of basis versors.

This represents in fact a simple decomposition of the configuration in terms of normal modes of oscillation in momentum space. The transformation of basis is represented by the matrix $F_{\kappa\iota}$, with the sites of coordinates n_μ represented by the index ι and the modes of coordinates k_μ by the corresponding index κ. In the case of periodical boundary conditions, according to the normalization convention defined before, this matrix is given by

$$F_{\kappa\iota} = \frac{1}{N^d} e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}.$$

It is easy to represent this explicitly in one dimension, where the index ι is simply the site coordinate $n = n_1$ and the index κ the momentum coordinate $k = k_1$. In this case we simply get

$$F_{\kappa\iota} = F_{kn} = \frac{1}{N} e^{\imath 2\pi kn/N}.$$

Up to the normalization convention adopted, in any dimension d the Fourier transformation is an unitary transformation and one can check that the transformation matrix is unitary, with a constant determinant, independent of the fields. In other words we have that $\mathbb{F}^\dagger \sim \mathbb{F}^{-1}$ up to the normalization convention. For the normalization that we adopt here we have in fact $\mathbb{F}^{-1} = N^d\mathbb{F}^\dagger$ and one can check (problem 2.9.2) that

$$N^d F^\dagger_{\iota'\kappa} F_{\kappa\iota} = I_{\iota'\iota},$$

model, the theory of the free scalar field, the introduction of a dimensionless external source j is implemented by the addition of a new term to the action, which becomes

$$S_0[\varphi] = \frac{1}{2}\sum_{\ell}(\Delta_\ell\varphi)^2 + \frac{\alpha_0}{2}\sum_s \varphi^2(s) - \sum_s j(s)\varphi(s). \tag{2.10.1}$$

The external source is a given function of the sites, over which we make no restrictions except that it have finite values on finite lattices. Our objective here is to determine how the introduction of this new term affects the classical solutions of the theory.

First of all, it is necessary to note that the introduction of this term, which is not necessarily positive, changes the local minima of the action without, however, causing it to become unbounded from below. It is easy to see that the action still has a global lower bound in the case in which j is a constant over the whole lattice and we adopt periodical boundary conditions, because in this case we have discrete translation invariance in the model. Under these conditions one can show (problem 2.10.1) that the minimum of the action must be achieved for a constant field. In this case the derivatives of the field, which can only contribute positively for S_0, are zero and the corresponding term of S_0 assumes its minimum. So long as α_0 is positive, the second-degree polynomial that remains in the actions certainly has a lower bound, which is located at $\varphi = j/\alpha_0$. Note that, due to the adoption of periodical boundary conditions, it is essential that α_0 be strictly positive, for in the case $\alpha_0 = 0$ there is no lower bound for S_0. In this case we may make $S_0 \to -\infty$ taking a constant φ over the whole lattice and making its value go to $\pm\infty$, depending on the sign of $\sum_s j(s)$. This is just another consequence of the fact that the $\alpha_0 = 0$ model has a zero mode on the torus.

Even for an arbitrary function $j(s)$, so long as it is finite, it is still true that there is a global minimum of the action, although in this case it is not so immediate to find it. This is due to the fact that, in order to make *infinitely* negative the only term of the action that can be negative, it is necessary to make φ tend to $\pm\infty$ at one or more points. However, in this case the quadratic terms at each site will always tend to $+\infty$ faster than the corresponding linear terms can tend to $-\infty$. Due to this it is not possible to make S_0 tend to $-\infty$ by any changes of the fields, but only to $+\infty$, which implies that S_0 has a lower bound. It is, however, possible to show rigorously that the action has a lower bound so long as $\alpha_0 > 0$, rewriting it in momentum space and completing a square (problem 2.10.2).

We can find the classical solution in the presence of the external source using the principle of minimum action, as we already did before for the free theory without external source. If we make an infinitesimal variation $\delta\varphi(s)$ of the fields, possibly different at each site, the corresponding variation of the action will be given by

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

Since the exponentials form a complete set of functions, in order for the linear superposition to be zero it is necessary that all the coefficients be zero, and from this we conclude that, for all $\vec{k}$,

$$\widetilde{\varphi}(\vec{k})\left[\rho^2(\vec{k})+\alpha_0\right]=\widetilde{j}(\vec{k}).$$

In this way the differential equation reduces to an algebraic equation for the Fourier components of the field. The solution may now be written explicitly both in momentum space and in position space, in this second case by means of a simple inverse transformation,

$$\begin{aligned}\widetilde{\varphi}(\vec{k}) &= \frac{\widetilde{j}(\vec{k})}{\rho^2(\vec{k})+\alpha_0},\\ \varphi(\vec{n}) &= \sum_{\vec{k}} e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\frac{\widetilde{j}(\vec{k})}{\rho^2(\vec{k})+\alpha_0}.\end{aligned}$$

We see in this way that it is possible to find the exact form of the classical solutions of the free theory in the presence of arbitrary external sources. The form of the solutions in momentum space is very simple, but it is not so easy to visualize the solutions in position space, because in this case the solutions are written as superpositions of all the Fourier modes. In order to be able to visualize the solutions in position space, we will examine a particularly simple case which is, however, of extreme importance. This is the case of an external source which is zero at all sites except one. We refer to this external source as a *point source* or as a *point charge*, a reference to its analogy with the familiar case of electrostatics. We write the point source of magnitude j_0 located at the site $\vec{n}'$ in the form

$$j(\vec{n})=j_0\delta^d(\vec{n},\vec{n}'),$$

where a Kronecker delta function appears. The finite Fourier transform of this point source is given by

$$\begin{aligned}\widetilde{j}(\vec{k}) &= \frac{1}{N^d}\sum_{\vec{n}} e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}j_0\delta(\vec{n},\vec{n}')\\ &= \frac{j_0}{N^d}e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}'}.\end{aligned}$$

The solution of the classical theory in momentum space may now be written as

$$\widetilde{\varphi}(\vec{k})=j_0\frac{1}{N^d\left[\rho^2(\vec{k})+\alpha_0\right]}e^{\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}'},$$

and the solution in position space reduces to

$$\varphi(\vec{n})=j_0\sum_{\vec{k}}\frac{1}{N^d\left[\rho^2(\vec{k})+\alpha_0\right]}e^{-\imath\frac{2\pi}{N}\vec{k}\cdot(\vec{n}-\vec{n}')}.$$

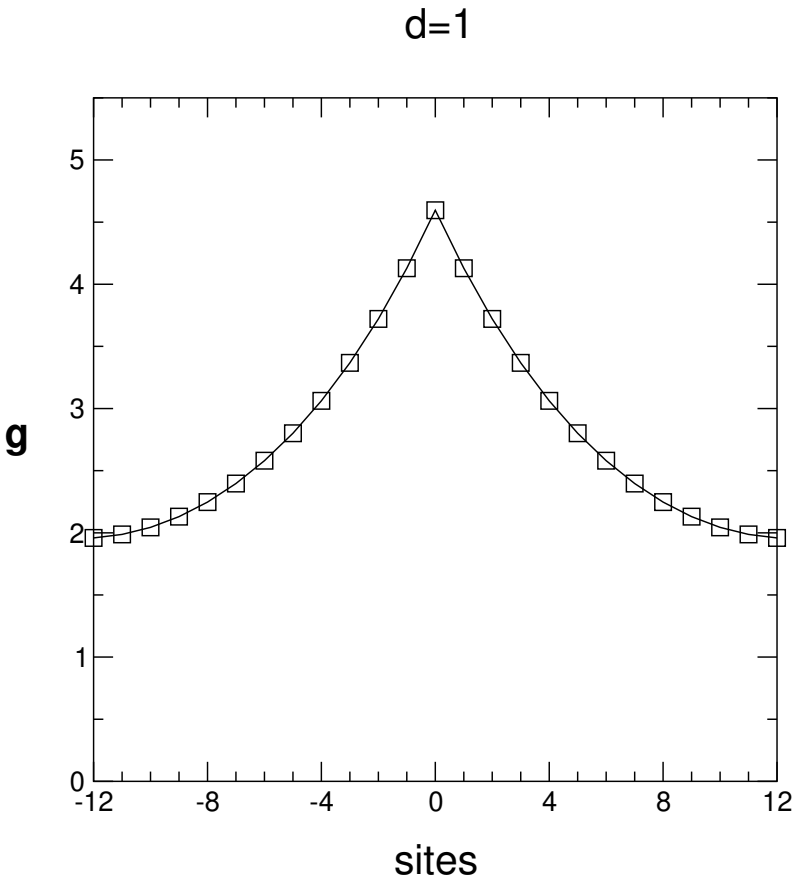

Figure 2.10.1: Periodical Green function in the case $d = 1$.

$$S_0[\phi] = \int \mathrm{d}^d x \left\{ \frac{1}{2} \sum_\mu \left[\partial_\mu \phi(\vec{x})\right]^2 + \frac{m_0^2}{2} \phi^2(\vec{x}) - J(\vec{x})\phi(\vec{x}) \right\} \tag{2.10.4}$$

it is necessary that the dimensionfull version of j be defined as $J = a^{-(d+2)/2} j$. On the other hand, we may define the dimensionfull version of g as $G = a^{2-d} g$ and, since with our normalization the functions and their Fourier transforms have the same dimensions, $\widetilde{G} = a^{2-d}\widetilde{g}$. With these definitions we have that

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

so that, in the continuum limit, the expression for the Green function is

$$\widetilde{G}(\vec{p}) = \frac{1}{V\,(p^2 + m_0^2)},$$

where, as we already saw in section 2.7, $\rho^2(\vec{k})/a^2 \to p^2$, with $\vec{p} = 2\pi\vec{k}/L$, and $\alpha_0/a^2 \to m_0^2$. In this way one can verify (problem 2.10.5) that our expression for

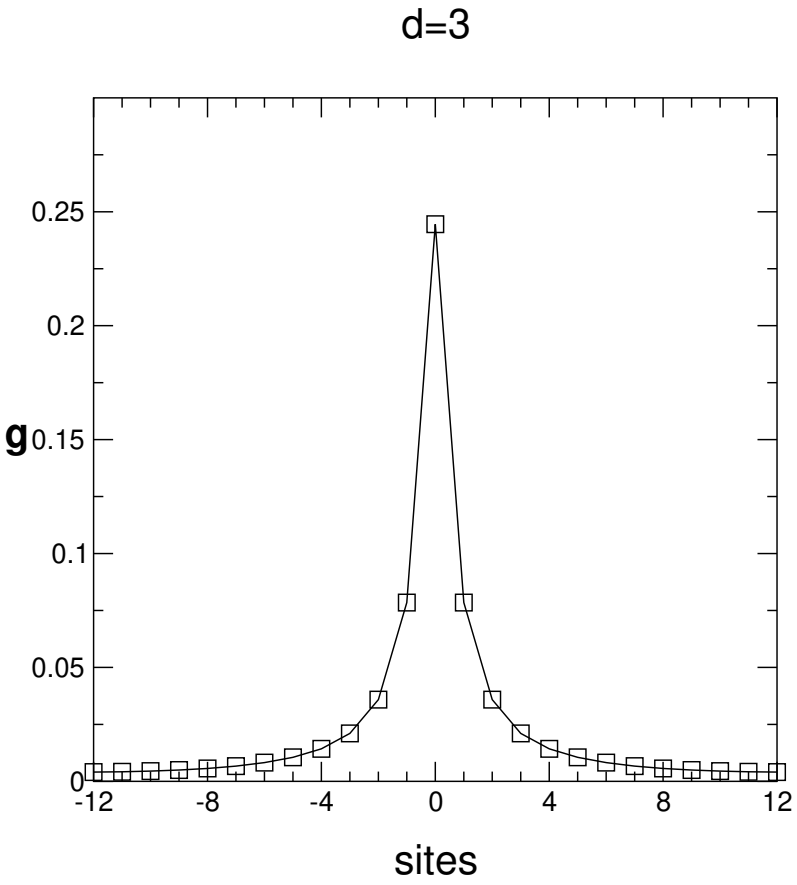

Figure 2.10.3: Periodical Green function in the case $d = 3$.

in figure 2.10.2, for the same values of α_0, N and j_0. In this case the functions falls off in a somewhat more pronounced way when we go away form the position of the point source. This is due to the larger number of neighbor sites that are connected by links to the site there the point source is located. This effect becomes more even pronounced in larger dimensions. In the graphs contained in figures 2.10.3 and 2.10.4 one can see similar examples for $d = 3$ and $d = 4$, still with the same values of α_0, N and j_0.

Note that the response of the system to an external point source is progressively more localized in the immediacy of the position of the source, as the dimension of space-time increases. For $d = 3$ in the continuum limit in infinite space, with appropriate boundary conditions and $m_0 = 0$, which is possible in this case due to the different boundary conditions, the solution becomes the Coulomb solution, the electrostatic potential of a point charge. In all cases the maximum value of the solution is proportional to j_0 and, in the limit in which j_0 goes to zero, the solution becomes identically zero, which is the solution that we discussed before for the theory without external sources. We see that the response of the system consists of a deformation of the field centered at the position of the charge, with an intensity

2.10.3. Show, starting from the general solution in momentum space given in equation (2.10.2), using the expressions for the direct and inverse Fourier transforms, and using the orthogonality and completeness relations, that the general solution in position space is the one given in equation (2.10.3).

2.10.4. Show, using the definition of the dimensionfull field in terms of the dimensionless one, as well as the other scaling relations, that the dimensionfull external source must be given by $J = a^{-(d+2)/2} j$ so that the action in the continuum limit may be written as shown in equation (2.10.4).

2.10.5. Starting from equation (2.10.3), and using the necessary scaling relations, show that the general solution in position space in the continuum limit is indeed the one given by equation (2.10.5).

2.10.6. ($\star$) Write a program to calculate the Green function $g(n)$ in position space in one dimension. Use it to plot a series of graphs of g like the one in the text, with $N = 25$, but using various values of α_0 between 1 and 10, so as to verify in a quantitative way how the range of the deformation of the field due to the presence of the external source varies as a function of this parameter.

2.11 Sources and Fixed Boundary Conditions

We may introduce external sources in systems with fixed boundary conditions, in the same way as we did for periodical boundary conditions. The form of the action of the free theory in this case is the same as before, as well as the form of the equation of motion,

$$(-\Delta^2 + \alpha_0)\varphi(\vec{n}) = j(\vec{n}). \tag{2.11.1}$$

The difference is that, in order to solve the equation in this case, we should use the basis of eigenfunctions $f^N_{\vec{k}}(\vec{n})$ which is appropriate to this type of boundary conditions,

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

which satisfy the orthogonality and completeness relations

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

The functions $\varphi(\vec{n})$ and $j(\vec{n})$ may be written in terms of their transforms as

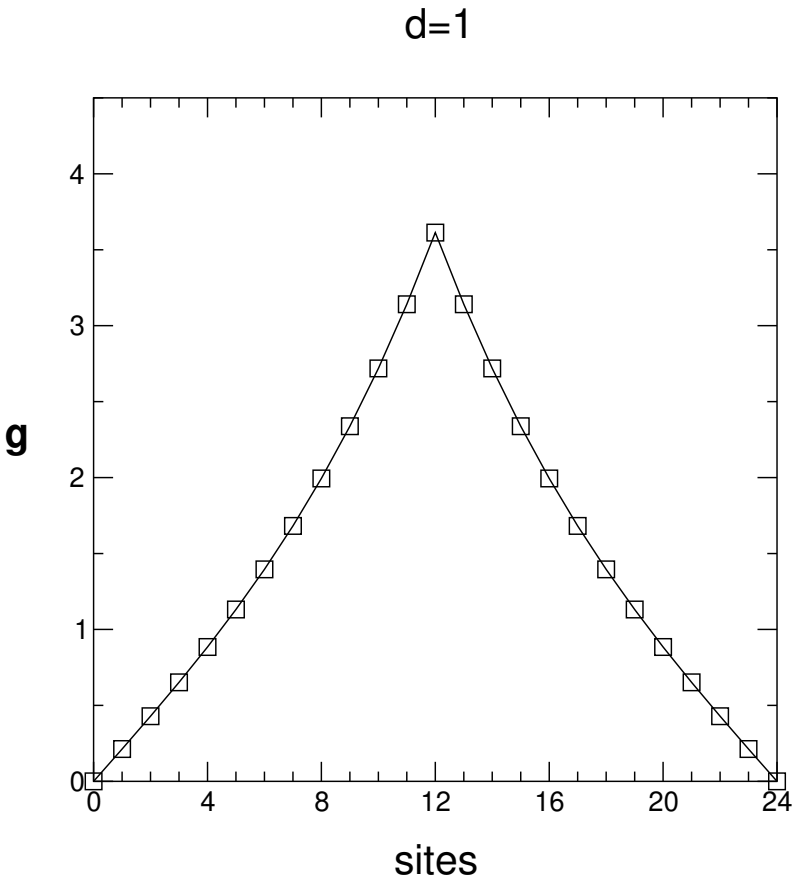

Figure 2.11.1: Green function with fixed boundary conditions for $d = 1$.

and the quantity that we will call the propagator or the Green function, in momentum space, is given by

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

while the Green function in position space is, as in the periodical case, defined as a double inverse transform of this function, involving the points $\vec{n}$ e $\vec{n}'$,

$$g_f(\vec{n}, \vec{n}') = \sum_{\vec{k}} \frac{f_{\vec{k}}^N(\vec{n}') f_{\vec{k}}^N(\vec{n})}{(N+1)^d \left[\rho_f^2(\vec{k}) + \alpha_0\right]}.$$

Just as in the periodical case, this function represents the response of the system to the presence of a unit external source, with $j_0 = 1$. Note that in this case g_f is not a function only of the difference $\vec{n} - \vec{n}'$ but rather of $\vec{n}$ and $\vec{n}'$ separately, because with fixed boundary conditions there is no discrete translation invariance on the lattice. We may also, just as in the periodical case, write the general solution for $\varphi(\vec{n})$ in terms of the Green function,

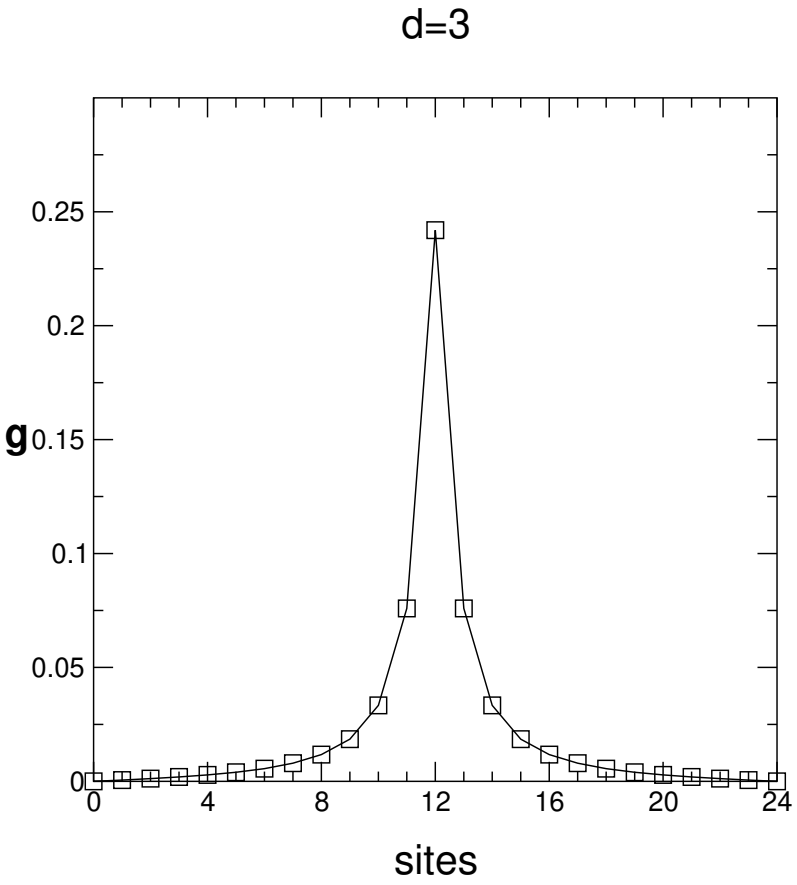

Figure 2.11.3: Green function with fixed boundary conditions for $d = 3$.

so that in the continuum limit we obtain once more

$$\widetilde{G}_f(\vec{p}_f) = \frac{1}{V\left(p_f^2 + m_0^2\right)},$$

where in this case we have $\vec{p}_f = \pi\vec{k}/L$.

Note that in this case, just as in the case of periodical boundary conditions, the Green function in momentum space always has the same form when written in terms of the eigenvalues of the Laplacian, be it on finite lattices, in the continuum inside a finite box or in infinite space. What changes is the number and character of these eigenvalues, of which there is a finite number on finite lattices, a discrete infinity in the continuum inside a finite box, and an uncountable, continuous infinity in infinite space. On the other hand, the Green functions in position space change significantly when one passes from one case to the other. Hence, we see that the transformation by the eigenfunctions of the Laplacian effectively filters out the detailed effect of the boundary conditions and of the finite volume of the box over the physically relevant results of the theory, and that these effects remain manifested in momentum space only by the existence of an infrared cutoff in finite boxes, which is removed when

lines, but in a way that is mathematically more solid, constructive and precise than the traditional approach. We will see that using this formalism one can recover all the results of the traditional formalism, in all that concerns the definition and calculation of the set of correlation functions of a given model.

The first two sections of this chapter are of a rather qualitative character, and constitute a survey of the important definitions and known phenomenological facts about the mathematical structure of the theory. The subsequent sections turn to a solid technical approach leading to the solution of the Gaussian model. Unlike the rest of this book, the last two sections of this chapter are developed in quite a general way, with applicability by no means limited to the Gaussian model.

3.1 Definition of the Quantum Theory

In this section we will define the mathematical object which we will denominate *quantum field theory* and enumerate some of its most important properties in a purely descriptive way. We will also mention a few points of fundamental importance for the physical interpretation of the theory. We will not make in this section any effort to justify these points of physical interpretation or to derive the properties of the theory from its definition. Essentially, all the rest of this book will be dedicated to such activities, and in future volumes we intend to explore other specific models and examples that may serve as illustration, with the objective of clarifying progressively the structure of the theory. With regard to this section, we will consider its objectives achieved if it becomes clear along it that a *complete definition* exists and that this definition is *constructive*, being given very explicitly by means of an algorithm, which specifies rules of procedures that, at least in principle, allow us to answer any questions formulated within the structure of the theory.

For the definition of the quantum theory of fields, we start from the same discrete mathematical structure in which we obtained the classical theory. Once again we will use the action S_0 to illustrate the definition. Is a way similar to that used to define the classical theory, we will first define a finite quantum theory on each finite lattice, and only after that consider the limit $N \to \infty$. As we shall see, a very important point is that, unlike the case of the classical theory, in this case it will *not* be necessary to introduce a dimensional scale, external to the model, when we take the continuum limit. We will define the quantum theory on each finite lattice of size N as a finite statistical model on that lattice. The quantities of more immediate physical interest, the *observables* of the theory, will be defined as statistical averages of functionals of the field within this statistical model. The statistical model establishes that all the possible configurations of the fields contribute to the statistical averages, with relative probabilities defined by the action functional of the model. These configurations of the fields are simply all possible field-functions that we can define on the lattice, which can be described either directly in position space or by means of their Fourier components in momentum space. The relative statistical weights are given by a Boltzmann factor involving the action functional.

$$\frac{[\mathbf{d}\varphi]\ e^{-S_0[\varphi]}}{\int [\mathbf{d}\varphi]\ e^{-S_0[\varphi]}},$$

defines a kind of *measure* over the space of configurations and is usually referred to as the measure of the model defined by the action S_0, or as the measure of S_0. As we will see later, this statistical structure, be it described as an ensemble, as a distribution or as a measure, constitutes in fact a representation of the *vacuum state* of the model in the context of the quantum theory.

Trivial examples of this kind of integration include the observation that the denominator of our definition in equation (3.1.1) guarantees that, if $\mathcal{O}[\varphi] \equiv 1$, then

$$\langle \mathcal{O} \rangle_N = \frac{\int [\mathbf{d}\varphi]\ 1\ e^{-S_0[\varphi]}}{\int [\mathbf{d}\varphi]\ e^{-S_0[\varphi]}} = 1,$$

for all values of N, which establishes the *normalization* of the expectation values. We also have, in the free theory defined by S_0, that if $\mathcal{O}[\varphi] = \varphi(s_0)$ for a certain given site s_0, then

$$\langle \mathcal{O} \rangle_N = \frac{\int [\mathbf{d}\varphi]\ \varphi\ e^{-S_0[\varphi]}}{\int [\mathbf{d}\varphi]\ e^{-S_0[\varphi]}} = 0,$$

also for all values of N, as can be easily verified (problem 3.1.1). Another example, and a far less trivial one, which is of great interest, would be the expectation value for the choice $\mathcal{O}[\varphi] = S_0[\varphi]$, which we will calculate in detail later on. The observables of greater interest to us will be those defined as the product of a finite number of values of the field at different sites,

$$\mathcal{O}[\varphi] = \varphi(\vec{n}_1) \dots \varphi(\vec{n}_n).$$

The expectation values of these observables will be refereed to as the *n-point functions* or as the *correlation functions*, which we shall denote by

$$g_N(\vec{n}_1, \dots, \vec{n}_n) = \langle \varphi(\vec{n}_1) \dots \varphi(\vec{n}_n) \rangle.$$

Their values define completely most of the physical characteristics of the models defined by each action functional. In the most general case we will be interested in functionals $\mathcal{O}[\varphi]$ that will be finite-order polynomials on the fields. One of the examples that we gave above, $\mathcal{O}[\varphi] = \varphi(s)$, is the one-point function and its expectation value $\langle \varphi \rangle$ is the expectation value of the field, which will have an important

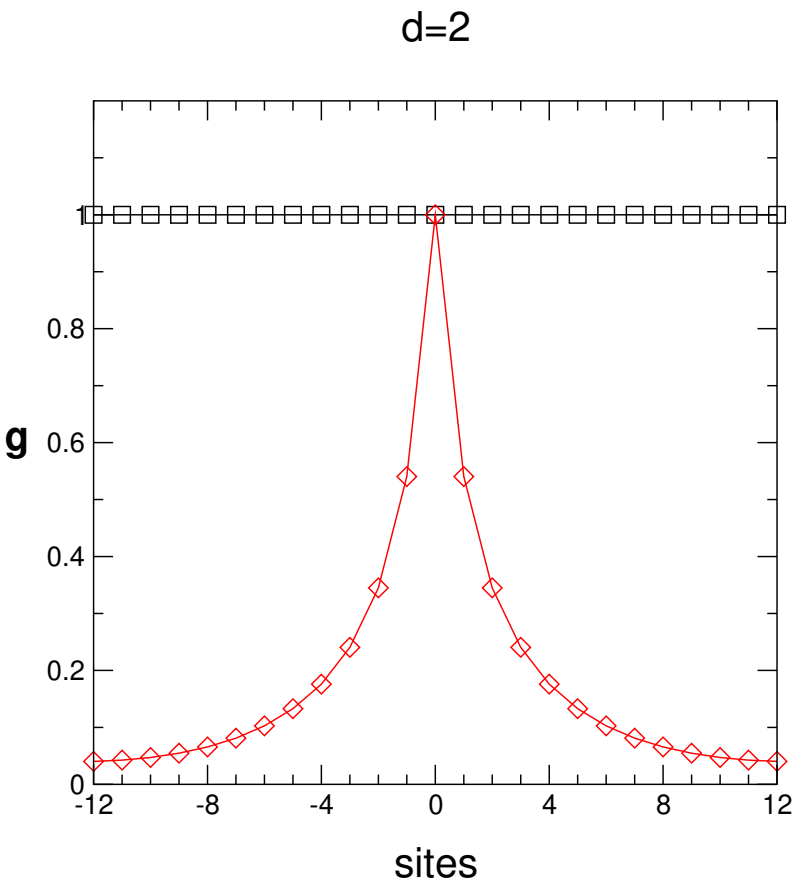

Figure 3.1.2: Periodical two-point correlation functions for $d = 2$.

decay of the two-point function does establish a *scale of distances* that is *intrinsic to the model*. In this case the sites which are the immediate neighbors of a given site are significantly correlated to it but, since the value of the function decays very fast for large distances, beyond a certain distance the sites become completely uncorrelated with the given site. Hence, this two-point *correlation function* establishes an intrinsic scale in the theory, given by the discrete distance within which the values of the fields at two different sites are appreciably correlated.

On a finite periodical lattice one can easily see this, because in this case the finite volume of the box causes the polynomial-decay cases not to decay at all over the finite extent of the lattice. For example, figure 3.1.1 shows two propagators of the free theory defined by S_0 in dimension $d = 1$ on a lattice with $N = 25$, one with infinite-range correlations, for which the correlations do not decay at all, and another one with finite-range correlations that clearly establishes a region of strong correlations of a given site with other sites which are close to it in terms of number of links. In these graphs the correlation functions have been normalized so as to be equal to one at the origin. The graphs were obtained calculating the correlation function in the case $\alpha_0 = 5$ to illustrate the exponential decay, and in the case

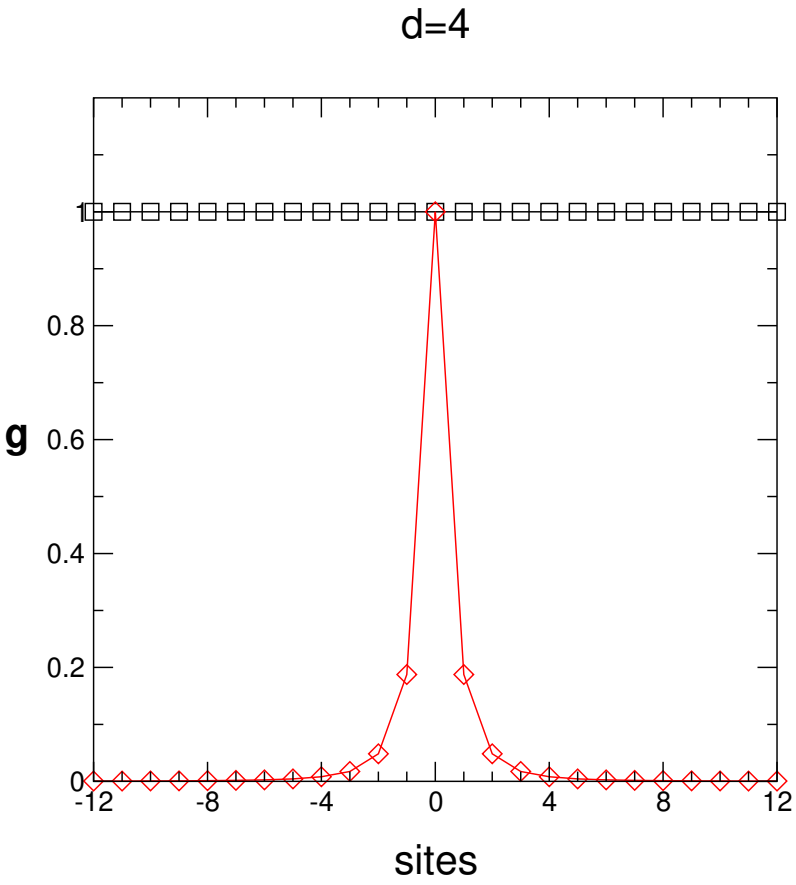

Figure 3.1.4: Periodical two-point correlation functions for $d = 4$.

point function is polynomial and not exponential, we say that the correlations have an infinite range or that the model has long-range correlations. In this case no length scale intrinsic to the theory is established. This is only the case, of course, if the correlations are long-range for *all* the different fields that are part of a given model. It suffices that *one* of the fields display an exponential decay of its two-point correlations for an intrinsic length scale to be defined in the model. Usually we will always have at least one field with finite-range correlations, thus providing the model with an intrinsic scale. Observe that in this case we may use the correlation length of this field as the physical unit of length, measuring in terms of it, for example, the size L of the lattice and the lattice spacing a. In this way we can define a system of physical units that is intrinsic to the model and not external to it.

As we will discuss in more detail later, most of the physical content of the theory will be encoded into the nature of the fields included in the models and in the nature and behavior of the set of n-point correlation functions among these fields. They will determine whether or not we have particles that in fact propagate dynamically, whether or not these particles have non-zero masses, whether or not these particles interact with each other in scattering processes, whether or not there are bound

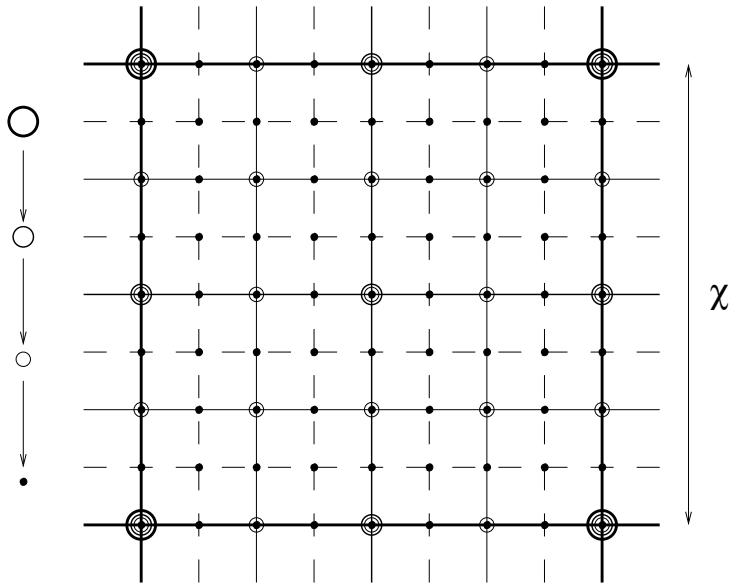

Figure 3.1.5: A sequence of lattices with decreasing lattice spacing.

Since χ defines the unit of length, it makes no sense to impose any conditions on its value, but only on ratios between it and other lengths. The condition with the most direct physical meaning would be that, if there is more than one parameter with dimensions of mass in a particular model, then the ratios between these should have finite and non-zero limits. In this way it would also be simpler to conceive limits in which the product of L by any of these parameters would go to infinity, corresponding to models defined in infinite, limitless space. In the simpler models, with only a single massive field, we have only the mass of the field and the size of the lattice to consider, of course, but conceptually the situation does not change. In figure 3.1.5 we show a sequence of superimposed lattices, with decreasing lattice spacings, together with a correlation length which is kept constant, hoping that this illustration will help the reader to visualize what should happen with the relation between the lattice spacing and the correlation length in the continuum limit.

The calculation of these continuum limits, which are always constrained by one or more conditions over the existing parameters, consists of two steps: first the calculation of the integrals on finite lattices of arbitrary size, and then the calculation of the limits for $N \to \infty$ under the required constraints. Although these are clearly defined mathematical operations, we will see that usually neither of them is easy to realize. As we shall see, we are able neither to calculate the integrals in exact form nor to take the limits in exact form except in the simplest model, the free theory, which we use here as an example. As we shall show in detail, the theory of the free scalar field can be solved exactly by the use of Fourier transforms. While the calculation of these high-dimensional integrals is simply a task of great complexity, which very quickly goes beyond our analytical possibilities, the calculation of the continuum limits is a mathematical operation full of subtleties and surprises.

It is important to observe here that not all elements that appear in the math-

$$S_0[\phi] = \int \mathrm{d}t \left[\frac{1}{2}(\partial_t \phi)^2 + \frac{m_0^2}{2}\phi^2(t) \right],$$

show that it is formally identical to the Euclidean action of the one-dimensional harmonic oscillator of mass M and elastic constant K, described by a coordinate X,

$$S[X] = \int \mathrm{d}t \left[\frac{M}{2}(\partial_t X)^2 + \frac{K}{2}X^2(t) \right],$$

mapping the variables and parameters of one model on those of the other. Show from this fact that the quantum theory of the free scalar field is formally identical to the quantum mechanics of the one-dimensional harmonic oscillator, that is, that one can map all the observables of one of these theories onto the observables of the other.

3.1.3. Recalling problem 1.3.1, where one considers making $\alpha_0 < 0$, show that in this case the integral

$$\int [\mathbf{d}\varphi]\ e^{-S_0}$$

does not exist even on finite lattices, where it is just a finite-dimensional integral.

3.1.4. Show that, for ultra-local actions S, that is, actions that do not depend on products of the fields at different sites, the correlation functions always factor out in terms of the expectation values of the fields at single sites,

$$g_N(\vec{n}_1, \ldots, \vec{n}_n) = \langle \varphi(\vec{n}_1) \ldots \varphi(\vec{n}_n) \rangle = \langle \varphi(\vec{n}_1) \rangle \ldots \langle \varphi(\vec{n}_n) \rangle.$$

3.2 Relation with Statistical Mechanics

The mathematical structure of quantum field theory, in the form in which it was defined in section 3.1, is formally identical to the mathematical formalism used in statistical mechanics for lattice systems. The mathematical difficulties that must be faced in the calculation of the averages are the same in either case and, in fact, the case $d = 3$ coincides completely with the formalism of the micro-canonical ensemble of statistical mechanics. In the case $d = 4$, particularly because there is then the additional issue of changing from Euclidean space to Minkowski space, we have only

of liquids and the spontaneous magnetization of certain metals and other materials are examples of phase transitions. The Ising model can be solved without too much difficulty in the case $d = 1$, but in this case it does not display critical behavior. On the other hand, in any dimension equal to or greater than $d = 2$ it does display critical behavior, but the exact solution of the model is unknown in the majority of these cases. The case $d = 2$ is extremely special because it is one of the very few models with critical behavior between two distinct phases that can be solved exactly, under certain conditions. It is necessary to emphasize here that all these models only display critical behavior in the $N \to \infty$ limit, that is, when we have extremely large lattices, as is the case for the real crystalline lattices of macroscopic quantities of materials.

Models like these, that display critical behavior, will be of extreme interest for quantum field theory. In the case of the Ising model the spins are discrete variables, but it is also possible to define similar models with continuous variables, which will be of even greater interest. One such example is the Heisenberg model, in which we consider that there exists at each site a three-dimensional classical spin, that is, a vector $\vec{\varphi}$ with three components and fixed modulus $\varphi = 1$. These are continuous variables that span the two-dimensional sphere $S_{(2)}$, rather than discrete variables as in the Ising model. In this case the Hamiltonian is given by

$$H[\vec{\varphi}] = -\sum_{\ell} \vec{\varphi}_{(-)} \cdot \vec{\varphi}_{(+)} - \vec{\jmath} \cdot \sum_{s} \vec{\varphi}(s),$$

where the dot denotes the scalar product of vectors. As we shall see in future volumes, this model also has close relations with the models of scalar fields of quantum field theory. An important difference between this type of model and the Ising model is that in this case H is invariant by a continuous set of symmetry transformations, the set of three-dimensional rotations, while in the discrete Ising model H is invariant by a discrete set of transformations, the sign reflections of the spins. In this continuous case the partition function is not given by a discrete sum, but rather by a functional integral

$$Z = \int_{S_{(2)}} [\mathbf{d}\sigma]\; e^{-\beta H[\vec{\varphi}]},$$

where $\mathrm{d}\sigma$ is the area element of $S_{(2)}$. These models only display critical behavior for $d > 2$, not for $d = 2$ or $d = 1$. In fact, it is a fairly well-established fact that in $d = 1$ there are no models with couplings only between next neighbors that display the long-range order which is characteristic of the type of critical behavior that is of interest for us in quantum field theory. The same is true in $d = 2$ for models which are invariant by continuous symmetry transformations, as is the case for the Heisenberg model. The particular case of the Ising model in $d = 2$ is not an exception to this rule, because in this very special case the invariance transformations are discrete, not continuous.

The behavior of the Heisenberg models for $d > 2$ may be described in a qualitative way as follows. The case of the Ising models is a little different due to the fact that

by a certain value T_c, the critical temperature, which is finite and non-zero for $d > 2$. The two phases have very different thermodynamical characteristics, which change abruptly at T_c. For example, the typical qualitative behavior of the scalar magnetization is given in the graph of figure 3.2.1, where $\beta_c = 1/(kT_c)$.

In the symmetrical phase the spins are distributed in a very random way across the lattice and the correlations between a site and its neighbors are weak, that is, if the spin at a certain site points in one direction the probabilities that the spin of one of its neighbors point in the same direction or in the inverse direction are practically the same. Sites which are more distant from one another than next neighbors are even less correlated. Clearly, this tends to make the average of $\vec{M}$ go to zero. We say that this phase is highly uncorrelated or that is has a short *correlation length*. In the broken-symmetrical phase the situation is the opposite of this one, the spins tend to be all aligned with each other, causing the average of $\vec{M}$ to be different from zero. In this phase there are long-range correlations in the system, that appear dynamically as *spin waves* that propagate along the crystalline lattice. If disturbed, the spins oscillate is a coordinated way, each one affecting significantly its neighbors and giving origin to perturbations that propagate like waves for long distances. Se say that in this case the system is highly correlated or that it has a long correlation length. The point $T = T_c$ is very special because this is the only point where we have at the same time $M = 0$ and long-range correlations.

As one can see in the graph of the scalar magnetization given in figure 3.2.1, at the critical point the magnetization has a singular behavior, and is not differentiable as a function of β. In general the systems that display phase transitions are characterized by some form of singular behavior at the critical point that separates the two phases. We may classify the critical systems according to the degree of singularity that they display at the transition point. The *first order* critical systems, of which boiling liquids are an example, are systems in which the order parameter, for example the density of the fluid, has itself a discontinuous behavior at the transition. Systems like the spontaneous magnetization models that we discuss here, in which the order parameter is continuous but not differentiable at the transition point, are denominated *second order* critical systems, and are the only ones of real interest for the quantum theory of fields. This is due to the fact that the first order systems, unlike the second order ones, do not have long range correlations at the critical point T_c. The existence of these long range correlations is essential for the very existence of the quantum field theories in the continuum limit. Due to this, only the immediacy of the critical points of models with second-order phase transitions are of interest for the quantum theory of fields, unlike what happens in statistical mechanics, where all the other regions of the space of parameters of the models also correspond to situations of physical interest.

In the classical theory of the free scalar field we saw that in order to obtain a finite mass m_0 in the continuum limit it is necessary to make the parameter α_0 go to zero in the limit. It was mentioned then that this was a special value of this parameter, the critical value. We will see that in the quantum theory this is in fact a critical point of the model. In this case there is no phase transition, properly

$$g(s_1, s_2) = \langle \varphi(s_1)\varphi(s_2) \rangle.$$

It has the property that follows: if, when $\varphi(s_1)$ has a positive value of typical magnitude, the probabilities that $\varphi(s_2)$ be positive or negative are similar, then the average value of the product tends to go to zero, resulting in a small or zero $g(s_1, s_2)$; on the other hand, if the fact that $\varphi(s_1)$ has a positive value of typical magnitude implies that the probability that $\varphi(s_2)$ is aligned with it is significantly larger than the probability that is has the opposite sign, then the average value tends to be positive and non-zero, resulting in a non-zero $g(s_1, s_2)$, with a magnitude related to the typical value of the fluctuations of the variables at the sites. Hence, the fact that this function is either large or small compared to the typical size of the fluctuations measures the level of statistical correlation between the variables associated to the sites s_1 and s_2. If s_1 and s_2 are the same site s, then $g(s, s) = \sigma^2$ is the square of the average magnitude of the fluctuations of the variables, a positive and non-zero number. Since we are not interested here in the absolute values of the fluctuations of these variables but rather in the correlations between two of them, it is natural to normalize the correlation function so that it is unity at the origin. In addition to this, in case the variables φ do not have zero averages, we can always calculate this average value $\bar{\varphi}$ and then describe the model in terms of new variables $\varphi' = \varphi - \bar{\varphi}$, that do have zero averages. With all these considerations we arrive at the final definition of the statistical correlation function. Given statistical variables $\varphi(s)$, we define the corresponding two-point correlation function as

$$\mathfrak{f}(s_1, s_2) = \frac{\langle \varphi'(s_1)\varphi'(s_2) \rangle}{\langle [\varphi'(s)]^2 \rangle},$$

where

$$\varphi'(s) = \varphi(s) - \langle \varphi(s) \rangle.$$

The function $\mathfrak{f}(s_1, s_2)$ has the property that $\mathfrak{f}(s, s) = 1$, which represents the trivial fact that the variable at a certain site is always completely correlated to itself. In homogeneous systems, that have discrete translational invariance on the lattice, $\mathfrak{f}$ is in fact a function only of the distance r between the sites, measured in terms of the number of links crossed in order to go from one site to the other. Besides, $\mathfrak{f}(r)$ is never an increasing function of the distance, usually it decreases or at most remains constant. In the great majority of systems $\mathfrak{f}(r)$ displays one of two general classes of behavior: it can display a decay with distance according to some inverse power of r, a situation which we denominate polynomial decay; or it can display an exponential decay with r, always much faster than any polynomial decay. In this case, for large distances r, we have that $\mathfrak{f}(r)$ assumes the general form

$$\mathfrak{f}(r) \sim \mathfrak{f}_0 \frac{e^{-\frac{r}{r_0}}}{r^p},$$

largest lattice for which it is still possible to run the program in a few minutes or less, for each value of β. How can you understand the results that you got?

3.2.2. Repeat the previous problem for the Ising model in two dimensions.

3.3 Gaussian Integration

The functional integral is a mathematical object whose complete analytical calculation is usually extremely difficult. There is a single case in which we can calculate the necessary integrals analytically on lattices of arbitrary size and dimension, and in fact take the continuum limit explicitly. This is the case in which the function to be integrated is the exponential of a quadratic form on the fields, that is, the case in which the action is quadratic on the fields. Such an exponential of a quadratic form is called a Gaussian function. Let us start by recalling how to calculate the integral of a Gaussian function in a single dimension, given by

$$g(x) = e^{-\alpha x^2},$$

where α is some positive real number. We want to calculate the integral

$$I_0(\alpha) = \int_{-\infty}^{\infty} \mathrm{d}x \; g(x),$$

as a function of the parameter α. Curiously, it is easier to calculate the square of I_0 than I_0 directly! We can write I_0^2 as

$$I_0^2(\alpha) = \left[\int_{-\infty}^{\infty} \mathrm{d}x \; g(x)\right] \left[\int_{-\infty}^{\infty} \mathrm{d}y \; g(y)\right].$$

This integral extends over the two-dimensional plane $\mathbb{R}^2$. Next, we make a change of variables in this plane, from the Cartesian coordinates (x, y) to polar coordinates (r, θ), where

$$x = r\cos(\theta), \;\; y = r\sin(\theta), \;\; g(x)g(y) = e^{-\alpha r^2},$$

obtaining for the square of the integral

$$I_0^2(\alpha) = \int_0^{\infty} \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta \; r \; e^{-\alpha r^2}.$$

This integral can be done immediately, due to the factor of r that appears from the integration element. Doing the integration we obtain

$$I[\mathbb{Q}] = \int_{-\infty}^{\infty} \mathrm{d}x_1 \ldots \int_{-\infty}^{\infty} \mathrm{d}x_n \; e^{-\sum_i \sum_j x_i Q_{ij} x_j}.$$

Observe that this integral is a functional of $\mathbb{Q}$. It is necessary to assume that the quadratic form is not degenerate, that is, that it does not have any zero or negative eigenvalues, because in this case the integral does not exist due to the existence of a direction in the space of the variables x_i in which the exponential does not decay, causing the integral to diverge. If all the eigenvalues are positive it follows that the quadratic form can be diagonalized by an orthogonal transformation of the variables x_i into another set of coordinates $y_i = T_{ij} x_j$ or, in matrix language, $\vec{y} = \mathbb{T}\vec{x}$. This transformation involves the introduction of a Jacobian determinant for the transformation of the integration volume but, since the transformation is linear, the Jacobian is constant, independent of the coordinates, so that it will always cancel out in the ratios of integrals that we are interested in. Hence, what matters is that in all cases of interest it is possible to reduce the integral, up to a normalization factor that it is not necessary to calculate, to the form

$$I[\mathbb{Q}] = \frac{1}{\det(\mathbb{T})} \int_{-\infty}^{\infty} \mathrm{d}y_1 \ldots \int_{-\infty}^{\infty} \mathrm{d}y_n \; e^{-\sum_i q_i y_i^2},$$

where q_i are the eigenvalues of $\mathbb{Q}$ and we see here why none of them can be negative or zero, since in that case one or more integrals would not exist. This multiple integral may now be written as the product of n one-dimensional integrals, one for each variable, so that the application of our previous result takes us immediately to the answer

$$I[\mathbb{Q}] = \frac{1}{\det(\mathbb{T})} \prod_{i=1}^{n} \sqrt{\frac{\pi}{q_i}}.$$

We see here, once more, why we cannot have zero eigenvalues. Since the determinant of a matrix is equal to the product of its eigenvalues, we may write this result in terms of the determinant of the quadratic form $\mathbb{Q}$, as

$$I[\mathbb{Q}] = \frac{\pi^{n/2}}{\det(\mathbb{T})} \sqrt{\frac{1}{\det(\mathbb{Q})}}. \tag{3.3.1}$$

We see, therefore, that we can calculate the integral of the product of any finite-order polynomial with the Gaussian exponential, for any dimension of the space over which we are integrating. We will now use these results in the quantum theory of the free field. The first thing to do is to write the action S_0 in terms of the Fourier transform of the field. We will see that in this way we will succeed in decoupling the degrees of freedom of the field, because in momentum space they consist of normal modes of oscillation that do not interact with each other. We start with the action in its usual form

related to two independent vectors, thus characterizing the fact that the normal modes are decoupled from each other. We might say that the action is diagonalized in this system of coordinates of the configuration space, but this would not really be a correct statement. In fact each field $\widetilde{\varphi}(\vec{k})$ is multiplied by its complex conjugate $\widetilde{\varphi}^*(\vec{k}) = \widetilde{\varphi}(-\vec{k})$, that is, the momenta are paired in the form $(\vec{k}, -\vec{k})$. We should say instead that the action has been *anti-diagonalized* by the transformation of coordinates. If we represent the fields by vectors in configuration space as we did before, using this time the basis formed by the Fourier modes (problem 3.3.3), the quadratic form of the action would be represented by a matrix that, rather than containing only diagonal terms, that relate each $\vec{k}$ with itself, would contain only anti-diagonal terms, that relate $\vec{k}$ with $-\vec{k}$. The diagonal and the anti-diagonal cross at the position of the zero mode $\vec{k} = \vec{0}$.

This is not really a problem, because the integral of a multi-dimensional Gaussian is related to the determinant of the operator that appears in the quadratic form, as we saw above. Up to a sign, this determinant may be written as either the product of the diagonal elements or as the product of the anti-diagonal elements of the matrix, as one can easily verify using the Laplace expansion for the determinant. The sign that remains undetermined depends only on the dimension of the matrix and is not important since it always cancels out in the ratios of two integrals that define the expectation values of the observables of the theory. However, since this is a very basic and important result, we will do in what follows a direct verification of this fact, calculating explicitly an integral of this type. We want to learn here how to deal with a functional integral written in momentum space, for example the following one[1],

$$I = \int \prod_{\vec{k}} \mathrm{d}\widetilde{\varphi}(\vec{k})\ \widetilde{\varphi}(\vec{k}')\widetilde{\varphi}(\vec{k}'')\ e^{-S_0[\widetilde{\varphi}]}.$$

Let us recall that there are always N^d independent field values, either with the field expressed in terms of $\varphi(\vec{n})$ or in terms of $\widetilde{\varphi}(\vec{k})$, since there are always exactly N^d possible values for either $\vec{n}$ or $\vec{k}$. However, the $\widetilde{\varphi}$ are complex, unlike the φ, which are real and, therefore, there are twice as many real parameters in the set of the $\widetilde{\varphi}$, since for each one of them we have

$$\widetilde{\varphi}(\vec{k}) = \mathfrak{R}(\vec{k}) + \imath\mathfrak{I}(\vec{k}).$$

On the other hand, these parameters $\mathfrak{R}$ are $\mathfrak{I}$ not all independent because, since φ is real, there are among them the constraints

$$\widetilde{\varphi}(-\vec{k}) = \widetilde{\varphi}^*(\vec{k}),$$

that is,

$$\mathfrak{R}(-\vec{k}) = \mathfrak{R}(\vec{k}) \quad \text{and} \quad \mathfrak{I}(-\vec{k}) = -\mathfrak{I}(\vec{k}).$$

[1]This calculation was developed originally in collaboration with Dr. Timothy Edward Gallivan.

since in this case we can factor out the terms involving the four modes $-\vec{k}'$, $\vec{k}'$, $-\vec{k}''$ and $\vec{k}''$. Since we now have two independent variables per mode, we end up writing eight integrals in explicit form,

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

where I' contains the integrals over all the other modes. We are assuming here that the modes indexed by $\vec{k}'$ and $\vec{k}''$ are complex and not real. We invite the reader to complete the deduction, taking into account explicitly the real modes and thus verifying that the results are correct in all cases. We may now use the four delta functions to do the integrals over the four variables $\Re(-\vec{k}')$, $\Im(-\vec{k}')$, $\Re(-\vec{k}'')$ and $\Im(-\vec{k}'')$, which appear only in the corresponding exponentials, obtaining

$$\begin{aligned}
I &= 4I' \times \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\Re(\vec{k}'') \int_{-\infty}^{\infty} \mathrm{d}\Im(\vec{k}'') \\
&\times \Big[\Re(\vec{k}')\Re(\vec{k}'') - \Im(\vec{k}')\Im(\vec{k}'') + \imath\Re(\vec{k}')\Im(\vec{k}'') + \imath\Re(\vec{k}'')\Im(\vec{k}')\Big] \\
&\times e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\Re^2(\vec{k}')+\Im^2(\vec{k}')\right]}\ e^{-N^d[\rho^2(\vec{k}'')+\alpha_0]\left[\Re^2(\vec{k}'')+\Im^2(\vec{k}'')\right]}.
\end{aligned}$$

We observe now that the remaining integrals may be decomposed in terms of factors that are integrals of odd functions over symmetrical domains of integration, being therefore zero. It follows that, for $\vec{k}' \neq \vec{k}''$ and $\vec{k}' \neq -\vec{k}''$, we have $I = 0$.

Let us examine now the case in which $\vec{k}' = \vec{k}''$. In this case, collecting the appropriate factors in a fashion analogous to the previous case, we have

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

$$\langle\widetilde{\varphi}(\vec{k}')\widetilde{\varphi}(-\vec{k}')\rangle = \frac{\displaystyle\int [\mathbf{d}\widetilde{\varphi}]\ \widetilde{\varphi}(\vec{k}')\ \widetilde{\varphi}(-\vec{k}')\ e^{-S_0[\widetilde{\varphi}]}}{\displaystyle\int [\mathbf{d}\widetilde{\varphi}]\ e^{-S_0[\widetilde{\varphi}]}}$$

$$= \frac{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}\mathfrak{R}(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\mathfrak{I}(\vec{k}') \left[\mathfrak{R}^2(\vec{k}') + \mathfrak{I}^2(\vec{k}')\right] e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\mathfrak{R}^2(\vec{k}')+\mathfrak{I}^2(\vec{k}')\right]}}{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}\mathfrak{R}(\vec{k}') \int_{-\infty}^{\infty} \mathrm{d}\mathfrak{I}(\vec{k}')\ e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\left[\mathfrak{R}^2(\vec{k}')+\mathfrak{I}^2(\vec{k}')\right]}}$$

$$= \frac{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}\mathfrak{R}(\vec{k}')\ \mathfrak{R}^2(\vec{k}')\ e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\mathfrak{R}^2(\vec{k}')}}{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}\mathfrak{R}(\vec{k}')\ e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\mathfrak{R}^2(\vec{k}')}} + \frac{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}\mathfrak{I}(\vec{k}')\ \mathfrak{I}^2(\vec{k}')\ e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\mathfrak{I}^2(\vec{k}')}}{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}\mathfrak{I}(\vec{k}')\ e^{-N^d[\rho^2(\vec{k}')+\alpha_0]\mathfrak{I}^2(\vec{k}')}}.$$

These two terms containing ratios of integrals are identical, as one can check with a simple change of the integration variable in one of them. We have then, using the trick seen before of differentiating with respect to the parameter in order to relate the integrals in the numerators with those in the denominators,

$$\begin{aligned}
\langle\widetilde{\varphi}(\vec{k}')\widetilde{\varphi}(-\vec{k}')\rangle &= 2\frac{\dfrac{\partial}{\partial\left[-N^d[\rho^2(\vec{k}')+\alpha_0]\right]}\sqrt{\dfrac{\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}{\sqrt{\dfrac{\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}} \\
&= -2\sqrt{N^d[\rho^2(\vec{k}')+\alpha_0]}\left(-\frac{1}{2}\right)\frac{1}{\sqrt{N^d[\rho^2(\vec{k}')+\alpha_0]}^3} \\
&= \frac{1}{\sqrt{N^d[\rho^2(\vec{k}')+\alpha_0]}^2}.
\end{aligned}$$

Using the fact that $\widetilde{\varphi}(-\vec{k}') = \widetilde{\varphi}^*(\vec{k}')$ in order to write the left-hand side as a square modulus, we have therefore the final result for the propagator of the free theory in momentum space,

$$\langle|\widetilde{\varphi}(\vec{k})|^2\rangle = \frac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}. \tag{3.3.3}$$

Note that this result for the propagator in momentum space is exactly equal to the Green function of the classical theory written in momentum space. The same is true for other boundary conditions, but this relation between the classical and quantum theories is a *specific property of the free theory*, not a general property of quantum field theory. It is interesting to mention that we may systematize this kind of calculation writing only the result for the integral

$n^{-n/2}$, while $\det(\mathbb{F}^{-1}) = n^{n/2}$. The first determinant is simply the Jacobian of the transformation from the basis $[\mathbf{d}\varphi]$ to the basis $[\mathbf{d}\widetilde{\varphi}]$ in the functional integral. Since it is independent of the fields and therefore cancels out in the ratio of integrals that defines the measure for the functional integration, we may write a generic functional integral, such as

$$\langle \mathcal{O} \rangle = \frac{\displaystyle\int [\mathbf{d}\varphi] \;\; \mathcal{O}\,[\varphi] \;\; e^{-S[\varphi]}}{\displaystyle\int [\mathbf{d}\varphi] \;\; e^{-S[\varphi]}},$$

in terms of the basis of Fourier components, as

$$\langle \mathcal{O} \rangle = \frac{\displaystyle\int [\mathbf{d}\widetilde{\varphi}] \;\; \mathcal{O}\,[\widetilde{\varphi}] \;\; e^{-S[\widetilde{\varphi}]}}{\displaystyle\int [\mathbf{d}\widetilde{\varphi}] \;\; e^{-S[\widetilde{\varphi}]}}.$$

Of course a similar result is valid for the expression of $\langle \mathcal{O} \rangle$ in terms of integrations involving the dimensionfull field ϕ.

Problems

3.3.1. Calculate, on a lattice with N^d sites in d dimensions, the multiple integral

$$I_0 = \int \prod_{\vec{n}} \mathrm{d}\varphi(\vec{n}) \; e^{-\frac{\alpha_0}{2} \sum_{\vec{n}} \varphi^2(\vec{n})}.$$

3.3.2. Show that $I_1(\vec{n}_1, \vec{n}_2) = C\delta(\vec{n}_1, \vec{n}_2)$ where $\delta(\vec{n}_1, \vec{n}_2)$ is the d-dimensional Kronecker delta function and

$$I_1(\vec{n}_1, \vec{n}_2) = \int \prod_{\vec{n}} \mathrm{d}\varphi(\vec{n}) \; \varphi(\vec{n}_1) \; \varphi(\vec{n}_2) \; e^{-\frac{\alpha_0}{2} \sum_{\vec{n}} \varphi^2(\vec{n})},$$

and calculate C.

3.3.3. Write, in the one-dimensional case, the matrix that represents the operator $\widetilde{K}(k, k')$ in configuration space, using as a basis the Fourier modes $\widetilde{\varphi}(k)$ of the field, in terms of which the action of the free theory in momentum space, as given in equation (3.3.2), is written as

$$S_0[\widetilde{\varphi}] = \frac{N}{2} \sum_{k} \sum_{k'} \widetilde{\varphi}(k) \widetilde{K}(k, k') \widetilde{\varphi}(k').$$

For simplicity, use lattices with odd N, enumerating the corresponding momenta from $-(N-1)/2$ to $(N-1)/2$, in order to verify that the matrix is anti-diagonal, and write explicitly the elements of the anti-diagonal. Using this fact and the result in equation (3.3.1), obtain the result in equation (3.3.4) up to a multiplicative constant.

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

where $\rho_f^2(\vec{k})$ was defined in equation (2.8.4).

3.4 Factorization of the Correlation Functions

One fundamental concept of the traditional theory is that the physical content of a model in quantum field theory is defined by the set of its correlation functions. Having developed the necessary calculational techniques, in this section we will discuss the properties of the correlation functions of the free scalar field on a finite periodical lattice. Through this simple model, that we use as our example, we may learn some things of general interest about the structure of correlations of the theory. The n-point functions are defined in position space as

$$g(\vec{x}_1, \ldots, \vec{x}_n) = \langle \varphi(\vec{x}_1) \ldots \varphi(\vec{x}_n) \rangle,$$

but we may also define corresponding functions in momentum space, doing Fourier transformations for each one of the n coordinates $\vec{x}_i$. Doing this we obtain n-point functions in momentum space, given by

$$\widetilde{g}(\vec{k}_1, \ldots, \vec{k}_n) = \langle \widetilde{\varphi}(\vec{k}_1) \ldots \widetilde{\varphi}(\vec{k}_n) \rangle.$$

As proposed in problem 3.1.1, it is not difficult to verify that, in the free theory defined by S_0, we have for the function of a single point in position space

$$g(\vec{x}_1) = \langle \varphi(\vec{x}_1) \rangle = 0,$$

by means of arguments of symmetry and parity applied to the functional integral, and using the fact that the action is symmetrical by the exchange of the sign of the field, that is, $S_0[\varphi] = S_0[-\varphi]$. In an analogous fashion, it is easy to verify (problem 3.4.1) that the same result is valid for any functions for which n is odd, independently of some of the factors $\vec{x}_i$ being equal or not, that is, that for any $i = 0, \ldots, \infty$ and any $\vec{x}_i$ we have

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

For example, we have that $\langle \varphi(\vec{x}_1)\varphi(\vec{x}_2)\varphi(\vec{x}_3) \rangle$, $\langle \varphi(\vec{x}_1)\varphi^2(\vec{x}_2) \rangle$ and $\langle \varphi^3(\vec{x}_1) \rangle$ are all zero, independently of the values of the vectors $\vec{x}_i$. Identical arguments may be applied in momentum space for expectation values of products of the Fourier components. In order to see this it suffices to write the action in terms of these components, as we already did before, verifying that it remains invariant by changes of

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

This is due to the fact that the degrees of freedom are decoupled *only* in momentum space, not in position space. Hence, in the first case the fact that $\langle\widetilde{\varphi}(\vec{k})\rangle$ is zero implies that $\langle\widetilde{\varphi}(\vec{k}_1)\widetilde{\varphi}(\vec{k}_2)\rangle = 0$ for $\vec{k}_1 \neq -\vec{k}_2$, but in the second case, although $\langle\varphi(\vec{x})\rangle$ is zero, we have $\langle\varphi(\vec{x}_1)\varphi(\vec{x}_2)\rangle \neq 0$, independently of the values of $\vec{x}_1$ and $\vec{x}_2$.

Of course the factorization relation (3.4.1) in momentum space has a counterpart in position space, but it is necessary to keep in mind that this equation is only valid for $\vec{k}_1 \neq -\vec{k}_2$ and not when the two momenta are equal and opposite. Doing the Fourier transformation of the left-hand side of this equation one obtains a relation for the two-point function in position space (problem 3.4.4), but it is not a factorization relation like the one suggested by equation (3.4.2). Instead of this, what one obtains is the relation

$$\langle\varphi(\vec{x}_1)\varphi(\vec{x}_2)\rangle = \sum_{\vec{k}} e^{-\imath\frac{2\pi}{L}\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}\langle|\widetilde{\varphi}(\vec{k})|^2\rangle. \tag{3.4.3}$$

The calculations involved in this kind of manipulation are usually simple but involve a few accounting subtleties involving the accounting of the terms in the sums over the modes in momentum space. This is a skill that it is very important to acquire in order to develop good control over the theory.

We will now calculate some of the examples that remain of non-zero correlation functions in momentum space, to illustrate the important phenomenon of the factorization of *all* higher-order correlation functions in terms of the propagator, which is characteristic of free field theories. A we already saw before, from equation (3.3.3) we have the following fundamental result for the two-point function, which *cannot* be factored in terms of the one-point function,

$$\langle|\widetilde{\varphi}(\vec{k})|^2\rangle = \frac{1}{N^d[\rho^2(\vec{k}) + \alpha_0]}.$$

Besides this, we have the result of equation (3.3.4) for the basic functional integral in momentum space,

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

starting from which it is easy to calculate all the others by means of differentiation with respect to the quantity $-N^d[\rho^2(\vec{k}) + \alpha_0]/2$. However, it is necessary to treat separately the cases in which $\widetilde{\varphi}(\vec{k})$ is real (such as, for example, the case $\vec{k} = \vec{0}$) and the cases in which $\widetilde{\varphi}(\vec{k})$ has a non-zero imaginary component, because there exists in the sum that defines $S_0[\widetilde{\varphi}]$ only one term containing a real component such as $\widetilde{\varphi}(\vec{0})$, but two identical terms containing a Fourier component that has non-zero imaginary part. As an example of this kind of calculation, let us consider the quantity

$$
\begin{aligned}
&= \frac{\left(\dfrac{-\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \displaystyle\prod_{\vec{k}'}\sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}{\displaystyle\prod_{\vec{k}'}\sqrt{\frac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}} \\
&= \frac{\left(\dfrac{-\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \dfrac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}}{\dfrac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}} \\
&= \frac{(-1)^2\,(-1)\,(-2)\,\dfrac{1}{\{N^d[\rho^2(\vec{k})+\alpha_0]\}^3}}{\dfrac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}} \\
&= 2\frac{1}{\{N^d[\rho^2(\vec{k})+\alpha_0]\}^2}.
\end{aligned}
$$

so that we obtain, in a way analogous to the previous one, the relation

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

showing once more that the four-point function factors into two two-point functions, but with a different coefficient. For higher-order functions one can obtain (problem 3.4.5) the general formula

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

for any integer n. In fact, in future volumes we will see that it will be convenient to build a small table of such relations between the functional integrals of the free theory, because they will show up repeatedly in the development of the perturbative theory for interacting theories, like the non-linear models that we will examine in the future.

We see therefore that the complete solution of the theory of the free scalar field, that is, the calculation of all its correlation functions, is reducible to the calculation of the propagator. It follows that all the physics of the theory is contained in the structure of this propagator. The factorization of the higher-order functions in terms of the propagator means that there are no physical interactions between the objects that propagate in this model. One way to understand this using our classical intuition is to remember that the theory is *linear*, being characterized classically by a linear equation of motion for which there is a *principle of linear superposition*, that is, the waves that propagate in space-time in the non-Euclidean version of the theory superpose linearly, going right through one another as in classical electrodynamics, *without interacting* with one another. The factorization of the correlation functions means that this linearity is preserved in the quantum version of the theory, that

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

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:

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

3.5 External Sources in the Quantum Theory

We studied before, in sections 2.10 and 2.11, the role of the external sources in classical field theory. We will examine in this section the behavior of the models when one introduces external sources in the quantum theory. We saw that, in the case of the classical theory, the effect of the introduction of external sources is a deformation of the classical solution, which depends of the specific form of the source which is introduced. This happens due to the change, in the space of configurations, of the position of the minimum of the action, which is caused by the introduction of the external source. We will see that something similar happens in the case of the quantum theory. It is clear that, in this case, it is not what happens to the position of the minimum of the action which is of immediate interest, but rather what happens with the relative statistical weights $\exp(-S)$ associated to all possible configurations.

We saw, in the example of the classical theory of the free scalar field on a periodical lattice, that the classical solution without sources was simply $\varphi \equiv 0$, and that it changed to a non-zero solution $\varphi[j]$ in the presence of the external source j. This is not a local point-by-point relation between φ and j, but rather a global relation, so that we may say that the solution $\varphi[j]$ is a type of functional of j: in order to determine $\varphi(s)$ at a site s it is not sufficient to know $j(s)$, instead it is necessary to know j at all lattice sites. In a similar way, we have that in the quantum theory of the free scalar field on a periodical lattice the expectation value $v = \langle\varphi\rangle$ of the field is zero in the absence of external sources. In this case the effect of the introduction of the external source is to cause $v(s)$ to be no longer zero, but rather a function of position that depends on the source j.

In order to exemplify these facts, let us calculate the expectation value of the field in the free theory, with periodical boundary conditions. When we have an external source the action is given by equation (2.10.1),

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

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 form. Another way to obtain the same result, which makes it easy to solve the equation, is to write all the functions of position in terms of their Fourier transforms. We will do this starting from equation (3.5.1). We have for the field φ', the expectation value v and the external source j,

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

so that we may write equation (3.5.1) as

$$\begin{aligned}
0 &= \sum_{\vec{n}}\sum_{\vec{k}}\sum_{\vec{k}'}\left[\sum_{\mu}\left(\Delta_\mu e^{-\imath\frac{2\pi}{N}\vec{k}\cdot\vec{n}}\right)\tilde{v}(\vec{k})\left(\Delta_\mu e^{-\imath\frac{2\pi}{N}\vec{k}'\cdot\vec{n}}\right)\widetilde{\varphi}'(\vec{k}')\right. \\
&\quad \left. +\alpha_0\ e^{-\imath\frac{2\pi}{N}(\vec{k}+\vec{k}')\cdot\vec{n}}\ \tilde{v}(\vec{k})\ \widetilde{\varphi}'(\vec{k}') - e^{-\imath\frac{2\pi}{N}(\vec{k}+\vec{k}')\cdot\vec{n}}\ \widetilde{\jmath}(\vec{k})\ \widetilde{\varphi}'(\vec{k}')\right] \\
&= \sum_{\vec{k}}\sum_{\vec{k}'}\left[\sum_{\vec{n}} e^{-\imath\frac{2\pi}{N}(\vec{k}+\vec{k}')\cdot\vec{n}}\right] \\
&\quad \times\left[-\tilde{v}(\vec{k})\ \widetilde{\varphi}'(\vec{k}')\sum_{\mu}\rho_\mu(\vec{k})\ \rho_\mu(\vec{k}')\ e^{-\imath\frac{\pi}{N}(k_\mu+k'_\mu)} + \alpha_0\ \tilde{v}(\vec{k})\widetilde{\varphi}'(\vec{k}') - \widetilde{\jmath}(\vec{k})\ \widetilde{\varphi}'(\vec{k}')\right] \\
&= \sum_{\vec{k}}\sum_{\vec{k}'} N^d\delta^d(\vec{k},-\vec{k}') \\
&\quad \times\left[-\tilde{v}(\vec{k})\sum_{\mu}\ \rho_\mu(\vec{k})\ \rho_\mu(\vec{k}')\ e^{-\imath\frac{\pi}{N}(k_\mu+k'_\mu)} + \alpha_0\tilde{v}(\vec{k}) - \widetilde{\jmath}(\vec{k})\right]\widetilde{\varphi}'(\vec{k}') \\
&= N^d\sum_{\vec{k}}\widetilde{\varphi}'(-\vec{k})\left[\tilde{v}(\vec{k})\sum_{\mu}\rho_\mu^2(\vec{k}) + \alpha_0\tilde{v}(\vec{k}) - \widetilde{\jmath}(\vec{k})\right],
\end{aligned}$$

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 same thing on the quantum case. In fact, the effects of the quantization process on the models, that is, the consequences of the quantum theory, can be explored by means of the examination of the functional relation between v and j in the quantum theory. As we shall see in what follows, this can most conveniently be done in terms of a functional that we will call the *effective action* of the model, which is a way to encode concisely this functional relation.

Problems

3.5.1. Show in detail that the only way to satisfy equations (3.5.1) and (3.5.2) for all possible field configurations $\varphi'(\vec{n})$ on the lattice is that the expressions in brackets that appear in these equations be zero. One way to do this, among many others, is to choose a particular set of functions $\varphi'(\vec{n})$ that can constitute a basis for the representation of any element of configuration space, which is a vector space with a large but finite dimension, $\mathbb{R}^{N^d}$.

3.5.2. Calculate the expectation value in the equation $\langle\varphi'(\vec{n})\rangle = 0$ and use it to derive the solution for v in terms of j in the quantum theory, showing that the answer coincides with the one derived in the text.

3.5.3. Calculate the inverse Fourier transform of equation (3.5.3) in order to obtain the solution in position space given in equation (3.5.4).

3.5.4. Show through the direct calculation of the expectation value that $K(\vec{n},\vec{n}')$ is the propagator of the model in position space, $\langle\varphi'(\vec{n})\varphi'(\vec{n}')\rangle$.

3.5.5. Show that the width of the distribution of values of the field at a single site, in the free theory with an external source j, which is given by

$$\sigma^2_{(j)} = \langle\varphi^2\rangle_{(j)} - \langle\varphi\rangle^2_{(j)},$$

where the index j indicates the presence of the external source, is equal to the width of the theory without the external source, which is given by

$$\sigma^2 = \langle\varphi^2\rangle - \langle\varphi\rangle^2,$$

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 classical field $\varphi_{(c)}$ as an observable of the quantum theory, and that will be enough for the purposes of this chapter. A deeper discussion of this topic will be presented later on, when we introduce the concept of block variables.

An important point about the functional relation between $\varphi_{(c)}$ and j is that it is a bijection, that is, given a $j(\vec{n})$ a certain function $\varphi_{(c)}(\vec{n})$ is uniquely determined, and vice-versa, given a certain $\varphi_{(c)}(\vec{n})$ there is a unique function $j(\vec{n})$ that corresponds to it. The first part of this statement is rather obvious, because a single cause j cannot produce two different consequences $\varphi_{(c)}(\vec{n})$. Regarding the second part, in the case of the classical theory this is a simple consequence (problem 3.6.1) of the uniqueness of the solution of a differential equation. In the quantum theory we may show this in the following way: since S is invariant by the transformation $\varphi \to -\varphi$, it follows that $S_{(j)}$ is invariant by the joint change of sign of φ and j, which also has the effect of changing the sign of $\varphi_{(c)}$. It is clear then that, if a certain j and a certain $\varphi_{(c)}$ are related by the functional relation established by the quantum theory, then $-j$ and $-\varphi_{(c)}$ are as well. In addition to this, it is clear that any non-vanishing external source affects the expectation value of the field in some way, so that only $j = 0$ is related with $\varphi_{(c)} = 0$. Given all this, it follows that there cannot be two different sources j_1 and j_2 that produce the same $\varphi_{(c)}$, because otherwise there would be a non-vanishing source $j = j_1 - j_2$ that is related to $\varphi_{(c)} = 0$ by the functional relation.

We will assume, for simplicity, that the models are defined on a finite lattice within a box, with periodical boundary conditions. The basic functional generator that we wish to define is a functional of the external source j, traditionally denoted by $Z[j]$,

$$Z[j] = \left\langle e^{\sum_{\vec{n}} j(\vec{n})\varphi(\vec{n})} \right\rangle = \frac{\int [\mathbf{d}\varphi] e^{-S_{(j)}}}{\int [\mathbf{d}\varphi] e^{-S}}. \tag{3.6.2}$$

Note that we have here an expectation value in the measure (or distribution) of S, without the term with the external source. One may also say that $Z[j]$ is the ratio of two measures, one with j present and the other without it. Given j, Z is a real number, a simple functional of j. As we will show later on, in general $\langle S \rangle$ diverges in the continuum limit, so that Z is a possibly singular ratio in that limit, except if $j = 0$, in which case $Z = 1$ both on finite lattices and in the continuum limit. However, the value of Z itself is not actually very important, what really matters is how it varies when we vary j. In any case it is a finite quantity on finite lattices, where it can therefore be used for the operations to be described below, and anyway we should always take the limit only at the final step of any given calculation, by

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 generates the full correlation functions $g_{1,\ldots,n}$, W generates functions that are called the *connected* correlation functions $g_{(c)1,\ldots,n}$. As we saw above, the first derivative of W with respect to j gives us the one-point function, the expectation value of the field. In order to examine in more detail the nature of these functions, let us take one more functional derivative of W. Starting from (3.6.3) we get,

$$\frac{\mathfrak{d}^2W[j]}{\mathfrak{d}j_1\mathfrak{d}j_2} = \frac{1}{Z[j]}\,\frac{\mathfrak{d}^2Z[j]}{\mathfrak{d}j_1\mathfrak{d}j_2} - \frac{1}{Z^2[j]}\,\frac{\mathfrak{d}Z[j]}{\mathfrak{d}j_1}\,\frac{\mathfrak{d}Z[j]}{\mathfrak{d}j_2} = g_{(j)1,2} - \varphi_{(c)1}\varphi_{(c)2} = g_{(c,j)1,2}. \tag{3.6.4}$$

Here $g_{(j)1,2}$ is the complete propagator in the presence of j and $g_{(c,j)1,2}$ is the connected propagator in the same conditions. Note that, for $j = 0$ in a theory which is symmetrical by reflection of the fields, as we assume here, we have that $\varphi_{(c)} = 0$ and then the two propagators coincide. However, for $j \neq 0$ or in cases where $j = 0$ does not imply that $\varphi_{(c)} = 0$, it is the connected propagator $g_{(c,j)1,2}$ given by W, not the full propagator $g_{(j)1,2}$ given by Z, which is the true correlation function of the theory, as we discussed in section 3.2. In order to obtain the correlations between φ_1 and φ_2 in circumstances in which $\langle\varphi\rangle \neq 0$ it is necessary to subtract the product of the expectation values of the two fields. We see therefore that W is a functional with a more direct significance than that of Z. In particular, the functional W can be used to write the functions of three, four or more points of the theory (problem 3.6.2), which are related in a more direct way to the existence within it of true physical interactions.

Up to this point, the structure that we have is that the functionals Z and W depend on the external source j and that functional derivatives with respect to it produce from these functionals all the correlation functions of the theory. Since the physics of a model in the quantum theory is encoded in the set of its correlation functions, these functionals may be understood as abbreviated condensations of all the properties of the model. To calculate completely these functional is equivalent to solve completely the theory, which usually is not an easy thing to do. We will proceed now with the development of the formalism of the functional generators, with the intent of obtaining a description of these properties in terms, not directly of j, but of the classical field $\varphi_{(c)}$ that appears as a consequence of the introduction of the external sources. Note that we may write the definitions of Z and W as

$$Z[j] = e^{W[j]} = \frac{\displaystyle\int [\mathbf{d}\varphi] e^{\sum_{\vec{n}} j(\vec{n})\varphi(\vec{n})} e^{-S}}{\displaystyle\int [\mathbf{d}\varphi] e^{-S}},$$

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

$$e^{W[j]} = e^{\sum_{\vec{n}} j(\vec{n})\varphi_{(c)}(\vec{n})} e^{-\Gamma[\varphi_{(c)}]} = \frac{\int [\mathbf{d}\varphi] e^{\sum_{\vec{n}} j(\vec{n})\varphi(\vec{n})} e^{-S}}{\int [\mathbf{d}\varphi] e^{-S}}.$$

At this point it starts to appear that $\Gamma[\varphi_{(c)}]$ has something to do with a kind of "classical action" for the "classical field" $\varphi_{(c)}$. The functional $\Gamma[\varphi_{(c)}]$ is called the *effective action* of the theory and we will see later on that this interpretation is correct and can be in fact very useful. We may write its complete definition in the form

$$e^{-\Gamma[\varphi_{(c)}]} = \left\langle e^{\sum_{\vec{n}} j(\vec{n})\left[\varphi(\vec{n}) - \varphi_{(c)}(\vec{n})\right]} \right\rangle = \frac{\int [\mathbf{d}\varphi] e^{\sum_{\vec{n}} j(\vec{n})\left[\varphi(\vec{n}) - \varphi_{(c)}(\vec{n})\right]}\ e^{-S}}{\int [\mathbf{d}\varphi] e^{-S}}.$$

Note that, since Γ is a functional directly of $\varphi_{(c)}$, not of j, the external sources that appear in this expression should be understood as functionals $j[\varphi_{(c)}]$. As we shall see in what follows, the effective action is related directly to the classical limit of the theory, as well as to its main properties relative to propagation phenomena and to the physical interactions that may exist in the theory.

Problems

3.6.1. Basing your arguments in the famous theorem relative to the uniqueness of the solution of a differential equation under certain conditions, show that the mapping between the classical solutions and the external sources in the classical theory of fields is a bijective or one-to-one map, that is, show that each external source j corresponds to a unique classical solution $\varphi_{(c)}$.

3.6.2. Using the definition of the connected three-point correlation function,

$$g_{(c,j)1,2,3} = \frac{\mathfrak{d}^3 W[j]}{\mathfrak{d} j_1 \mathfrak{d} j_2 \mathfrak{d} j_3},$$

in a theory with a non-vanishing external source j, show that it relates to the complete three-point and two-point functions by

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

Substituting the complete propagators $g_{(j)i,j}$ in terms of the connected propagators $g_{(c,j)i,j}$, with the use of the relation shown in equation (3.6.4), show

theory, the functional relation defined by this quantum theory. Clearly, this has to be some functional of $\varphi_{(c)}$, so that we may consider its variations when we vary $\varphi_{(c)}$ around the value defined by the quantum theory.

The objective of this section is to show that the effective action $\Gamma[\varphi_{(c)}]$ is such a functional, besides analyzing its properties and establishing its role as a kind of abstract of the properties of the quantum theory. Just as we did in section 3.6, we will establish these facts in a general way, for any models of scalar fields, not only for the free theory. We already saw in section 3.6 that the knowledge of the functionals $Z[j]$ and $W[j]$ allows us to obtain all the correlation functions of the quantum theory and, since from the physical standpoint the quantum theory may be understood as the set of its correlation functions, we have through these functionals a complete image of the quantum theory and its consequences. We will see here that the effective action also has this same role, but that it presents the structure of the quantum theory in a more synthetic and direct way. Obtaining Γ in closed form corresponds to the complete solution of the theory and, therefore, is not usually an easy task. However, it is often possible to formulate testable hypothesis about the form of Γ or of parts of it, based on symmetry arguments or other types of reasoning, that are very useful to guide us in our explorations of the structure of the models.

Our first task is to show that Γ is indeed related to the solution of the quantum theory through a minimization process. In order to put in a clearer perspective our procedure in this first part, let us point out that the classical theory and the quantum theory act on very different spaces of functions with respect to the field φ. When we study the classical theory through the principle of minimum action, we assume that, in the continuum limit, the possible fields are continuous and differentiable functions at almost all points, that is, all except a collection of isolated singularities, usually associated to the presence of point sources, which are no more than mathematically convenient fictions. In contrast to that, in the quantum theory we start by assuming that the fields can assume values in a much larger space, the space of all possible functions, without any restrictions of differentiability or even of continuity. As we shall see in detail later on, this space of configurations is a space of functions which are typically *discontinuous at all points*, even in the continuum limit. The imposition on it of the statistical distribution of a given model attributes to each element of the space different statistical weights but does not change the character typically discontinuous of the configurations.

On the other hand, the space of the expectation values $\varphi_{(c)}$ of the field in the quantum theory is much more limited than the space of the fields φ, because the statistical averaging process over all the possible configurations has a strong effect of eliminating the discontinuities and non-differentiabilities of the configurations, usually resulting, in the continuum limit, in continuous functions for $\varphi_{(c)}$, which in general are also differentiable except for a set of isolated singularities associated to singularities in the external sources j that are included in the theory. As we saw before, both the classical theory and the quantum theory establish functional relations between the sources j and the continuous and mostly differentiable fields. The relations among these spaces are illustrated in figure 3.7.1. In this figure J is

some other part of a more general model, representing a part of the physical world whose quantum behavior is not under direct scrutiny. Fundamentally, everything in nature has an underlying quantum behavior and an ultimate theory in its most fundamental form should describe the quantum interaction between all parts of nature without any explicit reference to external classical objects such as external sources.

It is in the context of this subspace of the possible configurations of the classical field $\varphi_{(c)}$, defined by the averaging process in the quantum theory, that we will study the behavior of Γ in the immediacy of the configuration $\varphi_{(c)0}$ associated to a given j_0 by the functional relation established by the dynamics of the quantum theory. At this point it is convenient to recall the definition of Γ,

$$\Gamma[\varphi_{(c)}] = -\ln\left\{\frac{\int[\mathbf{d}\varphi]\; e^{\sum_{\vec{n}} j(\vec{n})\left[\varphi(\vec{n})-\varphi_{(c)}(\vec{n})\right]}\; e^{-S}}{\int[\mathbf{d}\varphi]\; e^{-S}}\right\}, \tag{3.7.1}$$

as well as the fact that Γ is a functional of $\varphi_{(c)}$ alone, so that in this expression j should be understood as just a functional of $\varphi_{(c)}$, through the functional relation established between them by the quantum theory. Hence, given the effective action $\Gamma[\varphi_{(c)}]$ defined in this way for a given but otherwise arbitrary $\varphi_{(c)}$, we will now define the effective action in the presence of an arbitrary external source j_0, not necessarily the one that is related with $\varphi_{(c)}$ by the functional relation established by the quantum theory, as

$$\Gamma_{(j)} = \Gamma[\varphi_{(c)}] - \sum_{\vec{n}} j_0(\vec{n})\varphi_{(c)}(\vec{n}).$$

Note that this new external source is a source for $\varphi_{(c)}$, not for φ, so we are asking ourselves how would the action Γ behave as a *classical* action under the introduction of a source. Given a fixed j_0, this equation defines $\Gamma_{(j)}$ for an arbitrary $\varphi_{(c)}$, so that its functional variation is given by

$$\mathbf{d}\Gamma_{(j)} = \mathbf{d}\Gamma[\varphi_{(c)}] - \sum_{\vec{n}} j_0(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}).$$

In order to establish that the solution of the theory in the presence of j_0 is given by a local minimum of $\Gamma_{(j)}$, we will now consider the variations of this functional around the point $\varphi_{(c)0}$ which is the value of $\varphi_{(c)}$ that is related with j_0 through the functional relation established by the quantum theory. In this case the differential of $\Gamma_{(j)}$ is the expression given above with

$$\mathbf{d}\varphi_{(c)}(\vec{n}) = \varphi'_{(c)}(\vec{n}) - \varphi_{(c)0}(\vec{n}).$$

It is necessary to make very clear in which way we should analyze the variations of $\Gamma_{(j)}$. We assume that one makes small but otherwise arbitrary variations $\mathbf{d}\varphi_{(c)}(\vec{n})$ of the classical field and we ask what is the corresponding variation of $\Gamma_{(j)}$. In

$$= \sum_{\vec{n}} j_0(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}) - \ln\left[1 + \sum_{\vec{n}}\langle\varphi(\vec{n})\rangle_{(j)}\mathbf{d}j(\vec{n}) - \sum_{\vec{n}}\varphi'_{(c)}(\vec{n})\mathbf{d}j(\vec{n})\right]$$
$$= \sum_{\vec{n}} j_0(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}) - \ln\left[1 - \sum_{\vec{n}}\mathbf{d}\varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n})\right],$$

since we have that $\langle\varphi(\vec{n})\rangle_{(j)} = \varphi_{(c)0}$ and that $\mathbf{d}\varphi_{(c)} = \varphi'_{(c)} - \varphi_{(c)0}$. Expanding now the logarithm to first order we obtain

$$\mathbf{d}\Gamma = \sum_{\vec{n}} j_0(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}) + \sum_{\vec{n}}\mathbf{d}\varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}).$$

We have therefore for the variation of $\Gamma_{(j)}$, from its definition,

$$\mathbf{d}\Gamma_{(j)} = \sum_{\vec{n}} j_0(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n}) + \sum_{\vec{n}}\mathbf{d}\varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}) - \sum_{\vec{n}} j_0(\vec{n})\mathbf{d}\varphi_{(c)}(\vec{n})$$
$$= \sum_{\vec{n}}\mathbf{d}\varphi_{(c)}(\vec{n})\mathbf{d}j(\vec{n}).$$

If we recall now the result obtained in problem 3.6.3, according to which we may write for the variations of j and $\varphi_{(c)}$ at the same arbitrary point $\vec{n}$ that

$$\mathbf{d}j(\vec{n}) = \frac{1}{\sigma^2_{(j)}}\mathbf{d}\varphi_{(c)}(\vec{n}),$$

we see that we can write our final result for the variation of the effective action in the presence of external sources,

$$\mathbf{d}\Gamma_{(j)} = \sum_{\vec{n}}\frac{[\mathbf{d}\varphi_{(c)}(\vec{n})]^2}{\sigma^2_{(j)}},$$

which means that, given a certain external source $j_0(\vec{n})$ and a certain functional $\Gamma[\varphi_{(c)}]$, the corresponding functional $\Gamma_{(j)}$ always increases, for any variation $\mathbf{d}\varphi_{(c)}(\vec{n})$ around the function $\varphi_{(c)0}(\vec{n})$ determined by the quantum theory from $j_0(\vec{n})$. It follows that the functional $\Gamma_{(j)}[\varphi_{(c)}]$ is at a minimum when $\mathbf{d}\varphi_{(c)}(\vec{n}) \equiv 0$, that is, when $\varphi_{(c)}(\vec{n})$ is the function determined by the quantum theory.

In this way, we conclude that Γ describes how the quantum theory responds to the introduction of external sources, in the same way in which S does the same thing in the classical theory. We see therefore that, in the limit of large wavelengths, that is, for distances which are much larger than those finite correlation lengths that appear in the theory, in situations where the quantum fluctuations can be ignored, Γ is indeed the classical action that describes the classical limit of the model, thus describing its classical behavior, which exists as a consequence of the underlying quantum structure of the model.

In order to continue to elucidate the significance of Γ we will now examine its functional derivatives with respect to $\varphi_{(c)}$. We saw in section 3.6 that the functional

the effective action has exactly the same form as S_0, written in terms of the classical field,

$$\Gamma[\varphi_{(c)}] = \sum_{\vec{n}} \left\{ \frac{1}{2} \sum_{\mu} \left[\Delta_\mu \varphi_{(c)}(\vec{n}) \right]^2 + \frac{\alpha_0}{2} \varphi^2_{(c)}(\vec{n}) \right\}, \tag{3.7.4}$$

where we decomposed the sum over links as usual. This fact explains in a clear way why the propagator of the free quantum theory is equal to the Green function of the free classical theory. We may now take the functional derivatives of Γ, which we will do in a rather symbolic and formal way, leaving a more detailed approach to the reader, in problem 3.7.2. Taking the first functional derivative we obtain

$$\frac{\mathfrak{d}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}} = \sum_{3} \left\{ \sum_{\mu} \left[\Delta_\mu \varphi_{(c)3} \right] \left[\Delta_\mu \delta^d_{1,3} \right] + \alpha_0 \varphi_{(c)3} \delta^d_{1,3} \right\},$$

where we once again are using the notation of numerical indices for the dependencies on position, and we used the fact that the variables $\varphi_{(c)}$ are independent at all the points, so that

$$\frac{\mathfrak{d}\varphi_{(c)1}}{\mathfrak{d}\varphi_{(c)2}} = \delta^d_{1,2}.$$

Integrating the first term by parts, which does not produce any surface terms due to the periodical boundary conditions, we then use the delta functions to eliminate the sums and obtain

$$\frac{\mathfrak{d}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}} = \sum_{3} (-\Delta^2_{1,3} + \alpha_0 \delta^d_{1,3}) \varphi_{(c)3}.$$

The second functional differentiation is now immediate and results in

$$\frac{\mathfrak{d}^2\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)1}\mathfrak{d}\varphi_{(c)2}} = \sum_{3} (-\Delta^2_{1,3} + \alpha_0 \delta^d_{1,3}) \delta^d_{3,2} = -\Delta^2_{1,2} + \alpha_0 \delta^d_{1,2}.$$

We see that in this case the operator $\Box_{(c)}$ is directly related to the Euclidean Klein-Gordon operator. Note that, just as the Laplacian operator Δ^2, the operator $\Box_{(c)}$ is not diagonal. We may write the content of this result in the form of operators in configuration space,

$$\Box_{(c)1,2} = (-\Delta^2 + \alpha_0 I)_{1,2},$$

where I is the identity operator. The fact that this operator is the inverse of the propagator is translated in this language into the fact that the propagator is the Green function of the Euclidean Klein-Gordon operator, satisfying the finite-difference equation

$$\sum_{3} (-\Delta^2 + \alpha_0 I)_{1,3} g_{(c)3,2} = \delta^d_{1,2},$$

examine here, in more detail, the properties of this function, which describes how objects propagate in this model. Since propagation is in itself an important physical phenomenon, it is worth wile to focus for some time on a more detailed analysis of the structure of the propagator.

In momentum space this structure is very simple, it is just a function of the momenta that decays quadratically for large momenta. In the context of the acquisition of a better understanding of the inner workings of the quantum model, the exploration that is of most interest to us is that of the propagator in position space. The dimensionless propagator in position space,

$$g(\vec{x}_1, \vec{x}_2) = \langle \varphi(\vec{x}_1)\varphi(\vec{x}_2)\rangle,$$

is a function only of $\vec{x}_1 - \vec{x}_2$ and may be written as

$$\begin{aligned} g(\vec{x}_1 - \vec{x}_2) &= \sum_{\vec{k}} e^{-\imath \frac{2\pi}{L}\vec{k}\cdot(\vec{x}_1-\vec{x}_2)} \langle |\widetilde{\varphi}(\vec{k})|^2 \rangle \\ &= \sum_{\vec{k}} \frac{e^{-\imath \frac{2\pi}{L}\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}}{N^d[\rho^2(\vec{k}) + \alpha_0]}, \end{aligned}$$

as we saw in the derivation of equation (3.4.3). Our initial objective relative to this function is to calculate its value for $\vec{x}_1 = \vec{x}_2 = \vec{x}$, in which case we have the quantity

$$\sigma^2 = g(\vec{x} - \vec{x}) = g(\vec{0}) = \langle \varphi^2(\vec{x})\rangle,$$

a quantity that, by discrete translation invariance on the torus, is independent of position. Since we have that $\langle \varphi(\vec{x})\rangle = 0$, it follows that σ^2 is the square of the width of the distribution of values of the dimensionless field φ at a give site, that is, $\sigma = \sqrt{\sigma^2}$ is the average size of the fluctuations of the field around its average value of zero. We will refer to σ as the *local width* of the distribution of the fields. We may write for this quantity

$$\sigma^2 = \frac{1}{N^d} \sum_{\vec{k}} \frac{1}{\rho^2(\vec{k}) + \alpha_0}. \tag{4.1.1}$$

With the objective of determining whether or not this quantity has a finite limit in the continuum limit, we start by approximating it by an integral. Note that this is a mere approximation, which allows us to acquire a qualitative idea of the behavior of this quantity, and that the expression above for σ^2 does *not* converge to an integral in the continuum limit, since we are taking this limit within a finite box, where the Fourier modes and their momenta are always discrete. Since the smallest non-vanishing value for the momentum components inside the box is $2\pi/L$, the "element of volume" in momentum space is given by

$$\mathrm{d}^d p = \left(\frac{2\pi}{L}\right)^d, \quad \text{that is,} \quad \left(\frac{L}{2\pi}\right)^d \mathrm{d}^d p = 1.$$

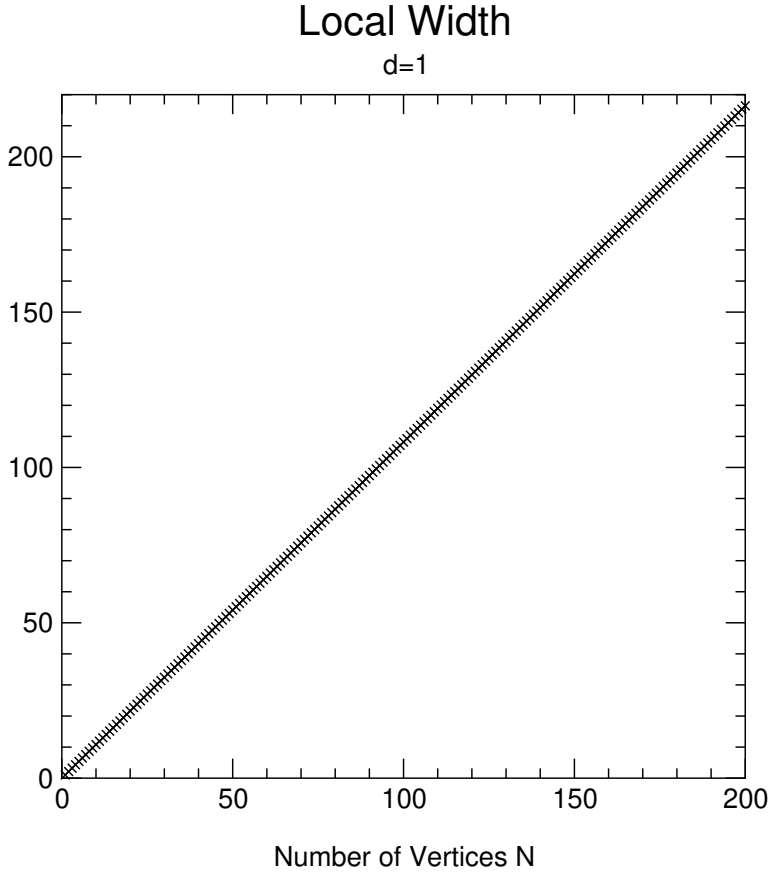

Figure 4.1.1: Behavior of the squared local width σ^2 with N in the case $d = 1$.

$$\sigma^2 \sim \frac{\Omega_{d-1}}{2^d \pi^2 (d-2)},$$

which is finite, for in our case here $d \geq 3$ and Ω_{d-1} is always a finite number different from zero, since it is the volume of a compact manifold, the surface of the d-dimensional unit sphere. For the case $d = 2$ the exponent of N vanishes, so that the factor in front of the integral neither diverges nor vanishes. It follows that in this case both the upper and the lower extremes of integration are in principle important. In this case we have $\Omega_1 = 2\pi$ and the integral results in

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

so that the upper extreme still dominates and in this case σ^2 diverges logarithmically with N, in fact a type of behavior that is very common in the case $d = 2$. In the case $d = 1$ the factor in front of the integral diverges as N, so that in this case we have the opposite of what happens in the other cases, and only the lower extreme

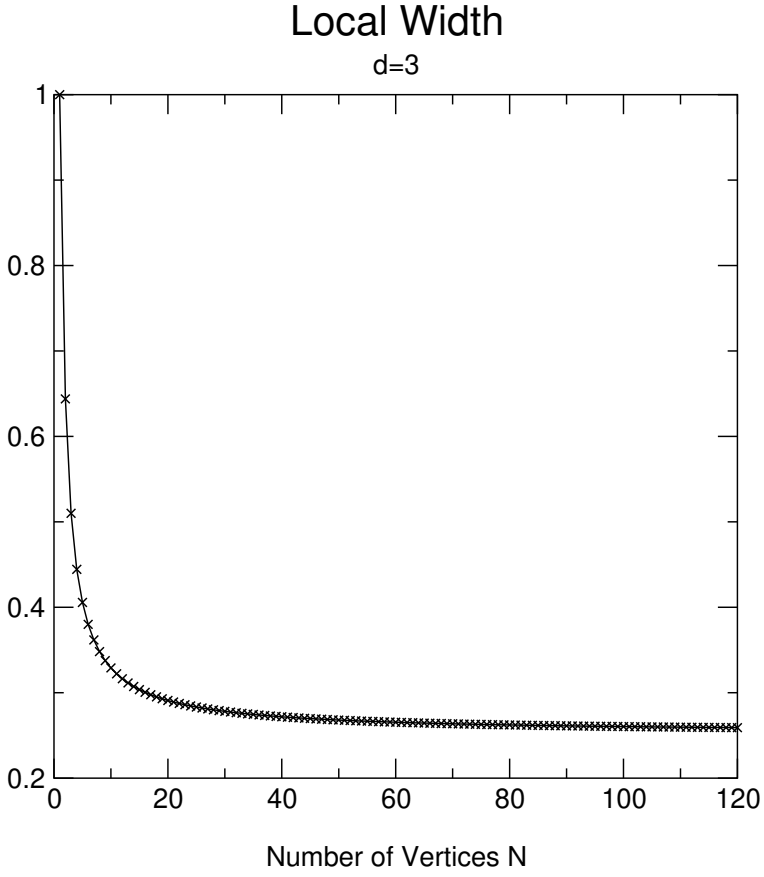

Figure 4.1.3: Behavior of the squared local width σ^2 with N in the case $d = 3$.

be emphasized that these are all just approximations that allow us to determine no more than the type of asymptotic dependency of σ^2 with N. This is still true even if we make the volume $V = L^d$ of the box go to infinity, so that the volume element $(2\pi/L)^d$ in momentum space goes to zero. The reason is that the quantity $\rho^2(\vec{k})/a^2$ that appears in the integrand only approaches p^2 if $N \to \infty$ with k_μ kept finite, while the sum over the momenta will always include terms in which $k_\mu \sim \pm N/2$. Hence, for terms close to the upper limit of the sum it is *not* true that $(\rho/a)^2$ approaches p^2. Note that for $d \geq 3$, since it is necessary that the integrals diverge in order for σ^2 not to vanish, the main contribution to the final result comes precisely from such terms. The same is true for $d = 2$, while for $d = 1$ the situation is reversed, and the main contribution comes from the lower extreme of the integral, so that in this case it is possible that the result of the approximation by the integral in fact becomes exact when we go to infinite space, if we do not make any further approximations.

For a precise calculation of the values of σ^2 in each dimension it is necessary to write programs to performs the sums on finite lattices with various sizes and then to extrapolate the results to the case $N \to \infty$. The graphs that can be found in the figures numbered from 4.1.1 to 4.1.5 show the values of σ^2 for sequences

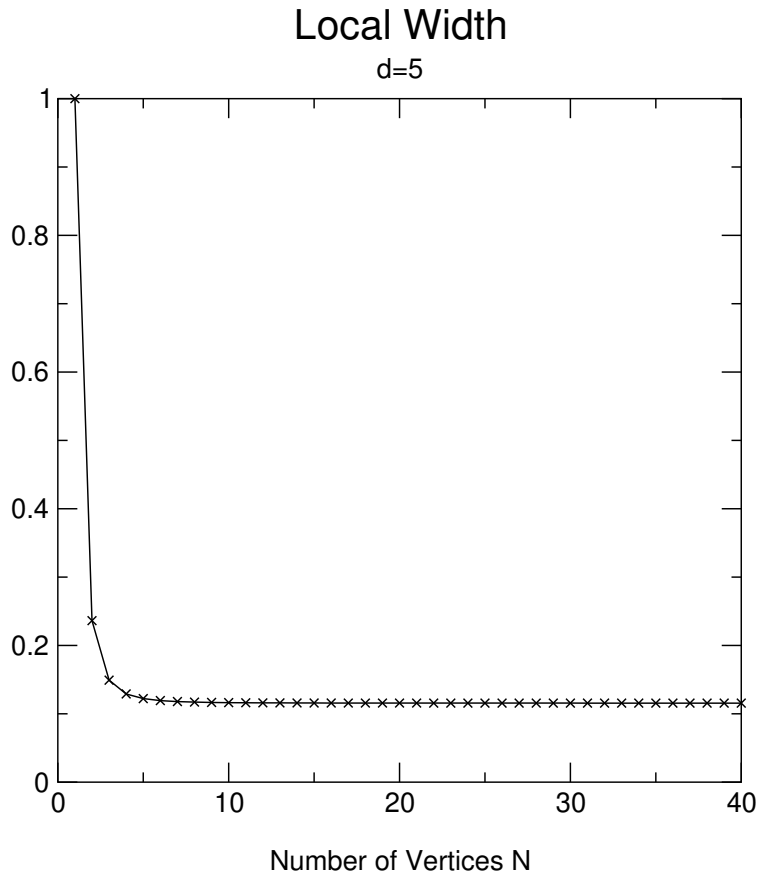

Figure 4.1.5: Behavior of the squared local width σ^2 with N in the case $d = 5$.

with the graphs of these functions that we saw before in section 3.5, which decay when $\vec{x}_1$ moves away form $\vec{x}_2$.

We will now examine the behavior of the dimensionfull versions of g and σ^2. Note that we can define a quantity Σ^2 for the dimensionfull field in a way analogous to the definition of σ^2. Given the scaling relations for the fields, we immediately have that $\Sigma^2 = a^{2-d}\sigma^2$, so that we may immediately deduce from table 4.1.1 the behavior of Σ^2. In $d = 1$ this quantity has a finite value proportional to L and for $d = 2$ it is equal to σ^2, and therefore it diverges in the same way, logarithmically. However, for $d \geq 3$ it diverges with some power of N, from which it follows that the dimensionfull field undergoes fluctuations of infinite magnitude in the continuum limit. This is the first sign indicating the extremely singular character of the behavior of the theory, and possibly the fact that the fundamental fields are not variables amenable to a direct physical interpretation.

Let us now continue our analysis by the examination of the behavior of the propagators in position space in the case in which $\vec{x}_1$ and $\vec{x}_2$ are two distinct points. Still from our scaling relations for the fields we have that those of the propagator should be $G = a^{2-d}g$, where $a = L/N$, so that we may write for G

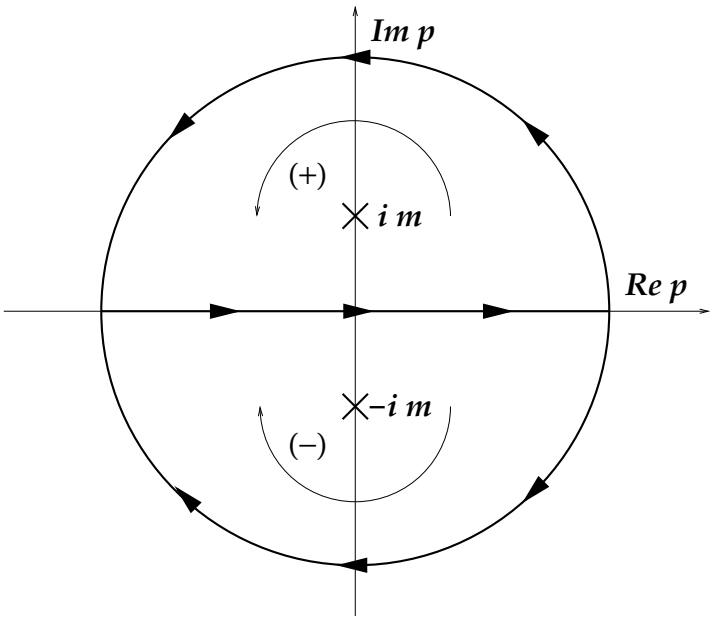

Figure 4.1.6: Integration contours in the complex p plane.

where the azimuthal angle ϕ goes from 0 to 2π and all the others go from 0 to π. Naturally, the total solid angle being a compact integration domain and the integrand a bounded function within it, the integration over the angles in (4.1.3) always gives finite results. In addition to this, as one can verify in detail in each case, the oscillations of the complex exponential cause the integration over p to converge, resulting always in a function that decays quickly for large r, as a decreasing exponential. Due to this, in this case it is always the lower integration extreme of the integral over p that dominates and, therefore, the results will depend on m_0 in any dimension d.

We will perform here the integrals in the cases $d = 1$ and $d = 3$, leaving the others to the reader (problem 4.1.7). For the time being, we restrict the discussion to the case $r \neq 0$. In the simplest case, $d = 1$, as well as in the case $d = 2$, it is really neither necessary nor useful to write the integral in the form of given in equation (4.1.3). In the case $d = 1$, with $x = x_1 - x_2$, we may calculate directly the integral in the form shown in (4.1.2),

$$G(\vec{x}_1 - \vec{x}_2) \sim \frac{1}{2\pi} \int_{-N\pi/L}^{N\pi/L} \mathrm{d}p \, \frac{e^{-\imath px}}{p^2 + m_0^2} = \frac{1}{2\pi} \int_{-N\pi/L}^{N\pi/L} \mathrm{d}p \, \frac{e^{-\imath px}}{(p - \imath m_0)(p + \imath m_0)}.$$

We may calculate this integral in the complex-p plane without difficulty, in the limit $N \to \infty$. In this case the integral runs over the real line and, if $x > 0$, we should close the circuit with an arc at infinity, of size π, in the lower half-plane, where the imaginary part of p is negative, so that the argument of the exponential, $-\imath px$, has a negative real part. Figure 4.1.6 illustrates the complex-p plane, with the integration contours and the poles of the integrand at $p = \pm \imath m_0$. In this case the integral is

d	$G(r)$	$m_0 \to 0$	$r \gg 1/m_0$
1	$\frac{1}{2m_0}\, e^{-m_0 r}$	$\to \infty$	$= \frac{1}{2m_0}\, e^{-m_0 r}$
2	$\frac{1}{2\pi}\mathrm{K}_0(m_0 r)$	$\to \infty$	$\sim \frac{1}{(8\pi m_0 r)^{1/2}}\, e^{-m_0 r}$
3	$\frac{1}{4\pi r}\, e^{-m_0 r}$	$\to \frac{1}{4\pi r}$	$= \frac{1}{4\pi r}\, e^{-m_0 r}$
4	$\frac{m_0}{4\pi^2 r}\mathrm{K}_1(m_0 r)$	$\to \frac{1}{4\pi^2 r^2}$	$\sim \frac{m_0^{1/2}}{2(2\pi r)^{3/2}}\, e^{-m_0 r}$
5	$\frac{1+m_0 r}{8\pi^2 r^3}\, e^{-m_0 r}$	$\to \frac{1}{8\pi^2 r^3}$	$\sim \frac{m_0}{8\pi^2 r^2}\, e^{-m_0 r}$

Table 4.1.2: Table of correlation functions in the continuum limit.

$$\begin{aligned} \frac{1}{8\pi^2 \imath r}\int_{-\infty}^{\infty} \mathrm{d}p\, \frac{p\, e^{\imath p r}}{(p-\imath m_0)(p+\imath m_0)} &= \frac{e^{-m_0 r}}{8\pi r}, \\ \frac{1}{8\pi^2 \imath r}\int_{-\infty}^{\infty} \mathrm{d}p\, \frac{p\, e^{-\imath p r}}{(p-\imath m_0)(p+\imath m_0)} &= \frac{e^{-m_0 r}}{8\pi r}. \end{aligned}$$

With this, we have the final result

$$G(r) = \frac{e^{-m_0 r}}{4\pi r}.$$

This function is the Yukawa potential that, in the limit $m_0 = 0$, reduces to the Coulomb potential of electrostatics. Just as in the case $d = 1$, for $m_0 \neq 0$ this function also falls off exponentially for large values of r, and it is finite at all points *except at $r = 0$, where it diverges*. Once more this is compatible with our previous calculation for $g(0)$, since we saw that $g(0)$ is finite and, for $d = 3$, we have that $G = g/a$, which means that $G(0)$ diverges when $N \to \infty$ and therefore $a \to 0$. In fact, one can verify that $G(r)$ is finite at the origin only for $d = 1$, and that in all the other cases, starting with $d = 2$, it diverges, typically with a negative power of r which is characteristic of each dimension d. The functions G calculated as in the examples above, for various dimensions d, are given in the table 4.1.2, which also contains the corresponding asymptotic behaviors for $r \to \infty$, that is, for $r \gg 1/m_0$, as well as for $m_0 \to 0$. The symbols K_0 and K_1 in this table are Bessel functions.

As one can see, these functions in infinite space have relatively simple forms in terms of known functions. In a finite box the form of the correlation functions is not so simple, and in general cannot be written in a simple way in terms of known functions, but only as infinite series (problem 4.1.8). However, they continue to be finite at all points $\vec{x}_2$ different from $\vec{x}_1$, so that there are no important qualitative differences between the two cases. One observes that the propagators in the cases

In order to have $m_0 \to 0$ in the continuum limit it suffices to make α_0 vary with N as

$$\alpha_0 = \frac{C}{N^{2+\varepsilon}},$$

where C is some positive constant and ε some positive number, which we imagine to be small. In this case the zero-mode term is

$$\frac{1}{N^d}\,\frac{N^{2+\varepsilon}}{C} = \frac{1}{C\; N^{d-2-\varepsilon}}.$$

We see that this term continues to go to zero for $d \geq 3$, so long as ε is smaller than 1. For $d = 2$, however, it becomes divergent as N^{ε}, that is, faster than the sum, while in $d = 1$ the situation is similar, since in this case it diverges as $N^{1+\varepsilon}$, also faster than the sum. Therefore, we see that for $d = 1$ and $d = 2$ σ^2 presents in fact infrared divergences similar to those of $G(r)$, when we make $m_0 \to 0$. These facts are peculiar of these low dimensions and should now worry us. The important thing is that there are no divergences in the expression of σ^2 in the cases $d \geq 3$, when we make m_0 go to zero, so that the results we obtained before continue to hold in these dimensions. This is not surprising because, as we discussed before, for $d \geq 3$ one can see that the main contributions to σ^2 come from the large-momentum terms of the sum, so that the results should not depend on m_0, which is a quantity characteristic of the low-momentum region. Since σ^2 cannot depend at all on m_0 under these conditions, it is clear that its behavior should not change when we make $m_0 \to 0$.

The graphs we showed before to illustrate the behavior of σ^2 as a function of N in each dimension were obtained using the value 1 for m_0, but we see now that this is not really a relevant fact. For the cases $d \geq 3$, the only ones in which σ^2 converges to a finite value in the limit, one can show (problem 4.1.9) that in fact the limits are completely independent of m_0.

We will end this section using the facts established do far in order to show a rather surprising fact relating to the behavior of the two-point correlation functions in quantum field theory. If we recall the basic definition of the correlation function in the context of statistical mechanics, discussed in section 3.2, we see that it does not really make any difference if we discuss the correlations in terms of the dimensionless function g or in terms of the dimensionfull function G, because in any case we should analyze the statistical correlations among the fields at various points by means of the homogeneous correlation function

$$\mathfrak{f}(r) = \frac{g(r)}{g(0)} = \frac{G(r)}{G(0)}.$$

We can calculate this function on finite lattices without any trouble and then take the continuum limit. Let us examine then how $\mathfrak{f}(r)$ behaves in this limit. It is clear that, by definition, $\mathfrak{f}(0)$ is always equal to one, both on finite lattices and in the continuum limit. For other values of r we saw that $G(r)$ is finite in the limit, while $G(0)$ diverges. It follows therefore that *in the continuum limit* $\mathfrak{f}(r)$ *vanishes for all*

Riemann $\zeta(z)$ function in terms of a sum of $1/k^z$ and look up in a table of integrals its value for $z = 2$.

4.1.2. From the result of the problem 4.1.1 show that Σ^2, as defined in the text, is bounded by a finite real number so long as L and m_0 are finite and not zero,

$$\Sigma^2 \leq \frac{L}{12} + \frac{L}{(m_0 L)^2},$$

as reported in one of the tables given in the text.

4.1.3. Write a program to calculate Σ'^2 numerically for lattices with increasing sizes. From its results produce an extrapolation to the limit $N \to \infty$ with constant m_0, and show that the result of problem 4.1.1 is exact within your numerical precision.

4.1.4. ($\star$) Consider the quantity Σ^2 in the case $d = 1$, in a finite interval of length L, for $m_0 \neq 0$ and an arbitrary N, which implies that $\alpha_0 \neq 0$ on each finite lattice, leaving open, however, the possibility that $\alpha_0 \to 0$ when $N \to \infty$. Build, for each finite N, two integrals I_M and I_m over the coordinates k of momentum space, extending them to real values, so that I_M is strictly larger and I_m strictly smaller than the sum that defines Σ^2. Calculate the integrals, take after that the limit $N \to \infty$ and demonstrate in this way that Σ^2 has a finite and non-vanishing limit in the continuum limit, assuming that $m_0 \neq 0$ in the limit.

4.1.5. Write a program to calculate the local width σ^2 of the fields in the case $d = 2$. Use the program to calculate $\sigma^2(N)$ for the values of N shown in the graph given in the text and plot the results as a function of $\ln(N)$, with constant m_0, verifying in this way that the results display indeed a logarithmic divergence in the continuum limit.

4.1.6. ($\star$) Write a program to calculate the local width σ^2 of the fields in the case $d = 3$. Use the program to calculate $\sigma^2(N)$ for as many values of N as possible with a reasonable amount of computer time, and make a numerical fitting of the resulting function to an expression of the form

$$f(N) = f_0 + \frac{f_1}{N^p},$$

where f_0, f_1 and p are unknown constants. Repeat the fitting for several subsets of the data, each with an increasing maximum value of N, in some convenient way, thus obtaining successive estimates for these three quantities, for increasing values of N. In this fashion, obtain an extrapolation of the result for these three quantities to the continuum limit $N \to \infty$, with constant m_0. Hint: try to start your fitting with $p \sim 1$, $f_0 \sim 1/4$ and $f_1 \sim 1$ and remember that the important thing is to adjust the function for large values of N.

a qualitative way our conception of the role played in the theory by mathematical concepts of a topological nature; it leads us in an emphatic way to the idea that only the block variables to be discussed later can actually be physical observables within the theory; it strongly suggests new quantization procedures on the lattice, which are of a very geometrical nature, for theories that have a curved internal symmetry space, as is the case for the very important non-Abelian gauge theories. Hence, this is a central and unifying concept, related to many of the difficulties that appear in the theory, difficulties that usually cause great confusion, specially among those trying to learn it.

In order to examine this important concept we must start by discussing what we mean by continuity of the configurations, because we will be taking the continuum limit from finite lattices, which are discrete mathematical objects in which there is no natural concept of continuity. Usually functions $\varphi(\vec{x})$, mappings from $\mathbb{R}^d$ into $\mathbb{R}$, are considered continuous in the direction μ of the domain if the finite difference

$$\Delta_\mu \varphi(\vec{x}) = \varphi(\vec{x} + \varepsilon \hat{x}_\mu) - \varphi(\vec{x})$$

approaches zero when $\varepsilon \to 0$ both by positive and by negative values. However, in quantum field theories defined by means of Euclidean functional integrals only averages of functionals of the fields on some particular ensemble can be calculated and used to extract the physically relevant properties of the theories. It is clear that, since the fields at sites are random variables that undergo constant fluctuations including changes of sign, the direct expectation value of the difference $\langle \Delta_\mu \varphi(\vec{x}) \rangle$ will be of no use to determine the character of continuity or discontinuity of the fields because, even if these differences never vanish, they can change sign, causing the average to vanish even for discontinuous fields. In fact, this average can be written as

$$\langle \Delta_\mu \varphi(\vec{x}) \rangle = \langle \varphi(\vec{x} + \varepsilon \hat{x}_\mu) \rangle - \langle \varphi(\vec{x}) \rangle,$$

so that its vanishing would only mean that the expectation value $\langle \varphi \rangle$ of the field is independent of position. It is clear that we need a quantity that vanishes only when the field is continuous, that is, of an observable that cannot change sign. In this situation we may use the quantity $\langle [\Delta_\mu \varphi(\vec{x})]^2 \rangle$, which is a measure of the average "jump" and hence of the average discontinuity of the fields in the direction μ, in order to define what we mean by continuity (problem 4.2.1). The fields will be considered typically continuous if this quantity vanishes when we make ε tend to zero. To be more precise, the configurations of $\varphi(\vec{x})$ are predominantly continuous at $\vec{x}$, in terms of the measure of the action, if and only if

$$\lim_{\varepsilon \to 0} \langle [\Delta_\mu \varphi(\vec{x})]^2 \rangle = 0.$$

However, this definition still does now exhaust the issue, because there is more than one form to take this limit. In the formulation of quantum field theory on the lattice, ε has to be some multiple of the fundamental lattice spacing a. The continuity of

$$
\begin{aligned}
&= -\sum_{\vec{k}}\sum_{\vec{k}'} \frac{\delta^d(\vec{k},-\vec{k}')}{N^d[\rho^2(\vec{k})+\alpha_0]}\ \rho_\mu(k_\mu)\ \rho_\mu(k'_\mu)\ e^{\imath\frac{\pi}{N}(k_\mu+k'_\mu)}\ e^{\imath\frac{2\pi}{N}(\vec{k}+\vec{k}')\cdot\vec{n}} \\
&= \frac{1}{N^d}\sum_{\vec{k}} \frac{\rho_\mu^2(k_\mu)}{\rho^2(\vec{k})+\alpha_0},
\end{aligned}
$$

where we substituted the result for the propagator and used the delta function to eliminate one of the sums over the momenta. Note that there is no sum over μ in this expression. Since both the lattice and this observable are symmetrical by permutations of the various directions μ, we may write this result in terms of $\rho^2(\vec{k}) = \sum_\mu \rho_\mu^2(k_\mu)$ as

$$
\langle[\Delta_\mu\varphi(\vec{n})]^2\rangle_N = \frac{1}{dN^d}\sum_{\vec{k}} \frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0}.
$$

It is not difficult to find upper and lower bounds to the sum that appears in this expression, which will hold for any value of N. In order to find an upper bound it suffices to take off the positive constant α_0 that appear in the denominator. It is interesting to note that, since $\alpha_0 \to 0$ in the continuum limit, it is reasonable to think that this change does not in fact affect the result in the limit. In order to find a lower bound it suffices to exchange the $\rho^2(\vec{k})$ that appears in the denominator by its maximum value, which is $4d$. With this we obtain the relations

$$
\begin{aligned}
\frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{4d+\alpha_0} \quad &< \quad \frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0} \quad \leq \quad \frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})} \quad \Rightarrow \\
\frac{1}{4d+\alpha_0}\frac{1}{dN^d}\sum_{\vec{k}}\rho^2(\vec{k}) \quad &< \quad \frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0} \quad \leq \quad \frac{1}{dN^d}\sum_{\vec{k}}1 \quad \Rightarrow \\
\frac{1}{4d+\alpha_0}\frac{1}{N^d}\sum_{\vec{k}}\rho_\mu^2(k_\mu) \quad &< \quad \frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0} \quad \leq \quad \frac{1}{d} \quad \Rightarrow \\
\frac{1}{4d+\alpha_0}\frac{1}{N}\sum_{k_\mu}\rho_\mu^2(k_\mu) \quad &< \quad \frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0} \quad \leq \quad \frac{1}{d} \quad .
\end{aligned}
$$

The sum that remains in the case of the lower bound can be calculated (problem 4.2.3) by the decomposition of the sines in terms of complex exponentials, followed by the use of the orthogonality and completeness relations. The result is simply the number $2N$, so that we have the final result for our sum,

$$
\frac{2}{4d+\alpha_0} < \frac{1}{dN^d}\sum_{\vec{k}}\frac{\rho^2(\vec{k})}{\rho^2(\vec{k})+\alpha_0} \leq \frac{1}{d}.
$$

In the limit $N \to \infty$ we have that $\alpha_0 \to 0$ and therefore we can write, recalling that there is no sum over μ,

for both the dimensionless field and the dimensionfull field, since they are in fact equal in this case,

$$\langle [\Delta_\mu \phi]^2 \rangle \to \frac{1}{2},$$

showing that in this case the discontinuities exist but are finite. In dimensions $d = 3$ and larger the discontinuities of the dimensionfull field diverge with powers that increase with the dimension,

$$\langle [\Delta_\mu \phi]^2 \rangle \sim \frac{1}{a^{d-2} d} \to \infty.$$

We see here two very important basic facts: first, that there is a *qualitative difference* between the behavior of quantum mechanics (the case $d = 1$) and the behavior of the quantum theory of fields (the cases $d > 1$); second, confirming what was already discussed in section 4.1, the fundamental dimensionfull fields display *extreme fluctuations* in the continuum limit, which puts immediately in great doubt any possibility that they may have any direct physical significance as observables. We will now explore a consequence of these facts that is directly related to the action. Since the action $S[\varphi]$ is itself a functional of the fields, we may consider the calculation of its expectation value $\langle S \rangle$. The result may help us to understand the behavior of the theory from another point of view. We know that the classical solution of the theory is the one that minimizes the action, whose minimum in the case of the action S_0 of the free scalar field is zero. This is the value that maximizes the relative statistical weight $\exp(-S)$ of the configuration within the ensemble. The average value of S will tell us something about the typical relative weights of the configurations that contribute in a dominant way to the averages. For the time being, we will limit ourselves to the calculation of the expectation value of the kinetic part S_K of the action S_0 of the free theory, the part that involves the derivatives,

$$S_K = \frac{1}{2} \sum_\ell (\Delta_\ell \varphi)^2,$$

which also appears in any model involving scalar fields. The expectation value of S_K is given by

$$\langle S_K \rangle = \frac{1}{2} \sum_\ell \langle (\Delta_\ell \varphi)^2 \rangle.$$

where we already know that the expectation value of the square of the finite difference converges to $1/d$ in the continuum limit. Since this limit does not depend on the link at which it is being calculated and there are dN^d links in the lattice, we obtain immediately that

$$\langle S_K \rangle \sim \frac{1}{2} N^d \to \infty,$$

seem surprising at first sight, but this surprise is due only to the fact that, when we examine these relative statistical weights, we are leaving aside another very important factor, the *number of configurations* with each value of the weight that exist in configuration space and that, therefore, contribute to the averages. Although the discontinuous configurations have, individually, negligible statistical weights as compared to the weights of continuous configurations such as the classical solution, their number is *immensely* larger, so that they end up dominating the situation completely. It becomes quite clear that the quantum-mechanical concept of the semi-classical approximation will have to be revised before one considers its application in quantum field theory. In future volumes we will also see that divergences like these are intimately connected to the divergences that appear pervasively in perturbation theory.

We might ask ourselves if this behavior could be just a peculiarity of the theory of the free scalar field. In future volumes we will see that it also applies to other free fields such as, for example, the free vector field of electromagnetism without sources, that is, without charges and currents. For the case of free electrodynamics this can be found in reference [1]. In the case of non-linear models, we do not know how to do a direct analytical verification, being in this case limited to extrapolations from computer simulations on finite lattices. We may, however, argue as follows to the effect that this is a property that must also hold in these models. The non-linear models in general contain a real parameter λ, the coupling constant, which is such that they converge to the free theory when we make λ go to zero. In fact, it is important for the physical interpretation of these models that they have the free theory as a smooth limit for $\lambda \to 0$. The property of discontinuity of the fields that we examined in this section depends only on the facts that $\langle(\Delta_\ell\varphi)^2\rangle$ and $\langle\varphi^2(s)\rangle$ have non-vanishing finite values in the limit. It is very reasonable to think, then, that they will still be finite and non-vanishing for $\lambda \neq 0$, although their values might vary with λ, so that the $\lambda \to 0$ limits of the expectation values of these observables may be smooth ones. In fact, despite the strong fluctuations and discontinuities of the fields, usually the expectation values are smooth or at least continuous functions of the parameters of the models.

Hence we see that the main facts described here are, in all probability, general properties of all quantum field theories. As we progress in our exploration of the subject, we will continue to verify and solidify this important notion.

Problems

4.2.1. Show, in the classical theory of fields, that the criterion that the quantity

$$[\Delta_\mu\varphi(\vec{x})]^2 = [\varphi(\vec{x} + \varepsilon\hat{x}_\mu) - \varphi(\vec{x})]^2$$

goes to zero when $\varepsilon \to 0$, by either positive or negative values, is equivalent to the condition that $\Delta_\mu\varphi(\vec{x}) \to 0$.

(a) Using the fact that the action is quadratic on the fields, and hence that it is homogeneous of degree 2 on the fields, show that the distribution of the theory can be written as

$$\int_{\Omega} [\mathbf{d}\varphi]\; e^{-S_0} = Z_0\; S_0^{\frac{N^d}{2}-1}\; e^{-S_0}\; \mathrm{d}S_0,$$

where Z_0 is a constant and we integrate over the manifold Ω, a kind of solid angle in configuration space, described by all the variables except S_0, which is a kind of radial variable.

(b) Defining the action per site by $s_0 = S_0/N^d$ and using the distribution in terms of S_0 given above, show that we have for its average value $\langle s_0 \rangle = 1/2$, which implies that $\langle S_0 \rangle = N^d/2$ diverges, as was seen in the text. Note that the integrals that appear can be written as Γ functions.

(c) Calculate also the width of the distribution of values of s_0, showing that $\langle s_0^2 \rangle - \langle s_0 \rangle^2 = 1/(2N^d)$. This quantity goes to zero in the continuum limit and this fact shows that the distribution of values of s_0 becomes a delta function centered at the value $1/2$, in that limit. This is another way to see that the continuous configurations, for which $s_0 = 0$, do not contribute to the expectation values of the theory in the continuum limit, being therefore of zero measure.

4.3 Block Variables and Observables

Block variables are defined as averages of some type, over the fields contained within finite regions of space-time, which we call blocks. The name comes from the realization of statistical-mechanic models on the lattice, where the regions consist of block of sites, having been introduced by Kadanoff in the study of statistical systems involving spins. In the example we will study here the average at issue will be a simple arithmetic average of the fields within the blocks but, in general, some other type of linear or even non-linear superposition may be involved. The block variables and the corresponding systems of linear superposition that define them play a central role in the definition of quantum field theories, because they determine the types of physical observables that can, in fact, be measured.

If we think about how we would go about measuring the instantaneous value of the field at a certain point in space-time, in the continuum limit, it will immediately become clear that we would not be able to do it at all. In order to do this it would be necessary to use as the instrument of measurement some object that could be completely localized at the point in question, so that we may detect exclusively the field at that point. However, the wave-like nature of all objects existing in nature, added to the uncertainty principle of quantum mechanics (or, equivalently, to the simple uncertainty principle of classical wave physics [2]), implies that this

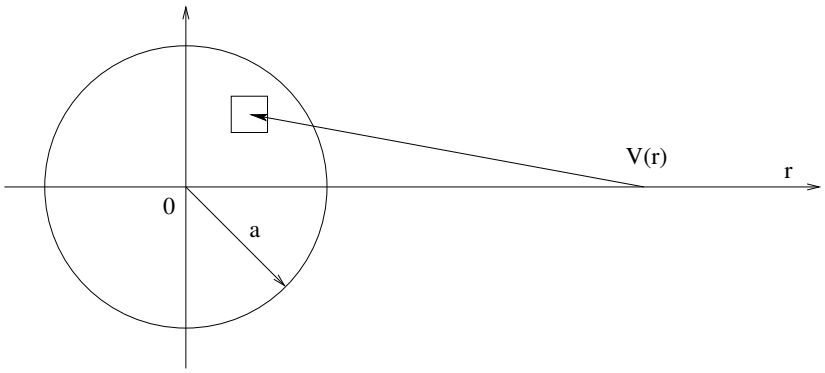

Figure 4.3.1: The problem of the calculation of the gravitational potential of a homogeneous spherical body.

field, by means of a judicious choice of the volume V_r of the blocks, and then discuss the theory in terms of these block variables, for all phenomena in the theory which are below that energy limit. In fact, one seldom does this, because usually the theory acquires a much more complex form when written in terms of these block variables, but in principle we may discuss the n-point correlation functions for these variables, in a way similar to the discussion of the correlation functions of the fundamental field,

$$g_r(\vec{n}_1, \ldots, \vec{n}_n) = \langle \bar{\varphi}(\vec{n}_1) \ldots \bar{\varphi}(\vec{n}_n) \rangle.$$

We will examine here in detail only the case of the two-point function in the free theory, that is, the block propagator. This will be useful to develop our understanding of the roles played by the dimensionfull and dimensionless versions of the fields, as well as to illustrate the reasons due to which we use, most of the time, the point variables rather than the block variables for the development of the theory, although the two-point function of these variables in position space has a singular behavior at the origin, in the continuum limit.

Let us consider then the calculation of the two-point function for block variables. Our objective here will be to verify how the block variables are correlated for short and long distances, relative to the size of the blocks. We will do the calculation both in position space and in momentum space, and in this second case we will be particularly interested in verifying whether or not the block propagator has a pole at the position of the renormalized mass, as is the case for the usual renormalized propagator that appears in perturbation theory. Observe that the usual renormalized propagator, written in terms of the fundamental field, is *not* the same as the block-renormalized propagator. The fact that both are referred to as "renormalized propagators" is just an example of the use of the term "renormalized" for multiple different ends. As we shall see, these two propagators have similar behavior for large distances and small momenta, but their behavior for short distances and large momenta is *very* different.

The calculations related to the block propagator will be done in the spirit of the

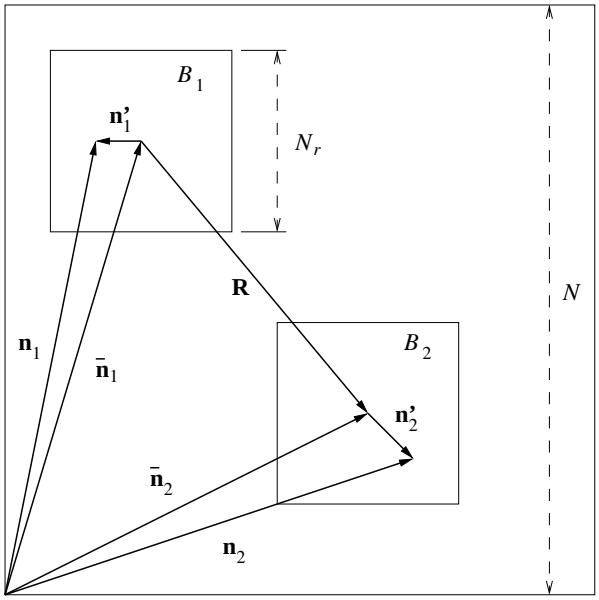

Figure 4.3.3: A cubical lattice with identical cubical blocks.

Consider then the free scalar field in a cubical d-dimensional lattice with N^d sites and periodical boundary conditions. Consider also in this lattice cubical blocks of sites, each with N_r^d sites and $N_r = N/r$ sites along each direction, for some number r such that $1 \leq r \leq N$. The geometrical situation is illustrated in figure 4.3.3. For simplicity of notation, in this section the vectors $\vec{n}$ and $\vec{k}$ will be represented by $\mathbf{n}$ and $\mathbf{k}$, while an upper bar will denote average over a block. The block variables are defined by arithmetical averages over the blocks. In terms of the dimensionless fields, for a block B centered at the position $\mathbf{n}$, we have

$$\bar{\varphi}(\bar{\mathbf{n}}) = \frac{1}{N_r^d} \sum_{\mathbf{n} \in B} \varphi(\mathbf{n}),$$

where the position $\bar{\mathbf{n}}$ of the block is given by

$$\bar{\mathbf{n}} = \frac{1}{N_r^d} \sum_{\mathbf{n} \in B} \mathbf{n}.$$

Note that, unlike $\mathbf{n}$, $\bar{\mathbf{n}}$ does not necessarily have integer components, depending on how the blocks are chosen. If we so wish, we may simplify this situation choosing the blocks in a more symmetrical way, with odd N_r and center at a site of the original lattice, but this is not actually important or necessary. The dimensionless block propagator in position space is given by

$$g_r(\bar{\mathbf{n}}_1, \bar{\mathbf{n}}_2) = \langle \bar{\varphi}(\bar{\mathbf{n}}_1) \bar{\varphi}(\bar{\mathbf{n}}_2) \rangle,$$

relating two blocks, a block B_1 at $\bar{\mathbf{n}}_1$ and another block B_2 at $\bar{\mathbf{n}}_2$. We may write this propagator in terms of the fundamental field as

where the form factor is defined within an arbitrary block B as

$$f_r^{(d)}(\mathbf{k}) = \frac{1}{N_r^d} \sum_{\mathbf{n}' \in B} e^{-\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{n}'}.$$

From the expression above for g_r we may read immediately its Fourier transform,

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

which is, therefore, the block propagator in momentum space. Note that, unlike what happens in position space, in momentum space no change is needed in the coordinates $\mathbf{k}$.

We have, then, the block propagator dully calculated, in terms of $f_r^{(d)}$, both in momentum space and in position space. In order to examine the properties of this propagator, we must first examine the properties of the form factor $f_r^{(d)}$. Observe, in the first place, that since $f_r^{(d)}$ is an average of complex phases it is always true that $|f_r^{(d)}(\mathbf{k})| \leq 1$, from which it follows that, in momentum space, the block propagator is always smaller than or equal to the propagator of the fundamental field. Observe also that, for simple cubical blocks like the ones we are using here,

$$\begin{aligned} f_r^{(d)}(\mathbf{k}) &= \frac{1}{N_r^d} \sum_{\mathbf{n}' \in B} e^{-\imath \frac{2\pi}{N} \mathbf{k} \cdot \mathbf{n}'} \\ &= \prod_{\mu=1}^{d} \left(\frac{1}{N_r} \sum_{n'_\mu \in B} e^{-\imath \frac{2\pi}{N} k_\mu n'_\mu} \right) \\ &= \prod_{\mu=1}^{d} f_r^{(1)}(k_\mu), \end{aligned}$$

so that it is enough to calculate $f_r^{(1)}(k) = f_r(k)$ in order to find out how the form factor behaves. Given the system of internal coordinates that we adopted for the blocks, we may write explicitly

$$f_r(k) = \frac{1}{N_r} \sum_{n' = -(N_r-1)/2}^{(N_r-1)/2} e^{-\imath \frac{2\pi}{N} k n'},$$

where n' spans N_r consecutive values, being half-integer if N_r is even and integer if N_r is odd, as is the case for a symmetrical choice of the blocks around the sites. We may execute the sum using the formula for the sum of a geometrical progression,

$$\begin{aligned} f_r(k) &= \frac{1}{N_r} \frac{e^{-\imath \frac{2\pi}{N} k \frac{N_r-1}{2}} e^{-\imath \frac{2\pi}{N} k} - e^{\imath \frac{2\pi}{N} k \frac{N_r-1}{2}}}{e^{-\imath \frac{2\pi}{N} k} - 1} \\ &= \frac{1}{N_r} \frac{e^{-\imath \frac{\pi}{N} k N_r} - e^{\imath \frac{\pi}{N} k N_r}}{e^{-\imath \frac{\pi}{N} k} - e^{\imath \frac{\pi}{N} k}} \end{aligned}$$

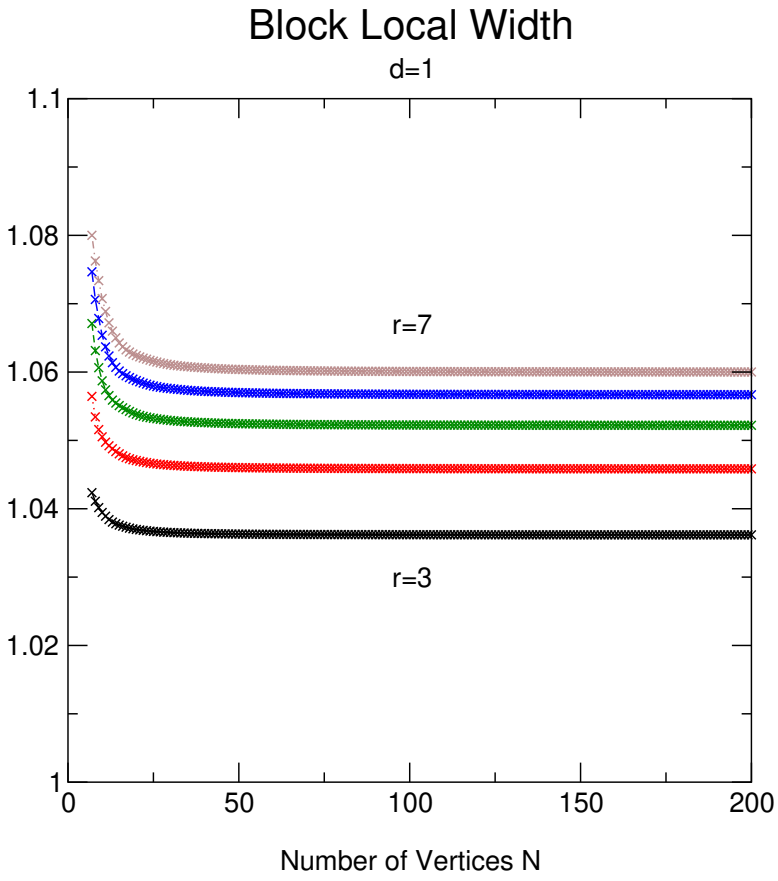

Figure 4.3.5: Behavior of the local block width as a function of N, for $d = 1$.

the high-frequency modes in the momentum space of the lattice. In position space this suppression has the effect of eliminating the singularity of the propagator at the origin, corresponding to a smearing of the fields by the blocking process. Figure 4.3.4 shows the fundamental propagator and the block propagator, on a logarithmic scale, along one of the directions in momentum space. The normalizations of the two propagators are arbitrary but consistent with each other. The graph is the same for any dimension d. One can clearly see the strong suppression of the block propagator for large momenta, as well as its oscillations due to resonances with the internal modes of the blocks.

We would like to discuss the results for g_r and $\widetilde{g}_r$ in two different limits, for $R \gg N_r$ and for $R = 0$. The first case turns out to be much simpler and we may discuss it directly from equation (4.3.1). If $R \gg N_r$ then it follows that $R \gg n_1'$ and $R \gg n_2'$ and we may neglect $\mathbf{n}_1'$ and $\mathbf{n}_2'$ in that equation, which makes $f_r = 1$ in equation (4.3.2) and therefore results in

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

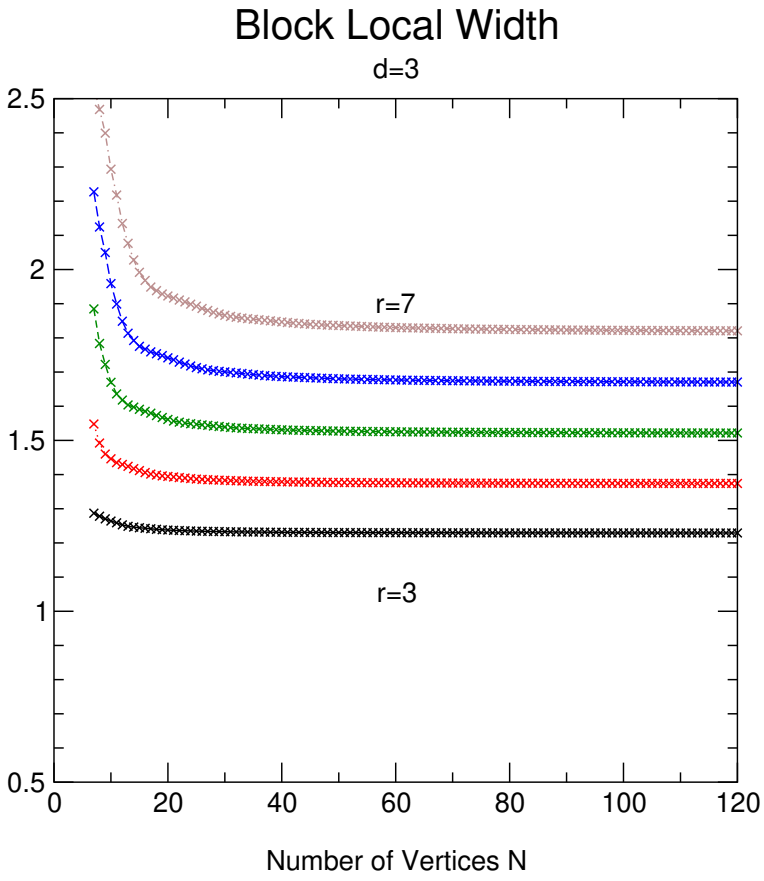

Figure 4.3.7: Behavior of the local block width as a function of N, for $d = 3$.

diverges at the origin. We should now verify how this block propagator behaves at the origin. Its value $G_r(\mathbf{0}) = \langle \bar{\phi}^2 \rangle$ at the origin is related to the average value of the fluctuations of the block variables, because since $\langle \phi \rangle = 0$ and the block field is a simple arithmetical average of the fundamental field over the block, it follows that we also have $\langle \bar{\phi} \rangle = 0$. The block propagator at the origin is given by

$$G_r(\mathbf{0}) = \Sigma_r^2 = \frac{1}{N^2 L^{d-2}} \sum_{\mathbf{k}} \frac{\left| f_r^{(d)}(\mathbf{k}) \right|^2}{\rho^2(\mathbf{k}) + \alpha_0} = \frac{1}{L^{d-2}} \sigma_r^2,$$

where Σ_r^2 is the local block width. In the graphs contained in the figures from 4.3.5 to 4.3.9 we present the corresponding dimensionless quantity σ_r^2, which is proportional to Σ_r^2 in finite boxes, with values from 3 to 7 for the ratio r between the sizes of the lattice and the blocks, for a mass $m_0 = N^2 \alpha_0 = 1$, in dimensions from $d = 1$ to $d = 5$, for sequences of lattices of increasing sizes.

We see that, in all cases, $G_r(\mathbf{0})$ converges to a finite value for each value of r, there being therefore no divergence at the origin. These values increase with r, meaning that, the smaller the blocks, the larger the fluctuations of the block

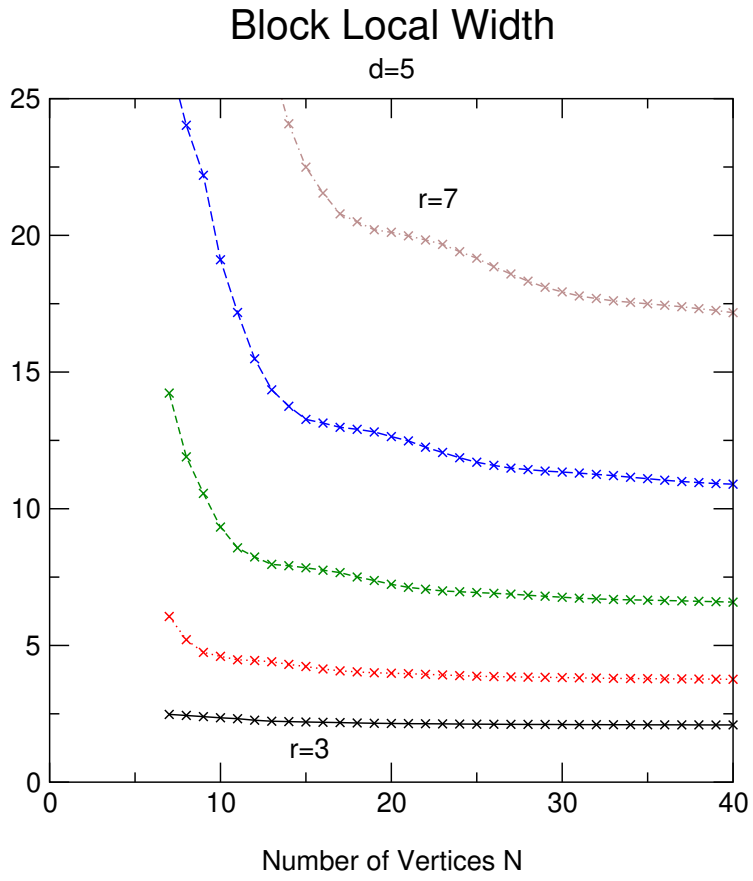

Figure 4.3.9: Behavior of the local block width as a function of N, for $d = 5$.

$$\mathfrak{f}_r(\mathbf{R}) = \frac{g_r(\mathbf{R})}{g_r(\mathbf{0})} = \frac{G_r(\mathbf{R})}{G_r(\mathbf{0})}.$$

The graphs contained in figures from 4.3.10 to 4.3.13 show the homogeneous correlation functions $\mathfrak{f}(\mathbf{R})$ calculated along one direction of the lattice, for dimensions d from 1 to 4, with $L = 1$, $m_0 = N^2\alpha_0 = 3$, $r = 5$ and different values of N in each case. We also put in these graphs parts of the corresponding dimensionfull propagators of the fundamental field in position space, which are divergent at the origin for $d \geq 2$, calculated for the same values of the parameters d, L, m_0 and N, and normalized consistently with $\mathfrak{f}(\mathbf{R})$, so as to permit the comparison of the results.

We see that, in general, the block propagator is smaller than the fundamental propagator, particularly near the origin, although this relation can be reversed in a slight way for larger values or R, specially for low dimensions, in which the infrared effects are more important. We see also that in the continuum limit $G_r(\mathbf{R})$ tends to a finite, continuous and differentiable function, at all points. One might be led to ask how can this happen, how is it possible that there are variables correlated

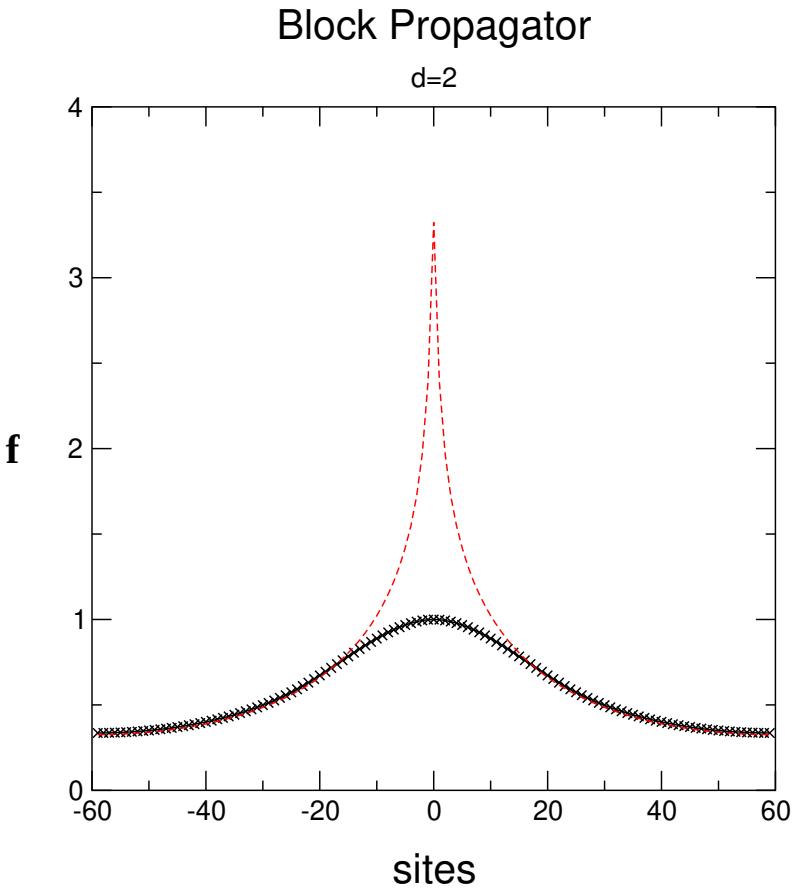

Figure 4.3.11: Block propagator in position space, for $d = 2$.

variables. For distances which are large compared to the size of the blocks, the propagator of the fundamental field coincides with the block propagator and we may use it directly to extract the physical results from the theory. We may say that the fundamental field encodes the information about how the models behave in *all* energy scales, from zero to infinity, but that in order to measure physical quantities it is necessary to define beforehand what is the proper energy scale of the physical situation one is dealing with, and then to choose block variables of appropriate size.

Note that the block variables do not necessarily have to be associated to cubical blocks centered at each point. Of course it is not essential that the blocks have any given form, they may be cubical, spherical, or of any other form adequate to each situation. Going even beyond that, the block variables may even be objects of a quite different nature such as, for example, the Fourier components of the fundamental field themselves. What matters is that they involve the superposition of an ever increasing number of values of the field as we take the continuum limit, as is the case for the Fourier components, and that there exist for them a fixed maximum limit for the momenta, as is the case for the Fourier transforms for fixed given momenta, which do not increase in the limit. Hence we see that the description in terms of

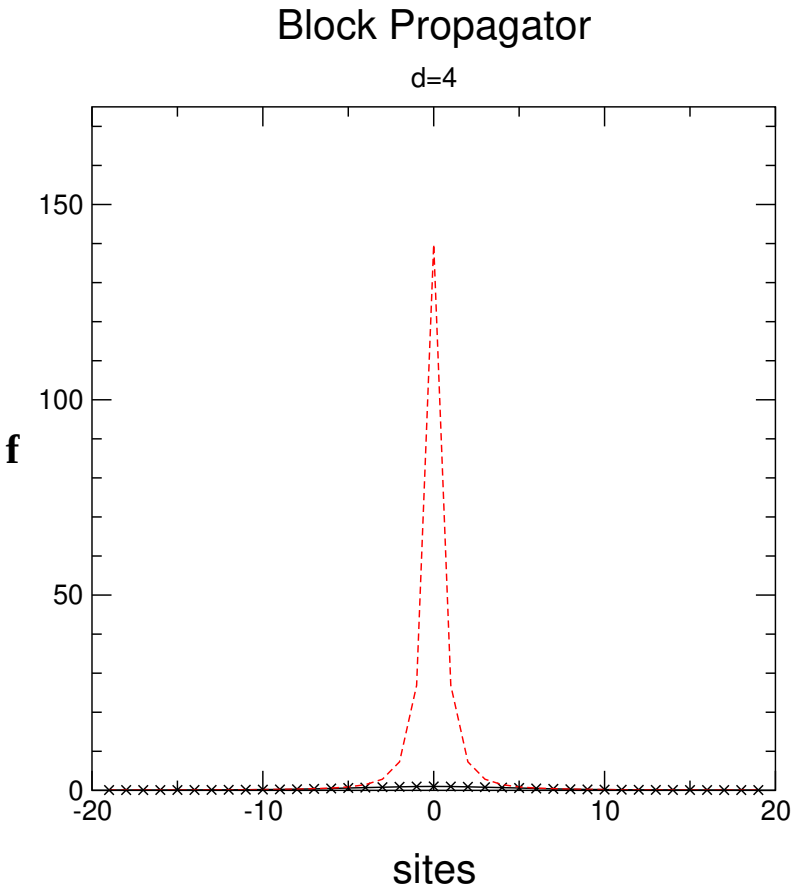

Figure 4.3.13: Block propagator in position space, for $d = 4$.

of N that it is possible to use in each dimension within a reasonable amount of computer time, varying r from 1 to N.

(b) Plot graphs of σ_r^2 as a function of r for this fixed value of N and make curve fittings in order to try to discover the dependency of this quantity on r.

(c) Use these results to find out how Σ_r^2 behaves in continuum limits in which both L and r increase with N as $\sqrt{N}$, so that the size $L_r = L/r$ of the blocks remains finite. Show in this way that Σ_r^2 has a finite and non-vanishing limit under these conditions, in the cases $d = 3$, $d = 4$ and $d = 5$.

(d) Find out the behavior of Σ_r^2 under these same conditions, in the cases $d = 1$ and $d = 2$. Remember that it is quite possible that the behavior is logarithmic in the case $d = 2$, in fact, this is likely to happen[2].

4.3.2. (a) Starting from the formula in equation (4.3.4) for the dimensionfull block

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

5.1 Connection with the Canonical Formalism

The concept of energy is introduced by means of what is denominated the *canonical formalism*, which is the one usually employed in the traditional presentation of the theory, and which is discussed in terms of states and operators in a Hilbert space. It is therefore necessary to discuss some aspects of the relation of the formalism of the Euclidean lattice with the canonical formalism of quantum field theory. Our main objective in this section is to introduce and examine the concept of energy from the point of view of the theory formulated on the Euclidean lattice. Later on we will try to see under what conditions it is possible to establish connections between the lattice formalism and elements of the operator formalism, such as particles states, the Hamiltonian operator and its eigenstates.

In this section we will construct the canonical formalism on the Euclidean lattice, introducing the concepts of conjugate momenta and of the energy. We will use the well-known case of quantum mechanics both as a guide for our construction and as a way to verify the correction of our results. Always using the free scalar field of a single component as our basic example, we have the action

$$S = \sum_s \mathcal{L},\ \mathcal{L} = \frac{1}{2}\sum_\mu (\Delta_\mu \varphi)^2 + \frac{\alpha_0}{2}\varphi^2,$$

where both S and $\mathcal{L}$ are dimensionless, $\mathcal{L}$ being the Lagrangian density. In order to build the canonical formalism it is necessary to separate one of the dimensions of the space, which we will call the time, from the other dimensions, which we will call spacial dimensions. To make things definite, we may think of the $d = 4$ case, but the formalism can be used in any dimension. We will denote the d-dimensional sums by $\sum_\mu$ and $\sum_s$, while those that do not include the time will be written as $\sum_i$ and $\sum_{\mathbf{x}}$, respectively, and then the sum over the temporal dimension will be denoted by $\sum_t$. The temporal variables will be denoted by an index 0 or T. The lattice will have N_L sites in the spacial directions and N_T sites in the temporal direction. In general these two numbers will be equal, but the possibility remains open that they be different, if and when this becomes necessary for future discussions. We may rewrite the action in this new notation, obtaining

$$S = \sum_t \sum_{\mathbf{x}} \mathcal{L},\ \mathcal{L} = \frac{1}{2}(\Delta_0 \varphi)^2 + \frac{1}{2}\sum_i (\Delta_i \varphi)^2 + \frac{\alpha_0}{2}\varphi^2.$$

Classically we may define the dimensionless conjugate momentum to the field φ, which we shall call $\bar{\pi}$, by means of

$$\bar{\pi} = \imath \frac{\partial \mathcal{L}}{\partial(\Delta_0 \varphi)} = \imath \Delta_0 \varphi,$$

which is the usual relation except for the factor of $\imath$, whose introduction is due to the fact that we are doing the construction in Euclidean space, as well as to the fact that $\bar{\pi}$ is the temporal component of a vector. This conjugate momentum may be

$\Delta_0\varphi$, with functional integrals involving both the variables $\bar{\pi}$ and the variables φ. As we shall see, the results are different in each case. We will adopt as the definition of the canonical version of the theory the following expression for the observables,

$$\langle\mathcal{O}\rangle = \frac{\displaystyle\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ \mathcal{O}[\varphi,\bar{\pi}]\ e^{\imath\sum_s(\bar{\pi}\Delta_0\varphi-\mathcal{H})}}{\displaystyle\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ e^{\imath\sum_s(\bar{\pi}\Delta_0\varphi-\mathcal{H})}}, \tag{5.1.2}$$

where $\mathcal{O}$ is a functional of $\bar{\pi}$ and φ, and $\mathcal{H}$ is the expression in (5.1.1). Observe that the dependency on $\bar{\pi}$ is always Gaussian in this definition, independently of the model under consideration, because we have

$$\imath(\bar{\pi}\Delta_0\varphi - \mathcal{H}) = -\frac{1}{2}\left[\bar{\pi}^2 - 2\imath\bar{\pi}\Delta_0\varphi + \sum_i(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

Note that, due to the introduction of the factor of $\imath$ in the definition of $\bar{\pi}$, the integrals on this variable converge in Euclidean space so long as the integrations are made over real values, exactly as in the case of φ. It is understood, therefore, that at each site we have the integrals

$$\int_{-\infty}^{\infty}\mathrm{d}\varphi \quad \text{and} \quad \int_{-\infty}^{\infty}\mathrm{d}\bar{\pi},$$

along the real axis of each one of the variables.

Hence we have a complete definition of all the observables of the theory in the canonical formalism on the Euclidean lattice. It is important to observe that when $\mathcal{O}$ does not depend on $\bar{\pi}$ this definition reduces to the previous one, since in this case we can do the integrations on $\bar{\pi}$ explicitly and return to the usual definition. In order to do this we start by separating the variables, writing

$$\langle\mathcal{O}\rangle = \frac{\displaystyle\int [\mathrm{d}\varphi]\ \mathcal{O}[\varphi]\ e^{-\frac{1}{2}\sum_s\left[\sum_i(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]}\int [\mathrm{d}\bar{\pi}]\ e^{-\frac{1}{2}\sum_s\left(\bar{\pi}^2-2\imath\bar{\pi}\Delta_0\varphi\right)}}{\displaystyle\int [\mathrm{d}\varphi]\ e^{-\frac{1}{2}\sum_s\left[\sum_i(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]}\int [\mathrm{d}\bar{\pi}]\ e^{-\frac{1}{2}\sum_s\left(\bar{\pi}^2-2\imath\bar{\pi}\Delta_0\varphi\right)}}. \tag{5.1.3}$$

We may then complete the square on $\bar{\pi}$ in the exponent of the second exponential, obtaining

$$\begin{aligned} \bar{\pi}^2 - 2\imath\bar{\pi}\Delta_0\varphi &= (\bar{\pi}-\imath\Delta_0\varphi)^2 + (\Delta_0\varphi)^2 \Rightarrow \\ \int [\mathrm{d}\bar{\pi}]\ e^{-\frac{1}{2}\sum_s\left[(\bar{\pi}-\imath\Delta_0\varphi)^2+(\Delta_0\varphi)^2\right]} &= e^{-\frac{1}{2}\sum_s(\Delta_0\varphi)^2}\int [\mathrm{d}\bar{\pi}]\ e^{-\frac{1}{2}\sum_s(\bar{\pi}-\imath\Delta_0\varphi)^2}. \end{aligned} \tag{5.1.4}$$

We now shift the variable $\bar{\pi}$, defining a new variable $\chi = \bar{\pi} - \imath\Delta_0\varphi$, and obtain for the integral on $\bar{\pi}$

$$\int_{-\infty}^{\infty}[\mathrm{d}\bar{\pi}]\ e^{-\frac{1}{2}\sum_s(\bar{\pi}-\imath\Delta_0\varphi)^2} = \int_{-\infty-\imath\Delta_0\varphi}^{\infty-\imath\Delta_0\varphi}[\mathrm{d}\chi]\ e^{-\frac{1}{2}\sum_s\chi^2}.$$

Drawing now the complex-χ plane we can identify the relevant integration paths.

$$\begin{aligned}\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}](\bar{\pi}-\imath\Delta_0\varphi)\; e^{-\frac{1}{2}\sum_s\left[\sum_i(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]}\; e^{-\frac{1}{2}\sum_s\left(\bar{\pi}^2-2\imath\bar{\pi}\Delta_0\varphi\right)}&\\ = \int [\mathrm{d}\varphi]\; e^{-S}\int [\mathrm{d}\bar{\pi}](\bar{\pi}-\imath\Delta_0\varphi)\; e^{-\frac{1}{2}\sum_s(\bar{\pi}-\imath\Delta_0\varphi)^2}&\\ = \int_{-\infty}^{\infty}[\mathrm{d}\varphi]\; e^{-S}\int_{-\infty-\imath\Delta_0\varphi}^{\infty-\imath\Delta_0\varphi}[\mathrm{d}\chi]\;\chi\; e^{-\frac{1}{2}\sum_s\chi^2},&\end{aligned}$$

where $\chi=\bar{\pi}-\imath\Delta_0\varphi$ and we used once more some of the manipulations used before. We may now modify the integration circuit as we did before, obtaining

$$\int_{-\infty}^{\infty}[\mathrm{d}\varphi]\; e^{-S}\int_{-\infty}^{\infty}[\mathrm{d}\chi]\;\chi\; e^{-\frac{1}{2}\sum_s\chi^2}=0,$$

by a simple symmetry argument. We see therefore that $\bar{\pi}$ and $\imath\Delta_0\varphi$ have the same expectation value,

$$\langle\bar{\pi}\rangle=\imath\langle\Delta_0\varphi\rangle.$$

However, we may verify that $\bar{\pi}\neq\imath\Delta_0\varphi$ in a simple way, calculating the second expectation value. Repeating the same procedures and calculations used previously, and executing some Gaussian integrations (problem 5.1.1), we obtain

$$\left\langle(\bar{\pi}-\imath\Delta_0\varphi)^2\right\rangle=1.$$

This means that, although $\bar{\pi}$ and $\imath\Delta_0\varphi$ have the same expectation value, the two quantities fluctuate around each other in such a way that the difference between them is, typically, a non-vanishing real number with a magnitude of the order of one.

We will now calculate the expectation value of the Hamiltonian $\mathbf{H}$ in this canonical version of the formalism. Since this corresponds to the calculation of the energy of the vacuum state, this is the first step for the determination of the role that the concept of energy plays in the theory. For starters, let us worry about the calculation of the integrals over the momenta. Starting from the definition of the expectation values in the canonical formalism, and repeating once more some of the previous operations, we may write for the expectation value of $\mathbf{H}$

$$\langle\mathbf{H}\rangle=-\frac{\imath}{2}\sum_{\mathbf{x}}\frac{\displaystyle\int[\mathrm{d}\varphi]\; e^{-S}\int[\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s\chi^2}\left[\bar{\pi}^2+\sum_i(\Delta_i\varphi)^2+\alpha_0\varphi^2\right]}{\displaystyle\int[\mathrm{d}\varphi]\; e^{-S}\int[\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s\chi^2}},$$

where $\bar{\pi}=\chi+\imath\Delta_0\varphi$, so that we may write for the expression of $\mathcal{H}$ in the denominator

$$\begin{aligned}-2\imath\mathcal{H} &= (\chi+\imath\Delta_0\varphi)^2+\sum_i(\Delta_i\varphi)^2+\alpha_0\varphi^2\\ &= \chi^2+2\imath\chi\Delta_0\varphi-(\Delta_0\varphi)^2+\sum_i(\Delta_i\varphi)^2+\alpha_0\varphi^2,\end{aligned}$$

The invariance by temporal translation implies that $\mathbf{H}_b$ and $\mathbf{H}$ have the same expectation value, but they are really two conceptually different observables. Observe that, in the spirit of the discussion in section 4.3, it is not possible to measure an energy at a perfectly well-defined instant, that is, on a vanishing temporal interval Δt, so that in any real situation we will always be making an average over a temporal block when we measure the energy. In our case here we simply adopted a maximal block, making an average over the whole extent of the lattice. Getting back to our calculation, due to the temporal translation invariance we may add over the temporal direction and then divide by N_T, without any change in the result, thus obtaining

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

We may now use Fourier transforms in d dimensions to calculate this in a simple way, writing the expression in the form

$$\langle \mathbf{H}' \rangle = -\frac{\imath}{2} N_L^{d-1} \frac{\displaystyle\int [\mathrm{d}\widetilde{\varphi}]\; e^{-S} \sum_p \left(-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0 \right) |\widetilde{\varphi}|^2}{\displaystyle\int [\mathrm{d}\widetilde{\varphi}]\; e^{-S}},$$

where the action S may be written in momentum space as

$$S = \frac{N_L^{d-1} N_T}{2} \sum_p \left(\rho^2 + \alpha_0 \right) |\widetilde{\varphi}|^2,$$

with $\rho^2 = \sum_\mu \rho_\mu^2$, that, in the general case in which we have $N_L \neq N_T$, may be written explicitly as

$$\begin{aligned} \rho^2 &= \rho_0^2 + \sum_i \rho_i^2 + \alpha_0 \\ &= 4 \sin^2 \left(\frac{k_0 \pi}{N_T} \right) + \sum_i 4 \sin^2 \left(\frac{k_i \pi}{N_L} \right) + \alpha_0, \end{aligned}$$

so that the expectation value of $|\widetilde{\varphi}|^2$ is given by

$$\langle |\widetilde{\varphi}|^2 \rangle = \frac{1}{N_L^{d-1} N_T} \; \frac{1}{\rho^2 + \alpha_0},$$

leading therefore to the result for the term we are examining,

$$\langle \mathbf{H}' \rangle = -\frac{\imath}{2N_T} \sum_p \frac{-\rho_0^2 + \displaystyle\sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0}.$$

It is possible, however, to establish analytically upper and lower bounds to the sum (problems 5.1.2, 5.1.3 and 5.1.4), showing that, for even N_T,

$$\frac{\omega}{2}\sqrt{\frac{(2N_T)^2}{(\omega T)^2+(2N_T)^2}} \leq \imath E \leq \frac{1}{T} - \frac{\omega^2 T}{(\omega T)^2+(2N_T)^2} + \frac{\omega}{2}\sqrt{\frac{(2N_T)^2}{(\omega T)^2+(2N_T)^2}},$$

a relation that, in the limit $N_T \to \infty$, results in

$$\frac{\omega}{2} \leq \imath E \leq \frac{\omega}{2} + \frac{1}{T}.$$

In order to examine the case $\omega \gg 1/T$ we may make an approximation of the sum by an integral, which is a good approximation for large N_T. In this case we have for the minimum variation of the momentum $dp = 2\pi/T$, so that we get

$$\begin{aligned} E &= -\frac{\imath}{T}\frac{T}{2\pi}\int_{-N_T\pi/T}^{N_T\pi/T} dp\, \frac{\omega^2}{\omega^2+p^2} \\ &= -\frac{\imath\omega}{\pi}\int_0^{N_T\pi/(\omega T)} d\xi\, \frac{1}{1+\xi^2} \\ &= -\frac{\imath\omega}{\pi}\arctan\left(\frac{N_T\pi}{\omega T}\right). \end{aligned}$$

In the limit $N_T \to \infty$ with finite ω and T the arc-tangent tends to $\pi/2$ and hence we obtain the expected result for the harmonic oscillator,

$$\imath E = \frac{\omega}{2}.$$

Note that this is the exact result only in the case in which the temporal box is infinite, with $T \to \infty$, so that the approximation by an integral is not sufficient to show the infrared effects due to the finite temporal box.

For a more detailed examination of the complete behavior of the energy as a function of N_T and ωT it is necessary to calculate the sum numerically (problem 5.1.5). The results of such a calculation appear in figures 5.1.1 and 5.1.2. The graph in figure 5.1.1 shows the energy in the continuum limit, as well as the upper and lower bounds that it is possible to establish analytically for it, in this limit. Besides the result in an infinite temporal box, the result in a finite box is also shown, to illustrate the infrared effects that exist in this case. In this graph the central straight line corresponds to the continuum limit in an infinite temporal box, that is, to the case $N_T \to \infty$ and $T \to \infty$. The other straight lines correspond to the upper and lower bounds which are proposed as problems to the reader. The lower straight line corresponds to the lower bound to which problem 5.1.2 makes reference, while the improved lower bound proposed in problem 5.1.3 coincides with the central straight line. The curved line corresponds to the numerical result for $N_T = 1000$.

The graph in figure 5.1.2 shows the energy in the continuum limit and on various finite lattices, illustrating the way in which these results approach their limit when

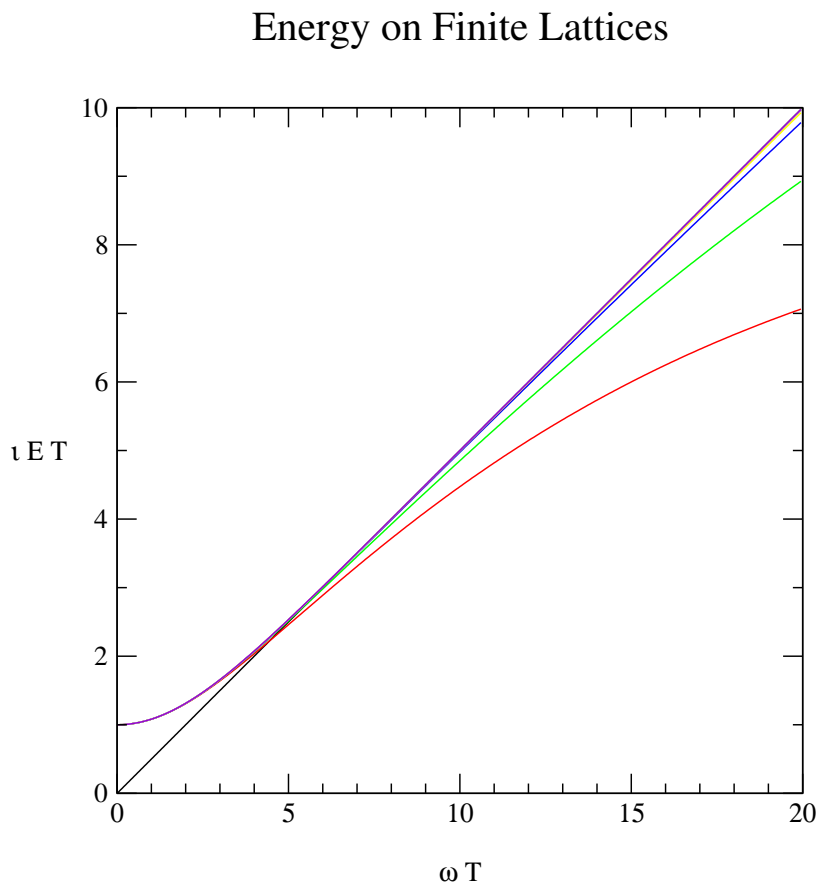

Figure 5.1.2: The energy as a function of the variable ωT. The straight line corresponds to the continuum limit in an infinite temporal box, that is, to the case $N_T \to \infty$ and $T \to \infty$. The curved lines correspond to the numerical results in progressively larger lattices, from $N_T = 10$ to $N_T = 1000$, showing how they approach the continuum result in the limit $N_T \to \infty$.

where $A^2 = \sum_i \rho_i^2 + \alpha_0$. Note that the sum in k_0 has the same form of the sum that we just discussed in the case of quantum mechanics. However, the continuum limit of this sum behaves in a way that is very different from what happens in the case $d = 1$, due to the way in which the quantity A, which contains the spacial components ρ_i of the dimensionless momentum, scales in the limit, for $d \geq 2$. In fact, the quantity $\imath ET$ diverges in this case, when we make $N_T \to \infty$ and $N_L \to \infty$.

One can understand this fact by observing that the result above is a sum, of something similar to the energy of the ground state of a harmonic oscillator, over all the N_L^{d-1} degrees of freedom of a $(d-1)$-dimensional section of the lattice, so that this sum is certainly divergent at least as N_L^{d-1}. In addition to this, the harmonic oscillators over which we are adding have all the possible frequencies in the temporal direction of the lattice, so that their ground state energies vary from values of the order of 1 to values of the order of N_T. For this reason, the quantity $\imath ET$ diverges

$$\imath eT = \frac{d-1}{d} + \frac{\alpha_0}{d}\sigma^2(N_T, d, \alpha_0),$$

where σ^2 is the local width of the field, a quantity that was extensively discussed in section 4.1. Since for $d \geq 2$ this quantity does not diverge faster than or as fast as N_T^2 in the $N_T \to \infty$ limit, while $\alpha_0 = m_0^2/N_T^2$, the second term goes to zero because α_0 goes to zero for finite m_0. The convergence is progressively faster for progressively smaller values of m_0.

Observe that, if we make $T \to \infty$ while we take the continuum limit, thus eliminating the infrared effects due to the finite size of the temporal box, the energy ceases to diverge as N_T^d and becomes divergent as N_T^p, with a power p in the range $d-1 < p < d$. This is due to the fact that we can make T go to infinity as N_T^q only with $0 < q < 1$, since $q = 0$ would of course correspond to keeping T finite, while $q = 1$ would imply that the lattice spacing a would be kept finite, in which case the limit $N_T \to \infty$ would would no longer be a continuum limit.

In the traditional formalism of quantum field theory the result for the energy of the vacuum is constructed as the sum of a collection of quantum-mechanical ground-state results, one for each mode. We can try to obtain, from the result for the energy shown in equation (5.1.7), a somewhat clearer relation between the results of quantum mechanics and of the quantum theory of fields. However, we will see that this relation cannot be established in a completely exact and precise form, for reasons related to the order in which the limits involved are to be taken, a subject that will turn out to be very important later on. In order that we be able to sketch an argument to this effect, it is necessary that we consider the symmetrical limit in which $N_T = N_L = N$. The result obtained in the case of quantum mechanics for the sum over k_0 that appears in equation (5.1.7), in the $N_T \to \infty$ limit, for a large temporal box, implies that we have

$$\sum_{k_0} \frac{A^2}{\rho_0^2 + A^2} \sim \frac{N_T A}{2},$$

so that we may write for the energy of the vacuum

$$E \sim -\frac{\imath N_T}{2T} \sum_{k_i} \sqrt{\sum_i \rho_i^2 + \alpha_0} \sim \frac{-\imath}{2} \sum_{k_i} \sqrt{\sum_i p_i^2 + m_0^2},$$

where we used the fact that $\alpha_0 N_T^2/T^2 = m_0^2$ and that, for large $N_T = N_L = N$, $\rho_i N_T/T \approx p_i = 2\pi k_i/T$, the dimensionfull linear momentum. In short, we may write that

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

which is a sum of the relativistic energies of free particles with rest mass m_0 and linear momentum $\mathbf{p}$, with an overall factor of $1/2$, there being one term in the sum

way is always larger that the result of the lattice formalism, for any value $d \geq 2$ of the dimension. In $d = 4$, for example, we obtain approximately 1.1938 for this result, to be compared to the lattice result $(d-1)/d = 3/4 = 0.75$.

We see in this way that the results of the quantum theory of fields have the potential to depend in a significant way on the order of the limits over N_T and N_L. In our case here this fact is of only secondary importance, because the energy of the vacuum diverges anyway, whatever the order of the limits, having therefore no direct physical relevance. We will see later on that, in order to define an energy that makes physical sense, it will be necessary to consider only the *variations* of the energy with respect to the energy of the vacuum, not the absolute value of the energy, a procedure that corresponds to what is called a subtractive "renormalization" of all the energies, exactly as is done in the traditional presentation of the theory. However, we see here that the usual argument of the traditional presentation, that this divergence is due to the sum of an infinite number of zero-point energies of harmonic oscillators, cannot be taken as more than an approximate intuitive argument, without exact mathematical validity.

Problems

5.1.1. Using the calculational techniques illustrated in the text, calculate the value at a give site s of the observable $\langle[\bar{\pi}(s) - \imath\Delta_0\varphi(s)]^2\rangle$, obtaining the result shown in the text. You will have to perform some Gaussian integrations. Remember that the extremes of integration of the integrals on $\chi = \bar{\pi} - \imath\Delta_0\varphi$ depend on φ until one makes the deformation of the integration contour in the complex χ plane.

5.1.2. Consider the expression of the energy derived in the text for the case of quantum mechanics, that is for $d = 1$, which is shown in equation (5.1.6). It contains the sum

$$\Sigma = \sum_{k_0=-k_m}^{k_M} \frac{1}{1 + \left(\dfrac{2N_T}{\omega T}\right)^2 \sin^2\left(\dfrac{k_0\pi}{N_T}\right)}.$$

Consider the case in which N_T is even, for which the limits of k_0 are $k_m = 1 - N_T/2$ and $k_M = N_T/2$. Show that this sum satisfies the inequalities

$$\begin{aligned}
\Sigma &\geq -1 + \frac{(\omega T)^2}{(\omega T)^2 + (2N_T)^2} + \frac{\omega T}{2}\sqrt{\frac{(2N_T)^2}{(\omega T)^2 + (2N_T)^2}}, \\
\Sigma &\leq 1 - \frac{(\omega T)^2}{(\omega T)^2 + (2N_T)^2} + \frac{\omega T}{2}\sqrt{\frac{(2N_T)^2}{(\omega T)^2 + (2N_T)^2}}.
\end{aligned}$$

5.1.5. Write a program to calculate numerically the sum that appears in the expression of the energy in the case of quantum mechanics, given in equation (5.1.6). Use your program to reproduce the data that are shown in the graphs of figures 5.1.1 and 5.1.2. Use lattices with sizes between 10 and 1000 and calculate $\imath ET$ for ωT from 0 to 20.

5.1.6. Write programs to calculate numerically the sum that appears in the expression of the energy per site for the cases $d \geq 2$, given in equation (5.1.8). Remember that in the quantum theory of fields we have $\alpha_0 = m_0^2/N^2$ and consider only the symmetrical case $N_T = N_L = N$. Use your programs to reproduce the data that are shown in the graph of figure 5.1.3.

5.1.7. Show analytically that the sum that you calculated in problem 5.1.6 tends to the value $(d-1)/d$ in the limit $N \to \infty$. Your demonstration does not have to be strictly rigorous and you may consider the case $m_0 \to 0$ it this simplifies things. However, be careful, because there is a term of the sum (the zero mode) which diverges for $m_0 = 0$. You can demonstrate this result by first showing that the energy per site may be written as

$$\imath eT = \frac{d-1}{d} + \frac{\alpha_0}{d}\sigma^2(N, d, \alpha_0),$$

where σ^2 is the local width defined in section 4.1, which has a finite limit in the continuum limit for $d \geq 3$. The case $d = 2$ has to be examined in separate, refer to the section mentioned in order to verify the behavior of σ^2 in this case.

5.1.8. Write a program to calculate numerically the sum that appears in the result of the traditional formalism for the energy per site,

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

where $\rho_i = 2\sin(k_i\pi/N)$. Remember that in the quantum theory of fields we have $\alpha_0 = m_0^2/N^2$. Use your program for progressively larger values of N and try to show that, in $d = 4$, the limiting value for this result is approximately 1.1938. Try to relate the fact that this result is larger than the corresponding result in the lattice formalism (0.75) with the behavior in the limit of the sum that appears in the lattice formalism in the case $d = 1$, which is shown in the graph of figure 5.1.2.

enough to define a single state in order for us to be able to define and calculate all the relevant observables of the theory, that is, all the correlation functions and any other observables, related to other functionals of the fields. However, the introduction of the direct representation of other states enriches our structure and permits a better understanding of its functioning.

In this section we are using the word "state" with a very general meaning, as a representation of the physical situation in a given region of space-time. We are going to make here *no* attempt to establish a definite formal relation with the concept of states as vectors in a Hilbert space. In fact, we are not going to talk at all about Hilbert spaces or the operators that exist in these spaces. We are going to talk only about physical states and observables. Later on we will see to what extent it is possible to establish a relation between our structure and the Hilbert spaces of quantum mechanics.

Very well, based on the experience we have with the traditional formalism it is not difficult to guess at the form that a one-particle state should have. Pushing ahead the connection between states and statistical distributions, we introduce the state of one particle with momentum $\vec{k}$ through the definition of a new statistical distribution of configurations,

$$|1,\vec{k}\rangle \sim \frac{[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}}{\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}},$$

or, in terms of the canonical formalism,

$$|1,\vec{k}\rangle \sim \frac{[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}}{\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}},$$

expressions where there appears the Fourier component of the field φ associated to the momentum-space mode $\vec{k}$. Observe that any expectation value of an observable on this state can be reduced to the ratio of two expectation values on the vacuum, by the simple division of both numerator and denominator by the normalization factor of the vacuum distribution,

$$\langle\mathcal{O}\rangle_{1,\vec{k}} = \frac{\left(\dfrac{\int[\mathrm{d}\varphi]\ \mathcal{O}\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}}{\int[\mathrm{d}\varphi]\ e^{-S[\varphi]}}\right)}{\left(\dfrac{\int[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}}{\int[\mathrm{d}\varphi]\ e^{-S[\varphi]}}\right)} = \frac{\langle\mathcal{O}\ |\widetilde{\varphi}_{\vec{k}}|^2\rangle_0}{\langle|\widetilde{\varphi}_{\vec{k}}|^2\rangle_0},$$

where the index 0 on the expectation values indicates that they are taken on the vacuum state. Hence we see that in fact the vacuum is sufficient for the calculation of any observables, a fact which is of great important, for example, to permit the computational calculation of the expectation values of observables on other states by reduction to expectation values on the vacuum state.

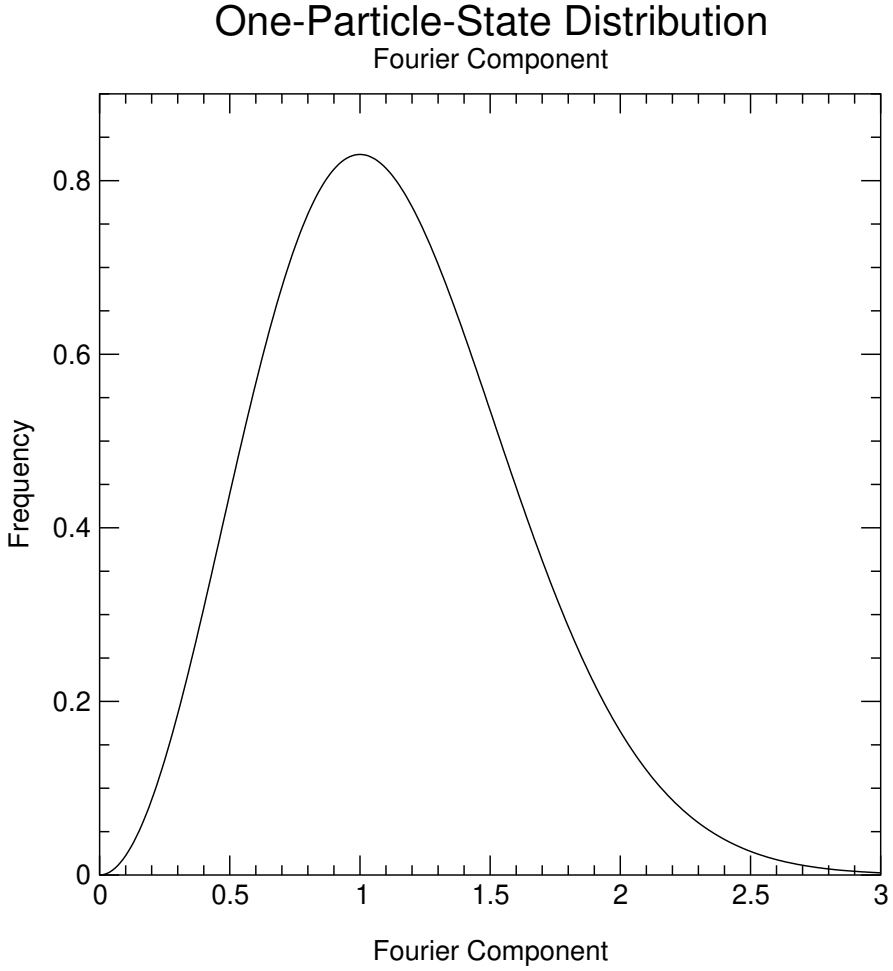

Figure 5.2.2: Qualitative diagram of the probability distribution $x^2 \exp(-x^2)$ of the Fourier component of the field that is singled out in the one-particle state with a given momentum vector $\vec{k}$, showing the point of maximum at 1.

through the criterion that the vacuum is the lowest-energy state that satisfies such conditions.

For the time being, we will limit ourselves to the examination of distributions containing the Boltzmann factor $\exp(-S)$ and powers of the Fourier components of the fields. Note that the effect of the introduction of the factor $|\widetilde{\varphi}_{\vec{k}}|^2$ in the distribution is intuitively clear. While the distribution given by the exponential $\exp(-S)$, where S is quadratic on all the Fourier components, concentrates the probabilities around the value 0, where it has its maximum value, as one can see in the graph of figure 5.2.1, the introduction of the factor $|\widetilde{\varphi}_{\vec{k}}|^2$ causes the displacement of this point of maximum to a finite and non-vanishing value, around which the probabilities become concentrated, as shown in the graph of figure 5.2.2. We will see that in the case of the state of n particles this maximum will be displaced to a value proportional to $\sqrt{n}$. Since this happens only for the part of the distribution related to the mode $\vec{k}$, through the introduction of the factor $|\widetilde{\varphi}_{\vec{k}}|^2$ we are favoring

where we already used in the second term the result

$$\langle|\widetilde{\varphi}_{\vec{k}}|^2\rangle_0 = \frac{1}{N_T N_L^{d-1}}\,\frac{1}{\rho^2_{\vec{k}}+\alpha_0}.$$

For the other expectation value, which appears in the third term, we have

$$\langle|\widetilde{\varphi}_{\vec{k}}|^4\rangle_0 = \frac{2}{\left(N_T N_L^{d-1}\right)^2}\,\frac{1}{\left(\rho^2_{\vec{k}}+\alpha_0\right)^2},$$

where we used the factorization relations given in section 3.4, for the case $\vec{k}\neq\vec{0}$, since the case $\vec{k}=\vec{0}$ would correspond to particles without any energy and without any $(d-1)$-dimensional momentum, being therefore of no interest. We may use these results in the third term and reorganize the terms in order to complete the sum of the second term in such a way that it runs over all possible values of $\vec{q}$, obtaining, after some manipulation,

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

One observes here that the first term is precisely the energy of the vacuum E_0, a quantity that diverges in the continuum limit. We may now define the quantity

$$\Delta E_{1,\vec{k}} = E_{1,\vec{k}} - E_0,$$

in which we subtracted from the energy its value in the vacuum state, obtaining

$$\imath\Delta E_{1,\vec{k}}T = \frac{-\rho_0^2(\vec{k})+\sum_i\rho_i^2(\vec{k})+\alpha_0}{\rho_0^2(\vec{k})+\sum_i\rho_i^2(\vec{k})+\alpha_0}. \tag{5.2.1}$$

Observe that this definition makes irrelevant the difference between the canonical definition and the usual definition, since this difference will always cancel out in the expression of ΔE. It is this quantity, the additional energy with respect to the energy of the vacuum that is contained within the state, that we will interpret as the physical energy to be associated to the state. This is equivalent to saying that the observable associated to the physical energy is a modified Hamiltonian,

$$\Delta\mathbf{H} = \mathbf{H} - \langle\mathbf{H}\rangle_0,$$

so that the dimensionless physical energy is given in terms of the expectation values of this observable,

$$\Delta\mathcal{E} = \langle\Delta\mathbf{H}\rangle,$$

on any state, while the dimensionfull energy is related to this dimensionless quantity by $\Delta E = \Delta\mathcal{E}/a = N_T\Delta\mathcal{E}/T$.

$\pm\sqrt{\mathbf{p}^2+m_0^2}$ either by smaller values or by larger values, thus changing the sign of the energy. The issue of the positiveness of the energy will remain open here because it cannot be solved in a theory of electrically neutral particles with spin zero as is the case for the real scalar fields we use here as an example. The resolution of this problem will have to wait until we are able to introduce into the structure of the theory other essential elements.

Observe that if our system is inside a box in which both T and L are finite then it may not be possible to satisfy an on-shell condition such as this one for arbitrary values of the mass m_0, because in this case both the values of p_0 and the values of $\mathbf{p}$ are quantized at discrete values, and there is no continuous variable except the mass that we may vary so that the equality can be satisfied. This problem disappears when we make T go to infinity, as we must, since in this case p_0 becomes a variable that can be varied continuously, and therefore it is always possible to satisfy the on-shell condition by varying p_0. If in addition to the limit $T\to\infty$ we also take the limit $L\to\infty$ then both p_0 and $\mathbf{p}$ become continuous variables and we obtain the usual on-shell condition for particles in infinite space-time.

If we keep L finite then the discrete character of $\mathbf{p}$ will be reflected, through the on-shell condition, on a corresponding discretization of the values of p_0. Thus we see here a simple example of the mechanism that leads to the appearance of energy quantization for bound states, which are confined to a finite region of the $(d-1)$-dimensional space. Note that making $T\to\infty$ while L is kept fixed is equivalent to taking the non-relativistic limit, since with $T\gg L$ only phenomena involving very small velocities will have world-lines that fit into the d-dimensional box. We therefore see here a very important fact, that the interpretation of relativistic particles as excitations of the modes of the d-dimensional cavity is reduced, in the non-relativistic limit, by means of the on-shell condition, to the association of physical particles to the energies and modes of the corresponding $(d-1)$-dimensional spacial cavity.

Adopting arbitrarily the first of the two possibilities above, we may impose that the $T\to\infty$ limit be taken in such a way that we have in this limit

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

for some finite, dimensionless and constant number A, so that

$$p_0(\vec{k})=-\frac{A}{T}+\sqrt{\mathbf{p}_{\vec{k}}^2+m_0^2}.$$

We see here that, for finite T, the on-shell condition is modified, that is, that the energy of each mode is modified by a term proportional to $1/T$, exactly as we verified for the energy of the vacuum in the case of quantum mechanics. This is, therefore, an infrared effect due to the finite size of the temporal box, exactly as before. Note that this comparison to the quantum-mechanical case already seems to indicate that the natural value for A is -1. We may now substitute this relation for $p_0(k)$ in the expression of the energy, obtaining in the $T\to\infty$ limit

$$\Delta E_{1,\vec{k}}=\frac{-1}{A}\sqrt{\mathbf{p}_{\vec{k}}^2+m_0^2}.$$

$$|n,\vec{k}\rangle \sim \frac{[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{\imath \sum_s [\bar{\pi}\Delta_0\varphi - \mathcal{H}(\varphi,\bar{\pi})]}}{\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{\imath \sum_s [\bar{\pi}\Delta_0\varphi - \mathcal{H}(\varphi,\bar{\pi})]}}.$$

One may now calculate the energy (problem 5.2.2), obtaining, as physically expected, the result

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

We see therefore that we obtain in fact a "ladder" of states, whose energies are integer multiples of a finite quantity, even on finite lattices, where both the dimensionless quantities N_T and N_L and the dimensionfull quantities T and L are finite. This ladder survives the continuum limit within an infinite temporal box so long as the on-shell condition is satisfied in the limit. For modes of the lattice that do not satisfy the on-shell condition the ladder collapses in the continuum limit and its steps become of vanishing height, so that all the collection of states related to it becomes energetically degenerate with the vacuum, not corresponding therefore to states of physically observable particles.

It is interesting to note here that the existence of this ladder of energies for the particle states in the non-linear $\lambda\varphi^4$ model, in $d = 4$, can be verified directly without too much difficulty by numerical means [3]. The rules for the construction of the Hamiltonian and of the particle states in the case of that model are exactly the same that we used here, the results being different, of course, but only due to the different form of the action. The measurement of the energies of the particle states on finite lattices can be made with great precision, leading to a very precise verification of the proportionality of the energy with the number n of particles. However, the determination of the energy of a particle in the continuum limit and the verification of the on-shell condition are much more difficult from the computational point of view and so far have been done only in a very rough and qualitative way. Whether or not the existence of such ladders of states is related to the phenomenon of the triviality of that model is currently unknown.

We will end this section showing that there exists in our structure an observable that gives, as its expectation values, the number of particles of a given state. This turns out to be the action of the model itself, which functions as a "number of particles" observable, so long as we subtract from it its expectation value on the vacuum, in analogy with what we did for the energy. Recalling once more that the form of the action of our free model in momentum space is

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

it is easy to calculate directly its expectation value on the vacuum, which has already been done as a problem proposed in a previous section, with the result

$$\langle \mathcal{N}_{\vec{k}} \rangle_{n,\vec{k}} = n,$$

while for $\vec{q} \neq \pm\vec{k}$

$$\langle \mathcal{N}_{\vec{k}} \rangle_{n,\vec{q}} = 0,$$

showing that the observable is, in fact, a projector for particles with momentum $\vec{k}$. Using these observables one can, for example, separate real particles, corresponding to modes satisfying the on-shell condition, from virtual particles corresponding to other modes. In non-linear theories it is not clear whether or not it is possible to define observables like this one in a general way.

Observe that we are not able to distinguish states of particles with momentum $\vec{k}$ from states of particles with momentum $-\vec{k}$, both with respect to the number of particles and with respect to the energy. This is due to the real nature of the scalar field of our simple model, which corresponds to particles without electrical charge. Both with respect to the positivity of the energy of the physical states and with respect to the complete definition of the observables that give us the number of particles, it is clear that, in order to go ahead with the physical interpretation of the theory, it would be necessary to introduce into it complex fields corresponding to charged particles, as well as the gauge fields of electrodynamics.

Problems

5.2.1. Calculate the expectation value of the Hamiltonian $\mathbf{H}$ on the state of one particle with momentum $\vec{k}$. During the calculation consider carefully the cases in which $\widetilde{\varphi}(\vec{k})$ is real and those in which $\widetilde{\varphi}(\vec{k})$ has a non-vanishing imaginary part.

5.2.2. Calculate the expectation value of the Hamiltonian $\Delta\mathbf{H}$ on the state of n particles with momentum $\vec{k}$. During the calculation consider carefully the cases in which $\widetilde{\varphi}(\vec{k})$ is real and those in which $\widetilde{\varphi}(\vec{k})$ has a non-vanishing imaginary part.

5.2.3. Calculate the expectation value of the action S on the state of n particles with momentum $\vec{k}$. During the calculation consider carefully the cases in which $\widetilde{\varphi}(\vec{k})$ is real and those in which $\widetilde{\varphi}(\vec{k})$ has a non-vanishing imaginary part.

5.2.4. Calculate the expectation value of the observable $\mathcal{N}$ on a state having n_1 particles with momentum $\vec{k}_1$ and n_2 particles with momentum $\vec{k}_2$, which is obtained by multiplying the Boltzmann factor by the appropriate factors involving the Fourier components of the fields relative to these two momenta,

$$|n_1, \vec{k}_1; n_2, \vec{k}_2\rangle \sim \frac{[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}_1}|^{2n_1} |\widetilde{\varphi}_{\vec{k}_2}|^{2n_2} e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}_1}|^{2n_1} |\widetilde{\varphi}_{\vec{k}_2}|^{2n_2} e^{-S[\varphi]}}.$$

$$\langle e|\mathcal{O}_{\rm op}^2|e\rangle = \langle e|\mathcal{O}_{\rm op}|e\rangle^2.$$

This is the statement that the dispersion or width of the distribution of values of the operator $\mathcal{O}_{\rm op}$ on the state $|e\rangle$ is zero,

$$\sigma_{\mathcal{O}}^2 = \langle e|\mathcal{O}_{\rm op}^2|e\rangle - \langle e|\mathcal{O}_{\rm op}|e\rangle^2 = 0.$$

In other words, the value of the observable $\mathcal{O}$ on the state $|e\rangle$ is completely well-defined, without fluctuations. This is a representation of the concept of eigenstate that we can translate directly to the lattice formalism,

$$\sigma_{\mathcal{O}}^2 = \langle \mathcal{O}^2\rangle_e - \langle \mathcal{O}\rangle_e^2 = 0.$$

Of course, in the representation of the structure on the lattice, one does not expect that the dispersion of the observable on its eigenstates is necessarily zero on finite lattices, but only that it goes to zero in the continuum limit, and possibly only if we take, besides this one, the $T \to \infty$ limit as well. For example, for the action per site s_0, an observable which was examined in the problems proposed in section 4.2, we know that this is true for the vacuum state, since we have that $\langle s_0\rangle_0 = 1/2$ and that the dispersion goes to zero in the limit $N_T = N_L = N \to \infty$. Of course, that observable is of no direct physical interest in the context of our discussion in this section.

We have then our criterion to determine whether or not a given state is an eigenstate of a given observable: it suffices to calculate the dispersion of the observable on the state and verify whether or not the result vanishes in the continuum limit. It is possible to define very singular statistical distributions for which the dispersion of any given observable is zero, even on finite lattices (problem 5.3.1), but these distributions do not correspond to physical states and are of little interest to us in the context of the quantum theory of fields. What we should verify is whether or not the vacuum state represented by the Boltzmann distribution is an eigenstate of the modified Hamiltonian $\Delta\mathbf{H}$, in the continuum limit. The same should be done with the observable number-of-particles $\mathcal{N}$. We should therefore calculate the dispersions of these observables in the vacuum state.

We will start by calculating the dispersion of the observable $\mathcal{N}$ and, therefore, of the action, because the calculations are simpler in this case, since these observables do not depend on $\bar{\pi}$ and we may, therefore, use directly the usual definition for the expectation values. In addition do this, these are dimensionless observables, which makes it simpler to take the continuum limit. Since we have that $\mathcal{N} = S - \langle S\rangle_0$, we can easily show that the dispersion of $\mathcal{N}$ is equal to the dispersion of S,

$$\begin{aligned}
\langle \mathcal{N}^2\rangle - \langle \mathcal{N}\rangle^2 &= \langle (S^2 - 2S\langle S\rangle_0 + \langle S\rangle_0^2)\rangle - (\langle S\rangle - \langle S\rangle_0)^2 \\
&= \langle S^2\rangle - 2\langle S\rangle\langle S\rangle_0 + \langle S\rangle_0^2 - \langle S\rangle^2 + 2\langle S\rangle\langle S\rangle_0 - \langle S\rangle_0^2 \\
&= \langle S^2\rangle - \langle S\rangle^2,
\end{aligned}$$

so that we have for the dispersion

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

which diverges in the continuum limit in the same way as before. Note that these results diverge even in the case $d = 1$, which corresponds to quantum mechanics. However, this fact does not cause much preoccupation because the concept of the observable number-of-particles does not play any fundamental role in quantum mechanics. For the case $d > 1$ it is also possible to calculate the dispersion of the operators $\mathcal{N}_{\vec{k}}$ (problem 5.3.4), which are given by

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

each one of which measures the number of particles with momentum $\vec{k}$. In this case we obtain, on the state of n particles with momentum $\vec{k}$,

$$\langle \mathcal{N}_{\vec{k}}\rangle_{n,\vec{k}} = n,$$

and

$$\langle \mathcal{N}^2_{\vec{k}}\rangle_{n,\vec{k}} = n^2 + n + \frac{1}{2},$$

so that we obtain for the dispersion

$$\langle \mathcal{N}^2_{\vec{k}}\rangle_{n,\vec{k}} - \langle \mathcal{N}_{\vec{k}}\rangle^2_{n,\vec{k}} = n + \frac{1}{2}.$$

In this case the result does not diverge, but we still have a value for the dispersion that does not vanish in the continuum limit, showing once more that the states of particles are not eigenstates of these observables.

In short, none of our states of particles are eigenstates of any of the observables that give, as their expectation values in these states, the corresponding numbers of particles. We will now proceed to the examination of the behavior of the observables related to the energy, which are the most important ones from the physical point of view. The observable of greatest relevance to us is the modified Hamiltonian

$$\Delta\mathbf{H} = \mathbf{H} - \langle\mathbf{H}\rangle_0,$$

recalling that the dimensionless physical energy is given by

$$\Delta\mathcal{E} = \langle\Delta\mathbf{H}\rangle,$$

and that the physical energy relates to this dimensionless quantity by

$$\Delta E = \Delta\mathcal{E}/a = N_T\Delta\mathcal{E}/T.$$

canonical definition of the observables. So that it be a positive quantity, recalling that $\mathbf{H}_b$ is purely imaginary in our formalism, we define the dispersion $\sigma_{\mathbf{H}_b}$ by means of

$$-\sigma^2_{\mathbf{H}_b} = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2.$$

As we saw in section 5.1, using the canonical definition of the expectation values we have for $\langle \mathbf{H} \rangle = \langle \mathbf{H}_b \rangle$ the result

$$\langle \mathbf{H}_b \rangle = -\frac{\imath}{2} N_L^{d-1} - \frac{\imath}{2N_T} \sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0},$$

with

$$\rho^2 = 4 \sin^2\left(\frac{k_0 \pi}{N_T}\right) + \sum_i 4 \sin^2\left(\frac{k_i \pi}{N_L}\right) + \alpha_0,$$

so that we have for the square of this quantity

$$\begin{aligned} \langle \mathbf{H}_b \rangle^2 \;\; = \;\; & -\frac{1}{4N_T^2} \left[\left(N_L^{d-1} N_T \right)^2 + 2 N_L^{d-1} N_T \sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right. \\ & \left. + \left(\sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right) \left(\sum_{\vec{q}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right) \right], \end{aligned} \quad (5.3.1)$$

where it is understood that the variables within each sum have as their argument the argument of the sum. Let us now calculate $\langle \mathbf{H}_b^2 \rangle$, starting by the integrals over $\bar{\pi}$,

$$\langle \mathbf{H}_b^2 \rangle = -\frac{1}{4N_T^2} \left\langle \left\{ \sum_{\vec{x}} \left[\bar{\pi}^2 + (\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right] \right\} \left\{ \sum_{\vec{y}} \left[\bar{\pi}^2 + (\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right] \right\} \right\rangle,$$

where, once more, it is understood that the variables within each sum have as their argument the argument of the sum. We may write this explicitly as

$$\begin{aligned} \langle \mathbf{H}_b^2 \rangle = & -\frac{1}{4N_T^2} \sum_{\vec{x}} \sum_{\vec{y}} \frac{1}{\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}] \; e^{\imath \sum_s (\bar{\pi} \Delta_0 \varphi - \mathcal{H})}} \int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}] \; e^{\imath \sum_s (\bar{\pi} \Delta_0 \varphi - \mathcal{H})} \\ & \times \left\{ \bar{\pi}_{\vec{x}}^2 \bar{\pi}_{\vec{y}}^2 + 2 \bar{\pi}_{\vec{x}}^2 \left[(\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right]_{\vec{y}} + \left[(\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right]_{\vec{x}} \left[(\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right]_{\vec{y}} \right\}, \end{aligned}$$

where the indices $\vec{x}$ e $\vec{y}$ indicate the dependencies with each one of these two sites, and we have used our freedom to interchange $\vec{x}$ and $\vec{y}$ within the sums. Recalling that the exponential can be written as

$$e^{\imath \sum_s (\bar{\pi} \Delta_0 \varphi - \mathcal{H})} = e^{-\frac{1}{2} \sum_s (\bar{\pi}^2 - 2\imath \bar{\pi} \Delta_0 \varphi)} e^{-\frac{1}{2} \sum_s \left[(\Delta_i \varphi)^2 + \alpha_0 \varphi^2 \right]}$$

where we used the expression of the Hamiltonian with $\bar{\pi}$ substituted by $\imath\Delta_0\varphi$,

$$\mathbf{H}'_b = \frac{1}{N_T}\sum_t \mathbf{H}' = \frac{1}{N_T}\sum_{\vec{x}} \mathcal{H}'.$$

We now observe that the result of equation (5.3.1) can be written in terms of $\mathbf{H}'_b$ as

$$\langle \mathbf{H}_b\rangle^2 = -\frac{1}{4}N_L^{2(d-1)} - \imath N_L^{d-1}\langle \mathbf{H}'_b\rangle + \langle \mathbf{H}'_b\rangle^2,$$

so that we may write for the dispersion of $\mathbf{H}_b$

$$-\sigma^2_{\mathbf{H}_b} = \langle \mathbf{H}_b^2\rangle - \langle \mathbf{H}_b\rangle^2 = \langle \mathbf{H}_b'^2\rangle - \langle \mathbf{H}'_b\rangle^2 - \frac{1}{2}\frac{N_L^{d-1}}{N_T} + \frac{1}{N_T^2}\sum_{\vec{k}}\frac{\rho_0^2}{\rho^2+\alpha_0}.$$

We can manipulate the last two terms of this expression and verify that they are proportional to the expectation value of $\mathbf{H}'_b$,

$$\langle \mathbf{H}'_b\rangle = -\frac{\imath}{2N_T}\sum_{\vec{k}}\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0},$$

so that we can write the dispersion of $\mathbf{H}_b$ in terms of the dispersion of $\mathbf{H}'_b$ as

$$-\sigma^2_{\mathbf{H}_b} = \langle \mathbf{H}_b^2\rangle - \langle \mathbf{H}_b\rangle^2 = \langle \mathbf{H}_b'^2\rangle - \langle \mathbf{H}'_b\rangle^2 - \frac{\imath}{N_T}\langle \mathbf{H}'_b\rangle = -\sigma^2_{\mathbf{H}'_b} - \frac{\imath}{N_T}\langle \mathbf{H}'_b\rangle,$$

that is,

$$\sigma^2_{\mathbf{H}_b} = \sigma^2_{\mathbf{H}'_b} + \frac{\imath}{N_T}\langle \mathbf{H}'_b\rangle.$$

We see here that the dispersions of $\mathbf{H}_b$ and of $\mathbf{H}'_b$, that is, the dispersions of $\mathbf{H}_b$ according to the canonical definition and according to the usual definition, are not too different, since the extra term is damped by a factor of $1/N_T$ and should not have much importance in the continuum limit.

We must now calculate, in explicit form, the dispersion of $\mathbf{H}'_b$, for which it is necessary to calculate $\langle \mathbf{H}_b'^2\rangle$. For this end it is convenient to first write $\mathbf{H}'_b$ in terms of the Fourier transforms of the fields,

$$\mathbf{H}'_b = -\frac{\imath}{2N_T}\sum_{\vec{x}}\left[-(\Delta_0\varphi)^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right] = -\frac{\imath}{2}N_L^{d-1}\sum_{\vec{k}}(-\rho_0^2+\rho_i^2+\alpha_0)|\widetilde{\varphi}|^2.$$

With this we can write for the expectation value of $\mathbf{H}_b'^2$

$$\langle \mathbf{H}_b'^2\rangle = -\frac{N_L^{2(d-1)}}{4}\sum_{\vec{k}}\sum_{\vec{q}}(-\rho_0^2+\rho_i^2+\alpha_0)_{\vec{k}}(-\rho_0^2+\rho_i^2+\alpha_0)_{\vec{q}}\langle|\widetilde{\varphi}_{\vec{k}}|^2|\widetilde{\varphi}_{\vec{q}}|^2\rangle.$$

$$\langle \mathbf{H}_b'^{\,2} \rangle = -\frac{1}{4N_T^2} \left[2 + 2 \sum_{\vec{k} \neq \vec{0}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 + \sum_{\vec{k}} \sum_{\vec{q}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)_{\vec{q}} \right].$$

The two remaining units in the first term may now be joined with the second term in order to complete the sum that appears in this one, resulting in

$$\langle \mathbf{H}_b'^{\,2} \rangle = -\frac{1}{2N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 - \frac{1}{4N_T^2} \left(\sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2$$

We observe now that the last term may be written in terms of $\langle \mathbf{H}_b' \rangle$ and we obtain

$$\langle \mathbf{H}_b'^{\,2} \rangle = -\frac{1}{2N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 + \langle \mathbf{H}_b' \rangle^2.$$

With this we finally obtain for the dispersion of $\mathbf{H}_b'$

$$-\sigma^2_{\mathbf{H}_b'} = \langle \mathbf{H}_b'^{\,2} \rangle - \langle \mathbf{H}_b' \rangle^2 = -\frac{1}{2N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2,$$

and, consequently, for the dispersion of $\mathbf{H}_b$

$$-\sigma^2_{\mathbf{H}_b} = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2 = -\frac{1}{2N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 - \frac{1}{2N_T^2} \sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0}.$$

We may join the two sums that appear in this expression into a single sum, thus obtaining

$$-\sigma^2_{\mathbf{H}_b} = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2 = -\frac{1}{N_T^2} \sum_{\vec{k}} \frac{(\rho_i^2 + \alpha_0)(-\rho_0^2 + \rho_i^2 + \alpha_0)}{(\rho^2 + \alpha_0)^2},$$

that is,

$$\sigma^2_{\mathbf{H}_b} = \frac{1}{N_T^2} \mathcal{S}_{\mathbf{H}_b},$$

with the definition of a symbol for the sum over the momenta,

$$\mathcal{S}_{\mathbf{H}_b} = \sum_{\vec{k}} \frac{(\rho_i^2 + \alpha_0)(-\rho_0^2 + \rho_i^2 + \alpha_0)}{(\rho^2 + \alpha_0)^2}.$$

Although this sum is not manifestly positive, it is in fact positive, as can be verified numerically. If we think about the symmetrical limit $N_L = N_T$ it becomes clearer

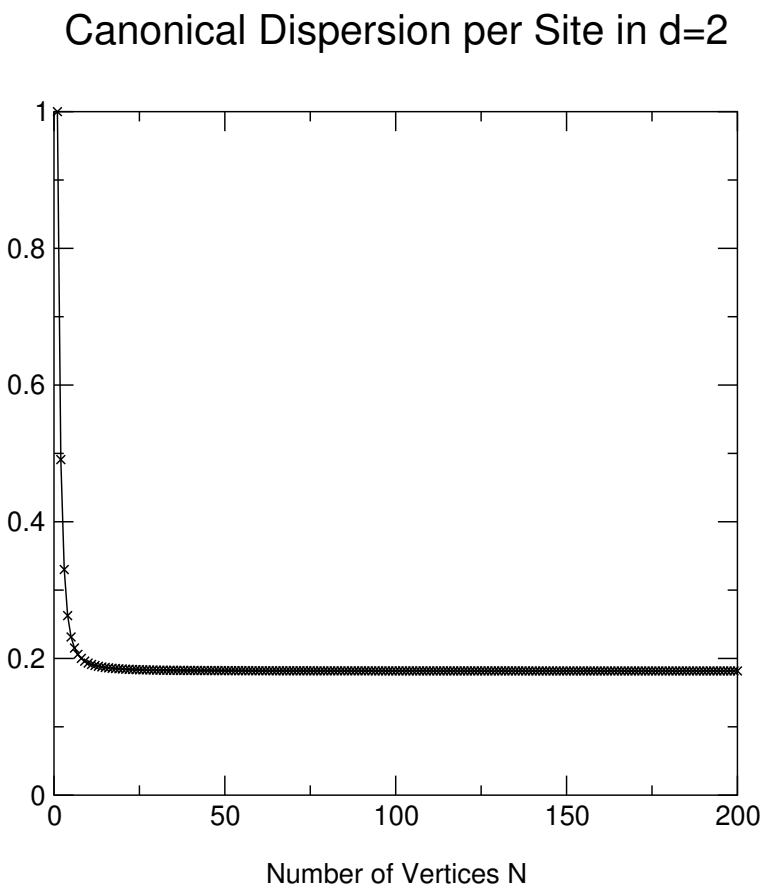

Figure 5.3.2: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 2$.

all cases we have that $\mathcal{S}_{\mathbf{H}_b} = 1$ for $N = 1$. In figure 5.3.1 we see that the case $d = 1$ differs from the others, because in this case the sum has a finite limit of the order of 1. In all the other cases the sum behaves as N^d, so that it is the ratio $\mathcal{S}_{\mathbf{H}_b}/N^d$ that is plotted in the graphs of figures from 5.3.2 to 5.3.5, a ratio which approaches a finite limit of the order of 1 in these cases.

Thus we see that the case $d = 1$ of quantum mechanics is the only one in which the vacuum is an eigenstate of the time-blocked Hamiltonian H_b. It suffices to observe that in this case we have for the dimensionfull dispersion $\Sigma_{\mathbf{H}_b} = \sigma_{\mathbf{H}_b}/a$, which is the one that corresponds to the dimensionfull physical energy, the behavior in the limit of large N_T,

$$\Sigma^2_{\mathbf{H}_b} \sim \frac{1}{T^2},$$

so that it is enough to make $T \to \infty$ for the dispersion to vanish. Note that we may take first the limit $N_T \to \infty$ and only after that make T go to infinity. In

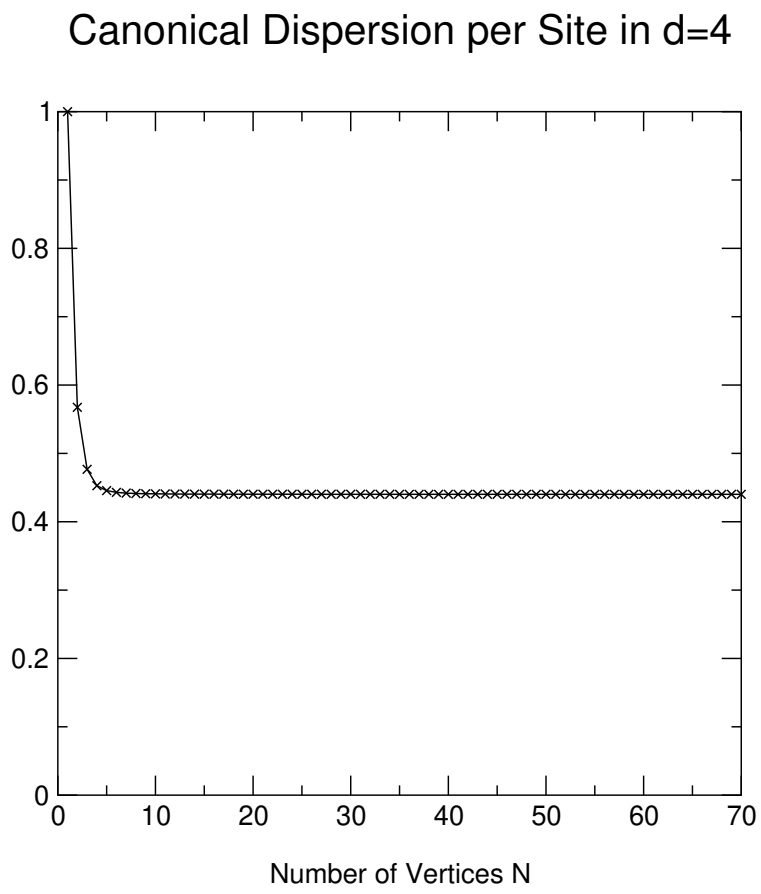

Figure 5.3.4: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 4$.

there is a qualitative difference in the results is the case $d = 1$, whose sum no longer has a finite value as was the case for the canonical definition. Note that figure 5.3.6 shows the dispersion per site, not simply the dispersion like figure 5.3.1 does. We see that according to the usual definition of the expectation values the sums behave as N^d in any dimension. All that one can conclude form these results, based on what happens in the case $d = 1$, is that the most sensible way to calculate the dispersion of the Hamiltonian is the canonical way. But there is no qualitative change in the situation in the case $d \geq 2$.

Note that in the case of quantum mechanics, although the sum now diverges as N_T, this still does not prevent us from making the dimensional dispersion go to zero in the limit, since in this case we have for $\Sigma_{\mathbf{H}'_b} = \sigma_{\mathbf{H}'_b}/a$

$$\Sigma^2_{\mathbf{H}'_b} \sim \frac{N_T}{T^2},$$

so that we can make the dispersion go to zero in limits in which we make T increase with N_T is a sufficiently fast way. This type of limit is the same that we are

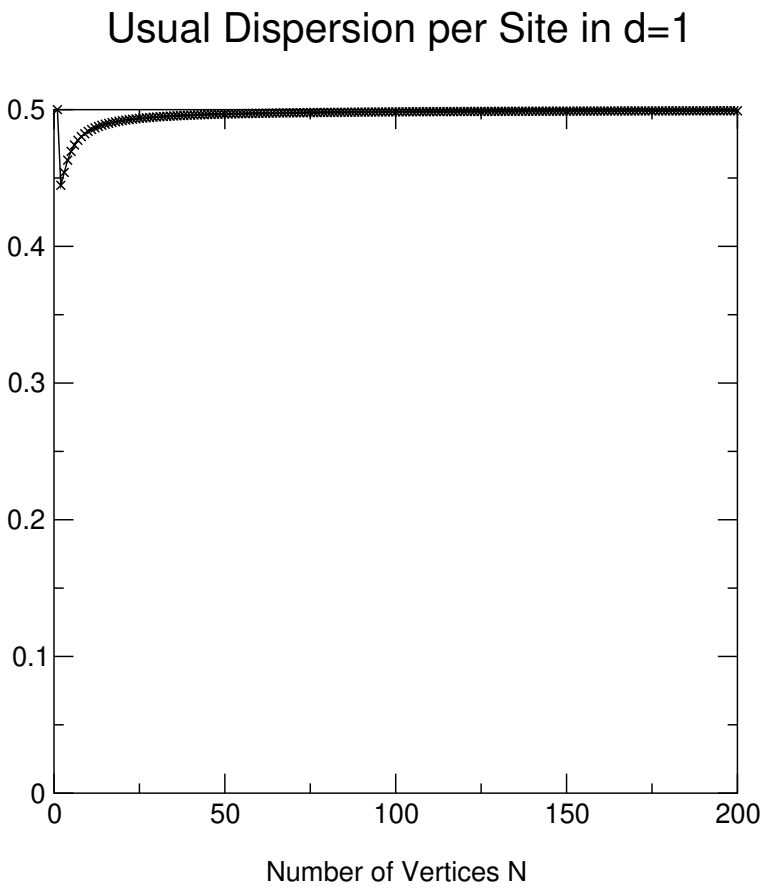

Figure 5.3.6: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 1$.

where we recall that T is the temporal size of the box. We see that in the case $d = 1$, since $\mathcal{S}_{\mathbf{H}_b}$ tends to a constant, the dispersion goes indeed to zero when we make $T \to \infty$, so that in this case the vacuum state is indeed an eigenstate of the blocked Hamiltonian. However, in all other cases the fact that the sum $\mathcal{S}_{\mathbf{H}_b}$ diverges as N^d means that we have $\Sigma^2_{\mathbf{H}_b} \sim N^d/T^2$, so that it is not possible to make the dispersion go to zero in the limit, and therefore in all these cases the vacuum state is *not* an eigenstate of the Hamiltonian. The borderline case is the case $d = 2$, in which we have

$$\Sigma^2_{\mathbf{H}_b} \sim \frac{N^2}{T^2}.$$

We see here that, if we make T increase in the continuum limit in a sufficiently fast way, in order to compensate the increase of N, we end up preventing the limit from being in fact a continuum limit, since in order to cause the dimensionfull width to vanish it is necessary to make $a \to \infty$ instead of $a \to 0$. We can see this if we recall that $T = Na$, so that the expression above can be written as

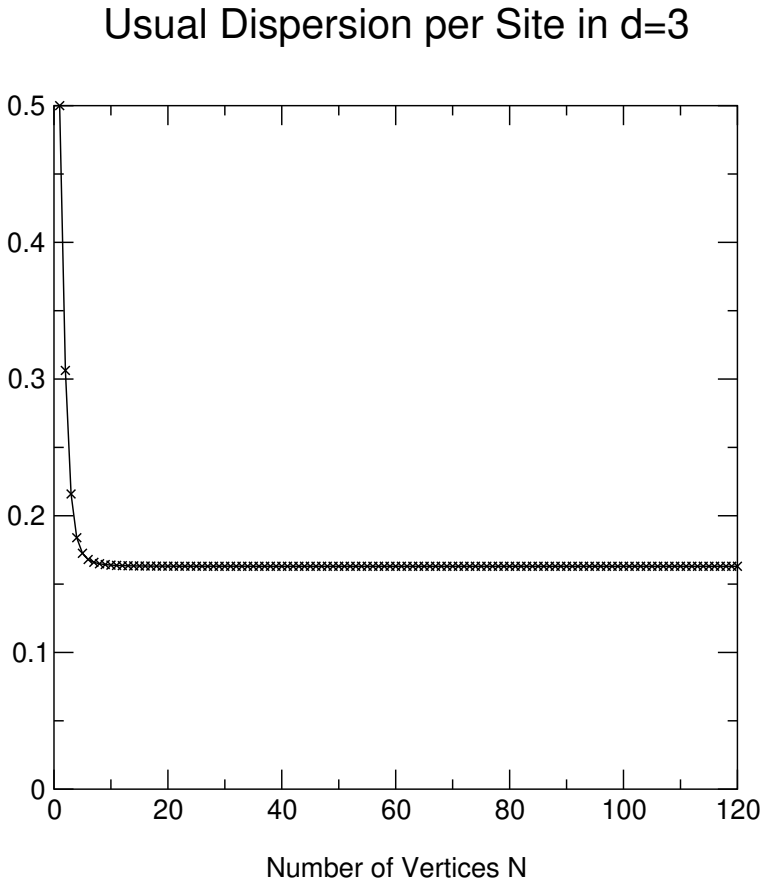

Figure 5.3.8: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 3$.

for $d \geq 2$ behave simply as N_T when we take the first limit. In fact, examining the behavior of the terms of the sums in the limit we can see that the sums tend to the value $N_L^{d-1} N_T$. Writing explicitly the general term $t(\vec{k})$ of the sum for the case of $\mathcal{S}_{\mathbf{H}'_b}$ we have

$$t(\vec{k}) = \left[\frac{-4 \sin^2\left(\frac{k_0 \pi}{N_T}\right) + \sum_i 4 \sin^2\left(\frac{k_i \pi}{N_L}\right) + \alpha_0}{4 \sin^2\left(\frac{k_0 \pi}{N_T}\right) + \sum_i 4 \sin^2\left(\frac{k_i \pi}{N_L}\right) + \alpha_0} \right]^2 .$$

Recalling that $\alpha_0 = m_0^2 a^2$ for some finite mass m_0, which implies that $N_T^2 \alpha_0 = m_0^2 T^2$, as well as that for finite k_0 and $N_T \to \infty$ the argument of the sine function goes to zero, so that we may approximate it by its argument in the first terms in the numerator and in the denominator, we may multiply numerator and denominator by N_T^2 and write, for most terms in the sum, that

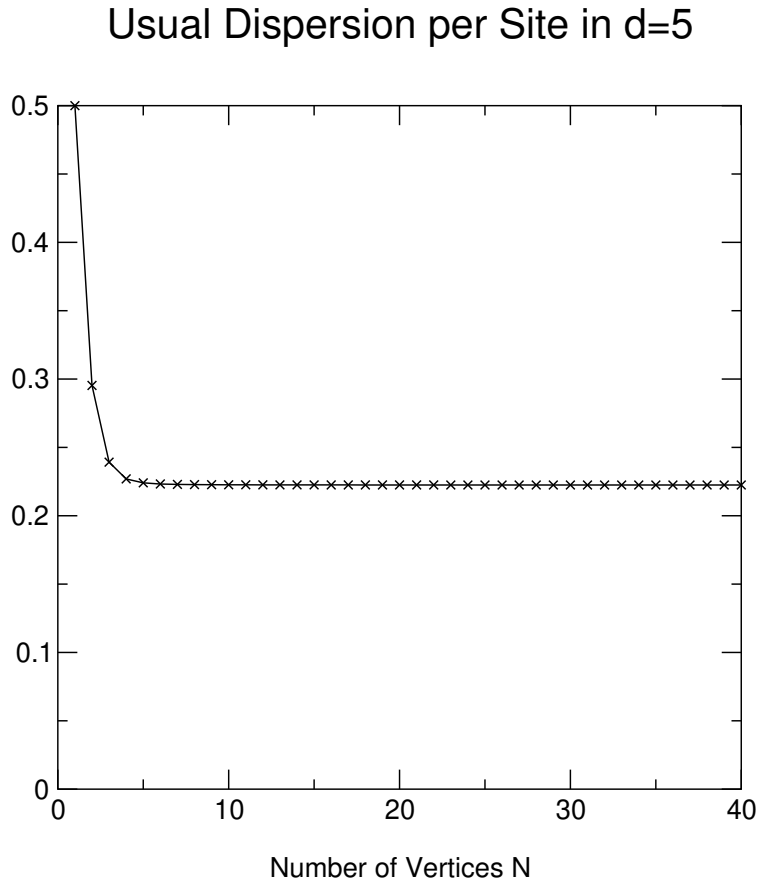

Figure 5.3.10: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 5$.

continuum limit. It follows that the term involving m_0 always becomes negligible in the limit, besides the fact that its presence would not change, in any case, the fact that the terms of the sum $\mathcal{S}_{\mathbf{H}'_b}$ tend to 1. As one can see, in this type of asymmetrical limit all the sums tend to $N_L^{d-1}N_T$ in the limit, diverging, therefore, as N_T in the first limit involved. The same type of behavior can be verified for the sum $\mathcal{S}_{\mathbf{H}_b}$ (problem 5.3.14).

Note that this argument for the evaluation of the sums is not completely rigorous, because it is clear that there are always some terms of the sums for which k_0 is of the order of N_T and for which we cannot approximate the sine function by its argument. If one examines the behavior of these terms one realizes that we may have over-evaluated the sums. However, with basis on the fact that these terms were not enough to avoid the divergent behavior of the sums as $N_L^{d-1}N_T$ even in the case of the symmetrical limit, in which they are relatively more important, we may expect that they do not change the divergent behavior of the sums in our limit here. At most, we may expect a change in the multiplicative constant, to the effect that

the same type of behavior that we saw before in the case of the fully asymmetrical limits. In this case, since both N_T and N_L increase in the limit, all the sine functions that appear in the terms of the sums can be approximated by their arguments. For example, in the case of $\mathcal{S}_{\mathbf{H}'_b}$, which we examined before, we now have

$$t(\vec{k}) \longrightarrow \left[\frac{-(2\pi k_0)^2 + (N_T/N_L)^2 \sum_i (2\pi k_i)^2 + (N_T/N_L)^2 m_0^2 L^2}{(2\pi k_0)^2 + (N_T/N_L)^2 \sum_i (2\pi k_i)^2 + (N_T/N_L)^2 m_0^2 L^2}\right]^2 .$$

Due to the factor $(N_T/N_L)^2 = N_T^{2(1-q)}$, which still diverges because $q < 1$ implies that the exponent is strictly positive, it is still true that, as before, the second and third terms of the numerator and of the denominator diverge with respect to the first, so that the terms approach 1 for finite $\vec{k}$. Combining these results with the increase of T in the limit, as was discussed before, we obtain for the dimensionfull dispersion $\Sigma_{\mathbf{H}_b}$, for example, the behavior

$$\Sigma^2_{\mathbf{H}_b} \sim \frac{1}{T^2} N_L^{d-1} N_T = \frac{1}{N_T^{2p}\mathcal{T}^2} N_T^{q(d-1)} N_T = \frac{1}{\mathcal{T}^2} N_T^{1+q(d-1)-2p},$$

so that in order for $\Sigma_{\mathbf{H}_b}$ to vanish in the limit we must have $2p > 1 + (d-1)q$. Since $0 < p < 1$ this condition results in

$$\frac{1 + (d-1)q}{2} < p < 1.$$

We may satisfy all the conditions over p and q with, for example, the choice $q = C/(d-1)$, with some constant C in the open interval $(0, 1)$ and p chosen in the open interval $((C+1)/2, 1)$. The conclusion is that there is no qualitative change in the results when we include this type of simultaneous asymmetrical limit. It is always possible to find limits in which the dispersion of the energy goes to zero, so long as we make N_L increase slower than N_T in the limit, and so long as we also make T increase without limit in the limit.

However, none of these asymmetrical limits helps us to solve completely the problem of how to make the vacuum state become an eigenstate of the Hamiltonian and at the same time keep intact all the fundamental physical characteristics of the theory. The reason for this is that any limit that is not symmetrical, that is, any limit in which one has $N_L = N_T^q$ with $q \neq 1$, destroys the on-shell condition and causes the theory not to contain any states of particles with energy different from zero, in the continuum limit. We can see this writing once more the expression, in Minkowski space, of the energy of the state of one particle with momentum $\vec{k}$ which we discussed in section 5.2,

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

Let us recall that, since $T \to \infty$, this energy does not go to zero only if one of the two factors in which the denominator can be factored vanishes as $1/T$ in the limit. Writing explicitly the ρ's we have

We can improve to some extent our understanding of the difficulties that we face in the definition of the quantum theory of fields if we once again turn our attention to the interpretation of our lattice structure in the terms of usual quantum mechanics. If we take the limit in the completely asymmetrical form, keeping N_L fixed, our structure is reduced to the quantum mechanics of a certain number of degrees of freedom associated to the sites. It becomes in fact a set of coupled harmonic oscillators with mass M, located at the sites, with frequency $\omega = m_0 = \sqrt{K/M}$, whose elastic constant K is associates to the term $\alpha_0\varphi^2$ of the action by

$$\alpha_0 = \omega^2 a^2 = \frac{K}{M}a^2 = \frac{K}{M}\left(\frac{T}{N_T}\right)^2,$$

where T/N_T is the lattice spacing a in the temporal direction. Note that finite M and K imply that α_0 goes to zero in the limit, as usual. On the other hand, in the asymmetrical limit we should look at the term $\beta_0(\Delta_i\varphi)^2$ of the action, with $\beta_0 = 1$, as a coupling term between two oscillators at neighboring sites, a term which naturally depends on the difference of position (or rather of elastic elongation) $\Delta\phi = \sqrt{M}\Delta x$ between the two neighboring oscillators. This is an elastic interaction with spring constant K' between these two neighbors, but the coefficient involved is simply

$$\beta_0 = \frac{K'}{M}a^2 = \frac{K'}{M}\left(\frac{T}{N_T}\right)^2 = 1,$$

which does not go to zero in the limit like α_0 does, so that these interactions between neighbors are infinitely strong from the point of view of quantum mechanics, corresponding to $K' \to \infty$ when $N_T \to \infty$.

In order to compensate for this fact, making the elastic interactions between the sites finite in the limit, it would be necessary to make K' finite, which implies making $\beta_0 \to 0$ in the limit, which is equivalent to violating completely the relativistic symmetries of the action of the corresponding quantum theory of fields. In order to understand the significance of all this from the point of view of field theory, let us observe that from the point of view of that theory the introduction of $\beta_0 \neq 1$ is equivalent to the introduction into the system of a velocity ν different from the velocity of light $c = 1$, through the relation $\beta_0 = \nu^2$, so that we can now write the action as

$$\begin{aligned} S &= \frac{1}{2}\sum_s \left[(\Delta_0\varphi)^2 + \beta_0\sum_i(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right] \\ &= \frac{1}{2}\int \mathrm{d}^d x \left[(\partial_0\phi)^2 + \nu^2\sum_i(\partial_i\phi)^2 + m_0^2\phi^2\right]. \end{aligned}$$

If we consider the case of the massless theory $\alpha_0 = 0$, then this parameter is indeed the velocity of propagation of waves in the system (in its de-Euclideanized version, of course), which ceases to be $c = 1$ and becomes equal to ν. We now see that our condition for the regularization of the asymmetrical limit, thus leading to a

5.3.1. Consider the delta-functional type of state, defined by a statistical distribution that attributes to a given configuration φ_0 of the fields the probability 1 and to all other configurations the probability 0. In other words, we can represent such a state by the distribution

$$|\varphi_0\rangle \sim \prod_{\vec{x}} \delta[\varphi(\vec{x}) - \varphi_0(\vec{x})].$$

Show that this state is an eigenstate of all the observables of the theory, including the Hamiltonian. In terms of the traditional formalism you will be showing, for example, that

$$\varphi_{\rm op}|\varphi_0\rangle = \varphi_0(\vec{x})|\varphi_0\rangle,$$

where $\varphi_{\rm op}$ represents the field operator, as well as

$$\mathbf{H}_{\rm op}|\varphi_0\rangle = \mathbf{H}[\varphi_0(\vec{x})]|\varphi_0\rangle.$$

Observe that a state like this corresponds to a situation in which the field does not fluctuate at all and is, therefore, devoid of any physical meaning in the quantum theory.

5.3.2. Calculate the dispersion of the action S on the vacuum state. Consider carefully and in separate the terms in which $\vec{q} \neq \pm\vec{k}$ and those in which $\vec{q} = \vec{k}$. Among these last ones, consider in separate the cases in which the momentum vector corresponds to a real mode and those in which the mode has a non-vanishing imaginary part.

5.3.3. Calculate the dispersion of the observable number of particles $\mathcal{N}$ on the state of n particles with momentum $\vec{k}$. Consider carefully and in separate the terms in which $\vec{q} \neq \pm\vec{k}$ and those in which $\vec{q} = \vec{k}$. Among these last ones, consider in separate the cases in which the momentum vector corresponds to a real mode and those in which the mode has a non-vanishing imaginary part.

5.3.4. Calculate the dispersion of the projector $\mathcal{N}_{\vec{k}}$ of the number of particles with momentum $\vec{k}$ on the state of n particles with momentum $\vec{k}$. Consider carefully and in separate the terms in which $\vec{q} \neq \pm\vec{k}$ and those in which $\vec{q} = \vec{k}$. Among these last ones, consider in separate the cases in which the momentum vector corresponds to a real mode and those in which the mode has a non-vanishing imaginary part.

5.3.5. Relate, in the case of the Hamiltonian without the average over the temporal block, the dispersion $\sigma_H^2 = \langle \mathbf{H} \rangle^2 - \langle \mathbf{H}^2 \rangle$ with the dispersion $\sigma_{H'}^2 = \langle \mathbf{H}' \rangle^2 - \langle \mathbf{H}'^2 \rangle$, doing the integration over the variable $\bar{\pi}$ and thus showing that

$$\sigma_H^2 = \sigma_{H'}^2 + \imath \langle \mathbf{H}' \rangle.$$

5.3.10. Write the dispersion $\sigma_{H'}$ of the non-blocked Hamiltonian in the $d = 1$ case of quantum mechanics, using the usual, non-canonical, definition of the expectation values. Evaluate the behavior of the sums that appear in this result in the $N_T \to \infty$ limit, just as was done in problem 5.3.9. Use your results to show that the corresponding dimensionfull dispersion behaves in the limit as

$$\Sigma^2_{H'} \sim \frac{N_T^2}{T^2},$$

showing in this way that, in this case, it is not possible to take the limits $N_T \to \infty$ and $T \to \infty$ in such a way that we have both that $a \to 0$ and that this dimensionfull dispersion vanishes in the limit.

5.3.11. Write a collection of programs to calculate, in the symmetrical case $N_L = N_T = N$, as a function of N, in dimensions from $d = 1$ to $d = 5$, the sums $\mathcal{S}_{H_b}$ that appear in the expression of $\sigma^2_{H_b}$. Also do the same for the sums $\mathcal{S}_{H'_b}$ that appear in the expression of $\sigma^2_{H'_b}$. Use your programs to reproduce the graphs which are shown in the text.

5.3.12. Calculate in detail the quantity $\langle H'^2_b \rangle$ in the case in which N is even, thus completing the argument presented in the text, where the calculation was presented in the case in which N is odd. Be mindful of the correct identification and counting of all the terms of the sums over the momenta, and remember that in this case both the value 0 and the value $N/2$ of the components k_μ are associated to real Fourier components of the fields.

5.3.13. Calculate the dispersion of the blocked Hamiltonian $\mathbf{H}_b$ on the state of one particle with momentum $\vec{k}$.

5.3.14. Show, examining the behavior of its terms, that the sums $\mathcal{S}_{H_b}$ tend to $N_L^{d-1} N_T$ in the asymmetrical limit, in which we make $N_T \to \infty$ with fixed N_L. Do the same in the case of the simultaneous asymmetrical limit, in which we make $N_L = N_T^q$ with $0 < q < 1$. In either case assume that we can limit the discussion to terms with finite k_0.

5.3.15. Write programs to calculate, in the asymmetrical case $N_L \neq N_T$, as functions of N_T and for a fixed value of N_L, in dimensions from $d = 2$ to $d = 5$, the sums $\mathcal{S}_{H_b}$ that appear in the expression of $\sigma^2_{H_b}$. Also do the same for the sums $\mathcal{S}_{H'_b}$ that appear in the expression $\sigma^2_{H'_b}$. Use your programs for values of N_L from 4 to 20 and values of N_T from 1 to 200, thus showing that these sums do in fact diverge as N_T in this type of asymmetrical limit.

respect to averages over the temporal direction. However, in a relativistic theory it is essential that the averages be over both the spacial and the temporal dimensions, because relativistic transformations mix the spacial and temporal coordinates, so that there can be no invariant meaning to a purely spacial average.

The introduction of external sources provided us with a solid handle to probe into the behavior of the models, both in the classical case and in the quantum case. It leads in the usual way to the introduction of the functional generators of the correlation functions, which we developed directly on the Euclidean lattice, and ultimately to the concept of the effective action. We managed to establish a rather complete physical interpretation of the effective action, not only as the functional generator of irreducible correlation functions, but also as a shorthand for the response of the models to the introduction of external sources. In either capacity the effective action can be seen as a useful condensation of the complete physical content of the model. Due to all this the effective action helps significantly with the interpretation of the classical limit of the quantum theory.

An exploration of the mathematical character of the dimensionless field configurations that contribute in a dominant way to the most important observables of the theory resulted in the unexpected and even surprising conclusion that these functions are typically discontinuous at all the points of their domains. One may say that the set of all continuous configurations is of zero measure within the ensemble of the theory, in the sense that their exclusion from the ensemble would not affect the expectation values which are physically relevant. However, most of the more direct consequences of the discontinuity of the field configurations will be found only in the second volume of this series.

Although this situation leads to the usual non-differentiable but still continuous behavior of the paths in the path-integral approach to non-relativistic quantum mechanics [5], in the case of quantum field theory with $d \geq 3$ it leads to infinite discontinuities of the dimensionfull field. This means that, while in the quantum-mechanical case it is possible to represent the configurations by random walks, any such representation in the case of quantum field theory is incorrect unless one takes the continuum limit in one of the asymmetrical ways described in section 5.3, in which case one looses in one fell blow both relativistic invariance and the complete structure of particle states, as discussed in that section.

Finally, a quite complete realization on the lattice of the concept of energy was also obtained. The situation regarding the energy of the vacuum state is qualitatively similar to the corresponding situation in the traditional approach. We also managed to define a complete set of particle states, which have the correct energy and momenta. In the continuum limit there are both virtual particles and real physical particles, which are clearly identified by the all-important on-shell condition, which must be satisfied by states representing relativistic particles. States that correspond to virtual particles can be shown to become energetically degenerate with the vacuum in the limit.

In this formalism the particles are closely associated to the normal modes of oscillation of the cavity represented by the lattice, and are thus more readily represented

direction from the very beginning.

One perceives that the formalism of Osterwalder and Schrader is built around the idea that the Hamiltonian is to be the generator of time translations, and assumes that states and operators are to be defined at completely sharp instants of time. The formalism assumes that there is a Hilbert space and that there is a Hamiltonian, both with the usual properties found in non-relativistic quantum mechanics, and proceeds to construct them. In order to do this it must require that $N_T = \infty$ from the start. One can have either a finite or an infinite N_L, but one absolutely must have an infinite N_T. By contrast, the states defined here are intrinsically d-dimensional objects, not $(d-1)$-dimensional objects existing at a sharply defined time. On the same token, observables can only be measured on the extent of d-dimensional boxes, not at sharply defined times or spacial positions.

It is important to emphasize that there is in fact no conflict between the results that we found here and those of the Osterwalder-Schrader formalism, because if we assume that the limits are to be taken in the asymmetrical way, then it is in fact possible to adjust things so that the vacuum becomes an eigenstate of the Hamiltonian, as we have shown in section 5.3. What is at issue here, due to the nature of the results we found, is not simply the existence or not of Hilbert spaces that can be associated to the structure of the theory, but their usefulness in representing systems of fundamental quantum fields of physical interest, having relativistic invariance and that contain relativistic particles with finite and non-vanishing additional energies above the energy of the vacuum.

One is inevitably led, then, to consider how the definition of the theory could possibly be changed in order to recover the usual Hilbert-space structure, without violating the basic precepts relating to the definition of the mathematical structure of a physical theory, that were discussed in the first chapter. However, it seems that any trial at this leads to some physically unacceptable loss. Taking the asymmetrical limit does the job, but leads to loss of relativistic invariance, and to the collapse of the whole structure of particle states into the vacuum. This is similar to trying to redefine states and observables at sharply defined times, as is done in the Osterwalder-Schrader formalism, and that leads to the loss of the connection between the particles and the modes of the d-dimensional cavity. Since this connection and the on-shell condition lead naturally, in the non-relativistic limit, to a corresponding connection between physical particles and the modes of the remaining $(d-1)$-dimensional cavities, the loss is a serious one.

It is a well-known experimental fact that physical particles are closely connected to the modes of oscillation of the corresponding fields when they are within a cavity. This can be shown experimentally by the introduction of excited atomic states into high-quality electromagnetic cavities [7]. If the cavity is tuned so that none of its modes has the frequency of the photon that the atom must emit in order to decay, then its spontaneous decay can be very effectively delayed or prevented. If, on the other hand, the cavity is tuned to the frequency of the photon, then the spontaneous decay can be stimulated, or a certain mode of decay can be stimulated at the expense of others. This shows in a decisive way that the photons, the particles of

circumstance we have phenomena involving only long wavelengths and long-range correlations, then we may use large blocks in order to analyze that situation, and hence the block variables will fluctuate very little, leading to a semi-classical or even to a classical limit, as the case may be.

However, we do loose something with the Hilbert-space formalism, namely its description of the temporal evolution process, in the usual way that works so well for non-relativistic quantum mechanics. We are faced therefore with the challenge of finding out how to define and handle the evolution in time of d-dimensional objects, which do not correspond to sharply-defined moments of time.

6.2 Blocked Temporal Evolution

Before anything else, the reader should be warned that this section contains material which is of a speculative nature, currently unsupported by either calculations or simulations. We mean here only to suggest an idea of how one of the remaining problems with the structure of the theory could be solved, thus seeding ideas for future research. No more than some intuitive reasoning will be offered here in support of the ideas presented.

One of the main remaining open problem in the basic structure of our formalism is the representation of temporal evolution. Now, one must realize that the loss of the Hilbert space formalism does not necessary imply the loss of the concept of temporal evolution, but only the loss of its usual representation within that formalism. We mean to propose here the substitution of the sharp-time temporal evolution of non-relativistic quantum mechanics by a blocked-time temporal evolution, which we will describe qualitatively on the Euclidean lattice. Of course, in order to represent temporal evolution in Euclidean space and be able to analyze it in any kind of detail, one would have to first understand in more detail than usual the relationship between the dynamics of the Euclidean and Minkowskian theories. However, here we will just propose the idea and ignore any such concerns.

On a fundamental level temporal evolution is a relationship between measurements made at different times. Since all measurements can only be done in the complete extent of d-dimensional regions of space-time, we will define the temporal evolution in terms of d-dimensional boxes. The idea is that temporal evolution will be a relationship between two consecutive d-dimensional regions of space-time, each holding a copy of a local quantum state. The transmission of information between them will be done through a $(d-1)$-dimensional surface, which is the interface between the two consecutive regions. We will propose the idea in the context of two identical lattices, each one contained in one of the two boxes, using the context of a stochastic simulation of the resulting system as a way to illustrate the ideas.

The drawing in figure 6.2.1 may help the reader to visualize the proposed system. In this figure the sets of 8 sites connected in circles are representations of the temporal directions of two d-dimensional lattices. The spacial dimensions of the lattices are omitted for simplicity of the drawing. In order to simplify the treatment of the

never the other way around, and hence we see that this scheme indeed implements an arrow of time.

Let us now discuss why would one think that such a $(d-1)$-dimensional boundary could have such a large effect, over the whole interior of the second box. The fact is that the effect of a $(d-1)$-dimensional boundary over a d-dimensional region of space is usually very large. One can consider, for example, the classical static case of electrical charges distributed over a two-dimensional surface: such a two-dimensional plane of surface charge will fill homogeneously the whole three-dimensional space with an electric field, while a line of charge and a point charge have an effect that decays with the distance. Contrary to what seems to be the popular belief in some quarters, the same is true in the quantum case. If a $(d-1)$-dimensional surface is covered with sources, then what is left as a propagation direction is the single remaining dimension, and in that direction there is therefore no solid-angle, that is, there is no angular increase with distance to promote the damping of the influence of the sources.

In the second box the $(d-1)$-dimensional boundary surface acts very much like an external source, except for the fact that it is dynamical and not static, that is, it is a fluctuating source with a dynamics comparable to the internal dynamics of that lattice. Hence, what will propagate from it into the second box is not a static field but a probability distribution of values for the field, which will therefore affect the distribution within the second box. It is interesting to note that this is a new kind of "fixed" boundary condition, in which the values of the field itself are not fixed, but the *distribution* of the values of the field is a fixed and given one. This is the only kind of fixed boundary condition that is physically realizable in the quantum theory, because one can never really fix the values of the intrinsically fluctuating fundamental field.

Although it should in principle be possible to deal with this whole scheme by analytical means in the Gaussian model, since all distributions are Gaussian, we currently do not know how to do this. The only treatment currently available would be by means of stochastic simulations, which puts the subject outside the scope of this book. But we may describe how one would go about doing this analytically. In order to determine which probability distribution should be implemented within the $(d-1)$-dimensional boundary surface of the second box, one must take the d-dimensional ensemble within the first box and integrate out all the variables except those within the chosen $(d-1)$-dimensional interface, thus producing an explicit representation of the distribution over this surface, which is a consequence of the distribution within the whole box. One can then use this distribution as a boundary condition for the second box.

It is currently difficult to guess any details about this new type of temporal evolution, but it is a distinct possibility that propagation into the second box may depend on the nature of the state in the first box, for example on whether it satisfies or fails to satisfy the on-shell condition. It is reasonable to think that only on-shell states should propagate, specially in the continuum limit. Note that on-shell waves necessarily correspond to modes with time-like momenta and hence have wave

the sigma models. In the next volume of this series we intend to present what is currently known about this. The most important consequences are related to a new insight into and interpretation of the perturbative scheme of approximation for such models, including a critical review of the process known as perturbative renormalization, and the discovery of a connection of the lattice formalism with the metrical geometry of space-time, including the phenomenon of the generation of metric curvature by the quantum fields, under certain circumstances.

Some of the central concepts involved in the theory certainly need further research and development, such as, for example, the process of passing from Euclidean space to Minkowski space and vice-versa. Another central issue is the complete definition of the concept of observables. In the development presented in this book we established some of the necessary conditions for a quantity to be an observable, but the sufficiency of these conditions is still open to question. This topic is certainly related to the concept of the measurement process in the quantum theory, which we have not touched at all, and which is probably one of the most difficult aspects of the theory. The question of the realization of the statistical interpretation of measurements within the structure of the theory is also related to the issue of the process of measurement, and therefore open to further exploration and discussion.

Finally, the extension of these explorations to more realistic types of field, such as vector fields and fermionic fields, would be a very important step towards the completion of the structure. While the realization of vector fields on the lattice is a very well-known subject, the same is not true for fermionic fields, which certainly represents one the major difficulties to be faced in future developments. The work in this area also lacks access to a sufficiently simple non-linear model that would not suffer from the triviality characteristic of the polynomial and sigma models of scalar fields. By the requirement of simplicity we mean a model that could be treated in a precise and complete way with what is currently known about the realization of fields on the lattice, which therefore must exclude fermionic fields. A model like this, containing true interactions between particles, and yet technically manageable on the lattice, would constitute an important tool for the further exploration and development of the theory.

It seems to us that there is ample room for further activity along the lines presented in this book. The use of lattices and of stochastic simulations not only establishes a practical calculational tool for the subject, it also constitutes a language in which one can discuss in a mathematically precise yet simple and clear way the issues and problems of the subject. This language allows for the free and profitable use of the imagination in the exploration of the underlying structure of the theory, followed when necessary by the computational effort needed to obtain precise answers to the questions posed. It is currently true, and may turn out to be the case permanently, that the routine use of computational resources on a large scale is an essential part of the research in this area. Fortunately, we live in a time when the availability of computer resources to the individual is increasing in an exponential way, so that the future prospects are very promising for those who acquire the necessary skills in the world of informatics.