The Gaussian Model

An Exploration into the Foundations of Quantum Field Theory

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Preface

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

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

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

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

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

Contents

Chapter 1

Conceptual Foundations

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

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

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

1.1 Philosophical Preliminaries

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

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

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

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

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

The next subject to be discussed here has to do with the nature of the limits involved in the mathematical definition of the theory. Although the mathematical structures involved in the theory will, by the end of the definition process, become *continuum* mathematical structures, we will require that such continuum structures be obtainable by means of limiting procedures starting from *finite* mathematical 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 freedom constantly, and we will arrive at a fairly complete definition of the observables only very slowly, using our mathematical and computational probes into the inner workings of the theory along the way.

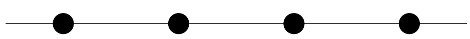
The last issue we would like to address here is that of the *closure* of the theory. By this we mean that, once it is defined completely in a concise way, all physical elements which are needed to describe objective physical reality must be contained within its structure, either directly as fundamental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

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

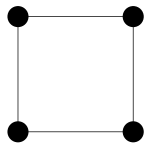
The complete description of the measurement process, including what is usually referred to as the reduction of the wave packet, and hence the complete definition of the physical observables, is probably only possible in the context of a complete and interacting theory, in which there are stable bound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

1.2 The Euclidean Lattice

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



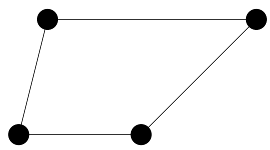
We have here four sites and five links in sequence, connecting sites which are neighbors to each other. Another lattice similar to this one could be obtained interconnecting the two loose ends of the outer links, resulting in the lattice



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,

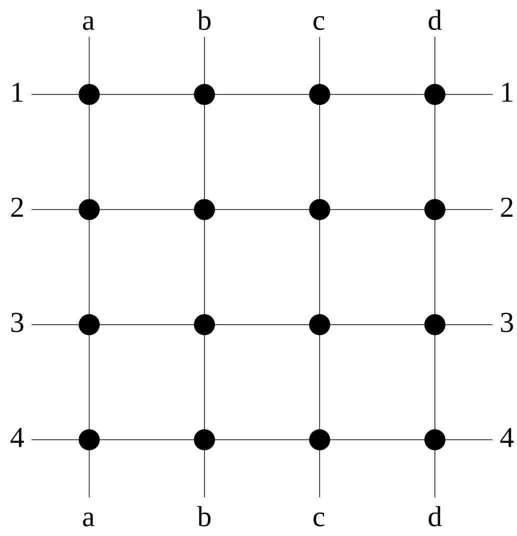


Figure 1.2.1: The basic elements of a typical two-dimensional lattice.

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

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

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

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

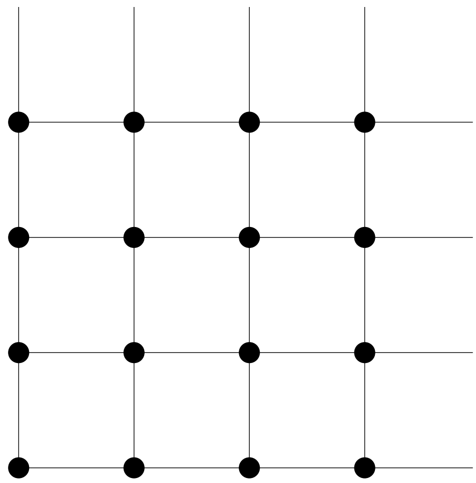


Figure 1.2.2: A simpler representation of a two-dimensional lattice with periodical boundary conditions.

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.

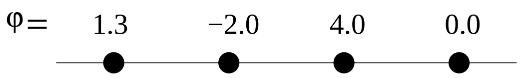
It is clear that the structure of the lattices can be generalized and made more complex in many different ways. We are taking here a small subset of the set of all possible lattices, which is particularly simple and symmetrical. Our strategy here is to focus attention only on the simplest cases, until 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.

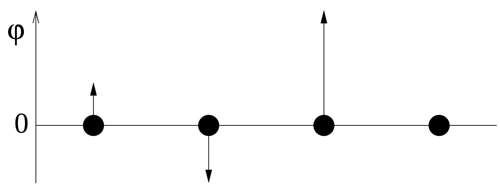
1.3 Fields on the Lattice

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

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

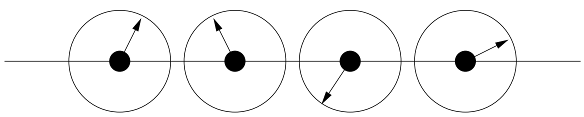


It is usual to represent this field by means of a set of arrows located at the sites, pointing along a real axis $\mathbb{R}$, with lengths given by the values associated by the field to each site,



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

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



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, $\mu = 1, \dots d$, 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

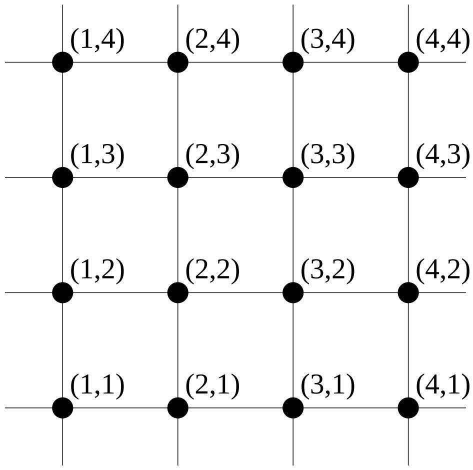


Figure 1.3.1: A system of integer coordinates in a typical two-dimensional lattice.

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

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

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

A possible example of an action S would be given by

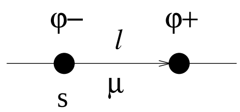
$$S[\varphi] = \sum_s \varphi^2(s).$$

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

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

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

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

Problems

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

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

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

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

Chapter 2

Classical Field Theory

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

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

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

2.1 Definition of the Classical Theory

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

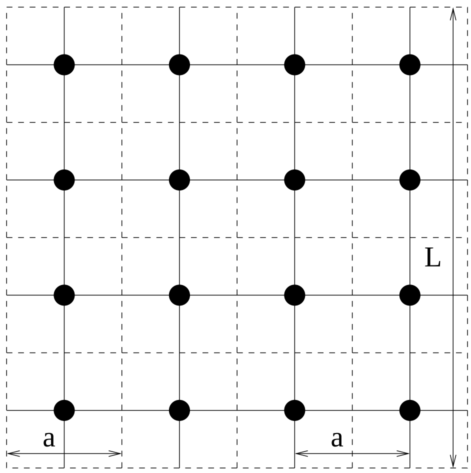


Figure 2.1.1: The geometrical elements of a periodical two-dimensional lattice.

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

We may now write the action S_0 in the form

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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).

2.2 Fixed Boundary Conditions

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

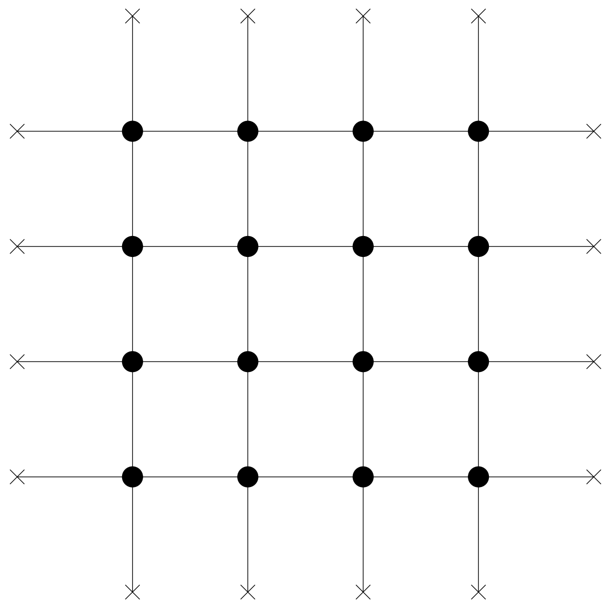


Figure 2.2.1: A two-dimensional lattice with fixed boundary conditions.

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

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

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

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

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

and we therefore have

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

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

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

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

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

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

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

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

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

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

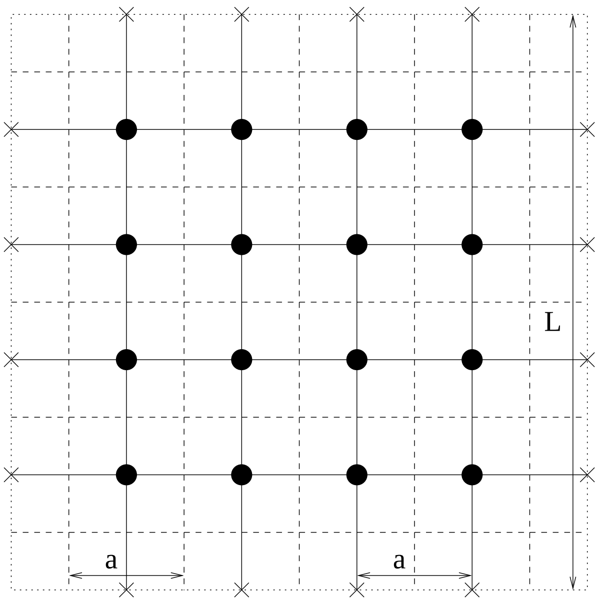


Figure 2.2.2: The geometrical elements of a two-dimensional lattice with a fixed boundary.

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

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

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

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

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

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

Problems

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

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

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

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

2.3 Finite-Difference Operators

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

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

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

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

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

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

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

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

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

In spite of the fact that in order to do this with the usual mathematical language of the continuum it may seem necessary to interpret the term $(\Delta_\mu\varphi)^2$ in a mixed 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, $\Delta_{(c)}^2$, related to the differences of second order given by

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

In the context of the classical theory this is related to a higher-order approximation $\Delta_{(c)}^2$ 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

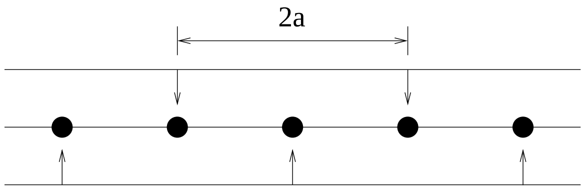


Figure 2.3.1: A one-dimensional double lattice.

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

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

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

Problems

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

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

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.

2.4 Space of Field Configurations

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

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

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

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

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

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

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

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

$$\left[\begin{array}{c} \varphi_1 \\ \cdot \\ \cdot \\ \cdot \\ \varphi_\iota \\ \cdot \\ \cdot \\ \cdot \\ \varphi_{N^2} \end{array}\right],$$

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

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

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

and the inversion operations are (problem 2.4.2)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Problems

2.4.1. 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.

2.5 Momentum Space

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

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

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

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

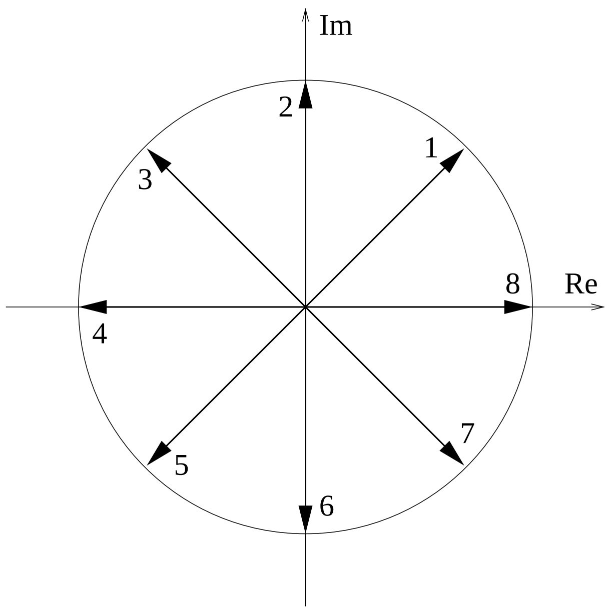


Figure 2.5.1: Example of a complex unit circle for $N = 8$.

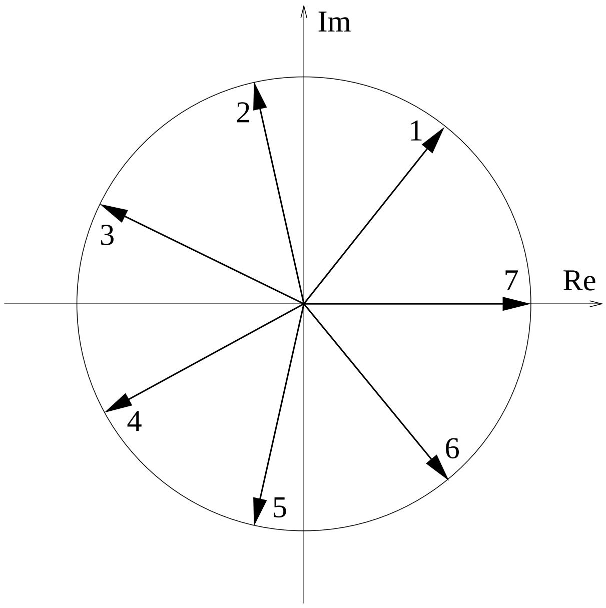


Figure 2.5.2: Example of a complex unit circle for $N = 7$.

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,

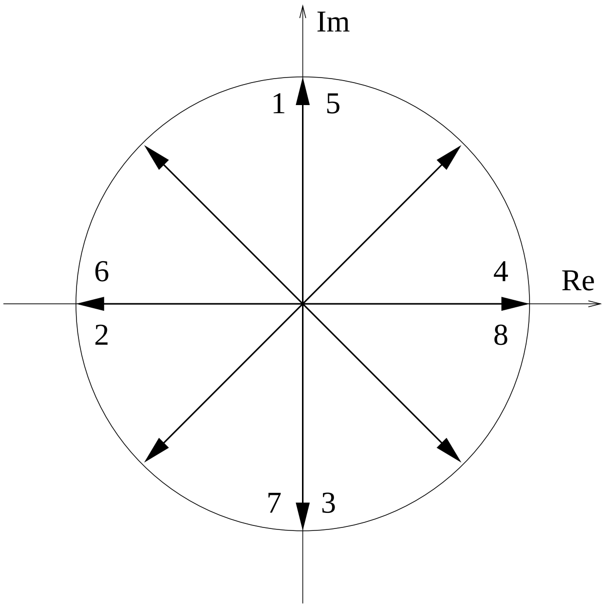


Figure 2.5.3: A double lap on the complex unit circle with $N = 8$.

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

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

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

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

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

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

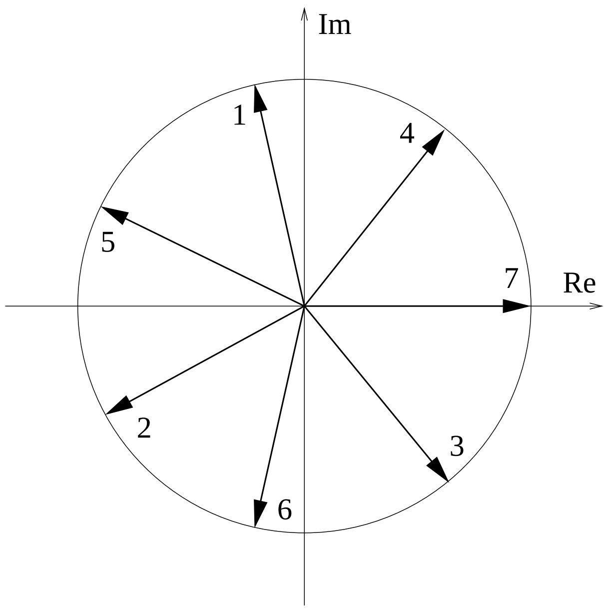


Figure 2.5.4: A double lap on the complex unit circle with $N = 7$.

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

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

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,

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

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

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

and *relation of completeness*,

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

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

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

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

Problems

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

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

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

2.5.4. 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

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

is contained within the set of phases given by

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

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.

2.6 Finite Fourier Transforms

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Problems

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

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

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 $\Delta_\mu^{(c)}$, 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

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

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

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

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

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

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

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

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

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

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

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

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

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

where ρ^2 is given by

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

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

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

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

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.

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

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

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

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

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

Observe that in this case, unlike the case of periodical boundary conditions, we cannot make $k_\mu = 0$ for any value of μ, since the corresponding eigenfunction would be identically zero. Besides this, for any μ the change $k_\mu \to -k_\mu$ will only change the sign of the eigenfunction and therefore does not produce an independent eigenfunction. Due to this, we do not have here the freedom we had in the periodical case, of choosing the range of variation of k_μ, which must be as given above. This 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 $f_{\vec{k}}^N(\vec{n})$ on finite lattices satisfy the orthogonality and completeness relations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}\widetilde{\varphi}(\vec{k}) &= \frac{1}{V}\int_V \mathrm{d}^d x f_{\vec{k}}^N(\vec{x})\varphi(\vec{x}),\\ \varphi(\vec{x}) &= \sum_{\vec{k}} f_{\vec{k}}^N(\vec{x})\widetilde{\varphi}(\vec{k}).\end{aligned}$$

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 $f_{\vec{k}}^{N}(\vec{n})$ given in equation (2.8.1) are eigenfunctions of the finite-difference Laplacian. Derive also the expression for the corresponding eigenvalues ρ_f^2.

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 $f_{\vec{k}}^{N}(\vec{n})$ 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 $f_{\vec{k}}^{N}(\vec{n})$ 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

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

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

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

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

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

2.9 Basis Transformations in Configuration Space

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

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

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

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

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

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

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

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

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

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

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

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

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

Problems

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

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

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

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

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

2.10 External Sources and Green Functions

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

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

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

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

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

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

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

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

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

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

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

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 $\vec{k}$,

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

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,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

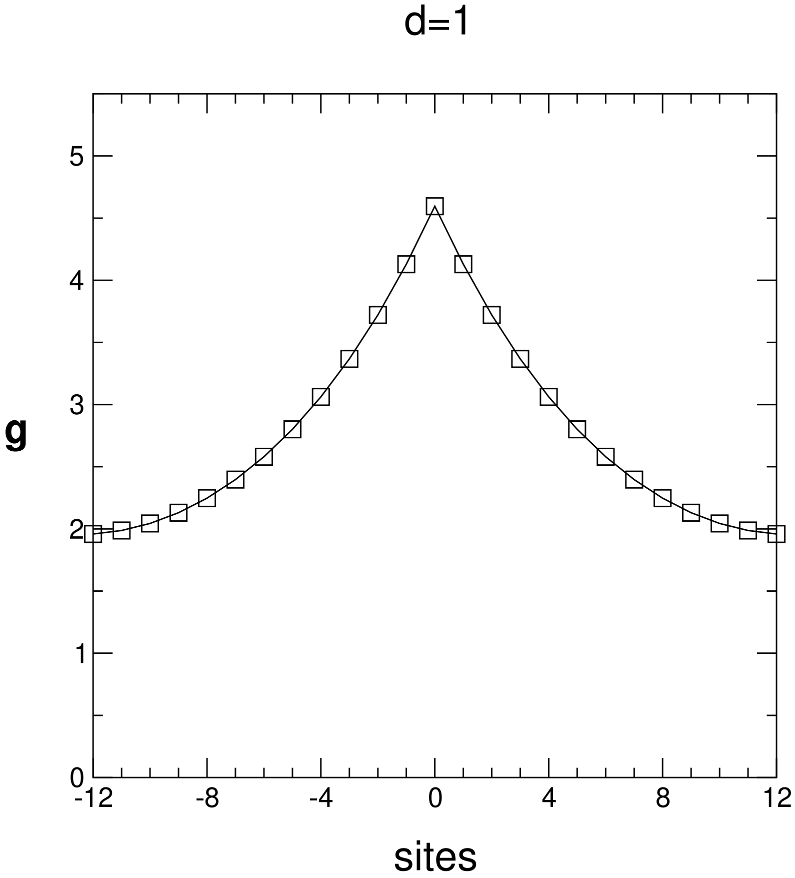


Figure 2.10.1: Periodical Green function in the case $d = 1$.

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

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

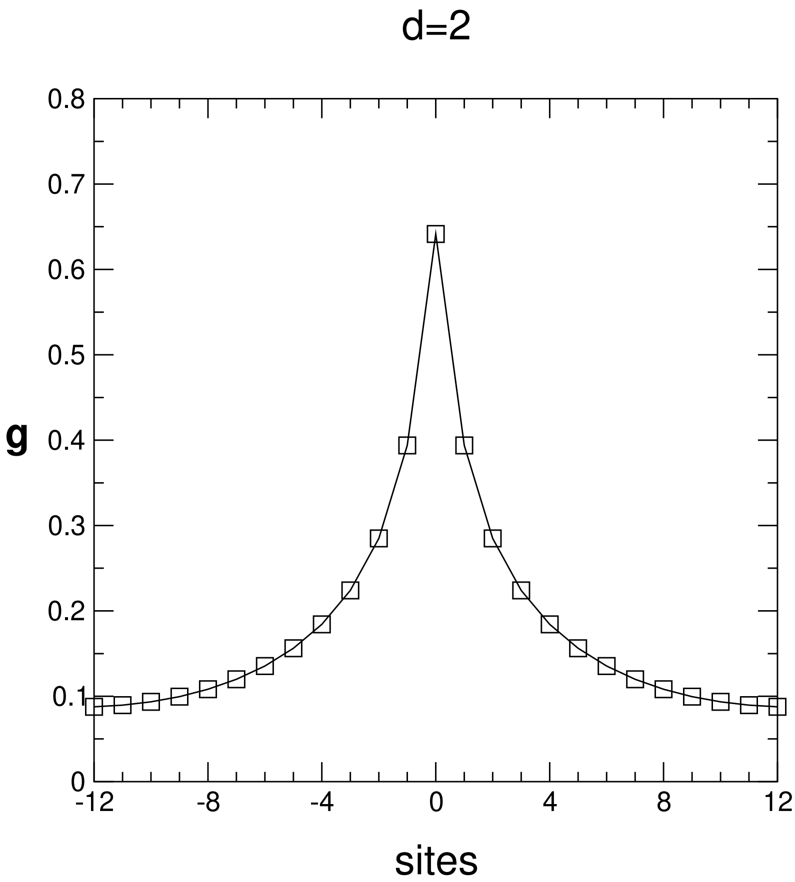


Figure 2.10.2: Periodical Green function in the case $d = 2$.

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

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

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

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

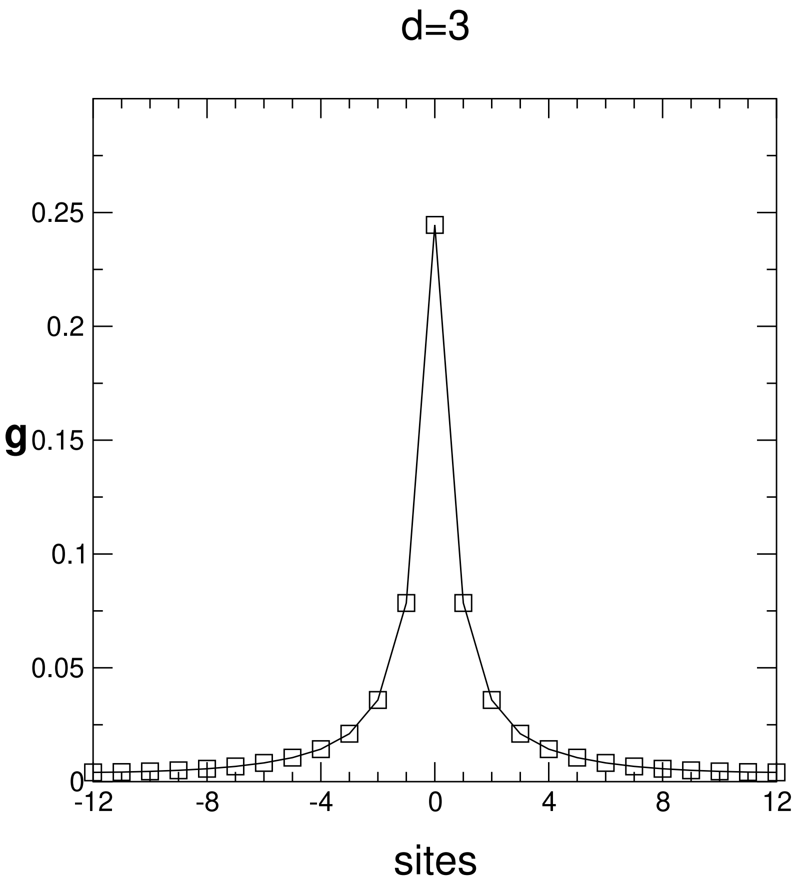


Figure 2.10.3: Periodical Green function in the case $d = 3$.

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

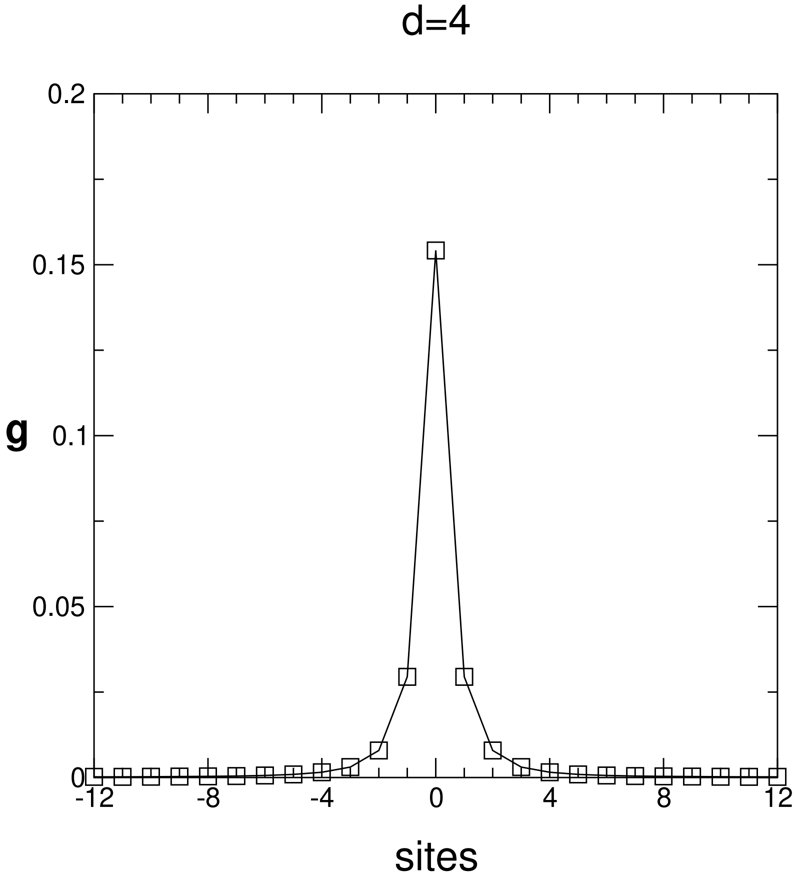


Figure 2.10.4: Periodical Green function in the case $d = 4$.

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

Problems

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

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

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 $f_{\vec{k}}^N(\vec{n})$ which is appropriate to this type of boundary conditions,

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

which satisfy the orthogonality and completeness relations

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

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

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

Substituting these expressions in (2.11.1) we have

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

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

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

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

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

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

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

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

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

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

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

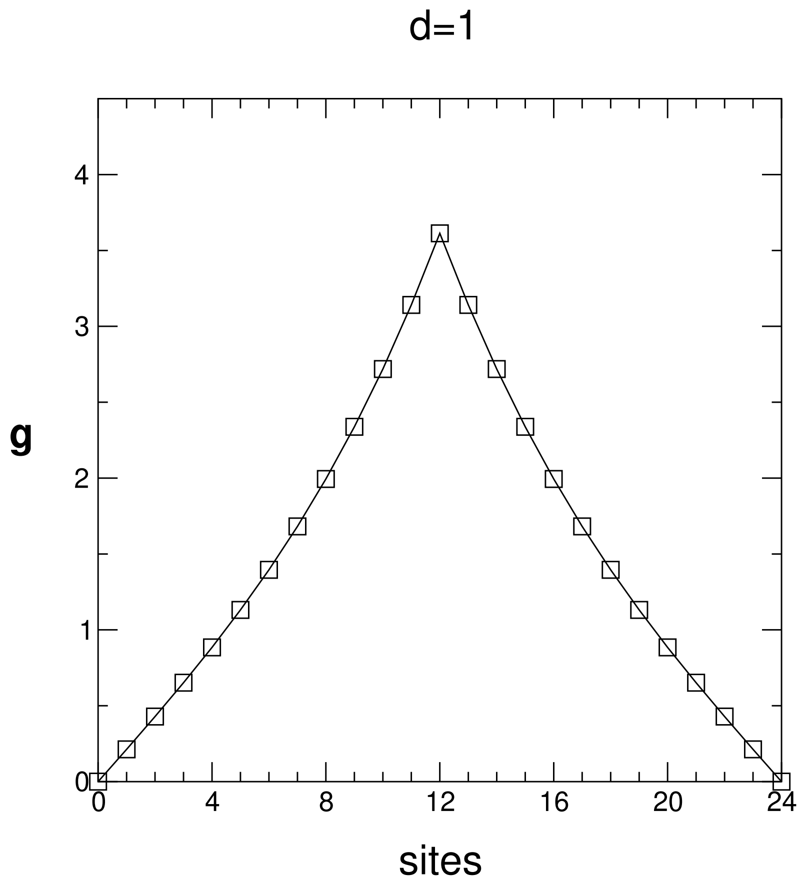


Figure 2.11.1: Green function with fixed boundary conditions for $d = 1$.

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,

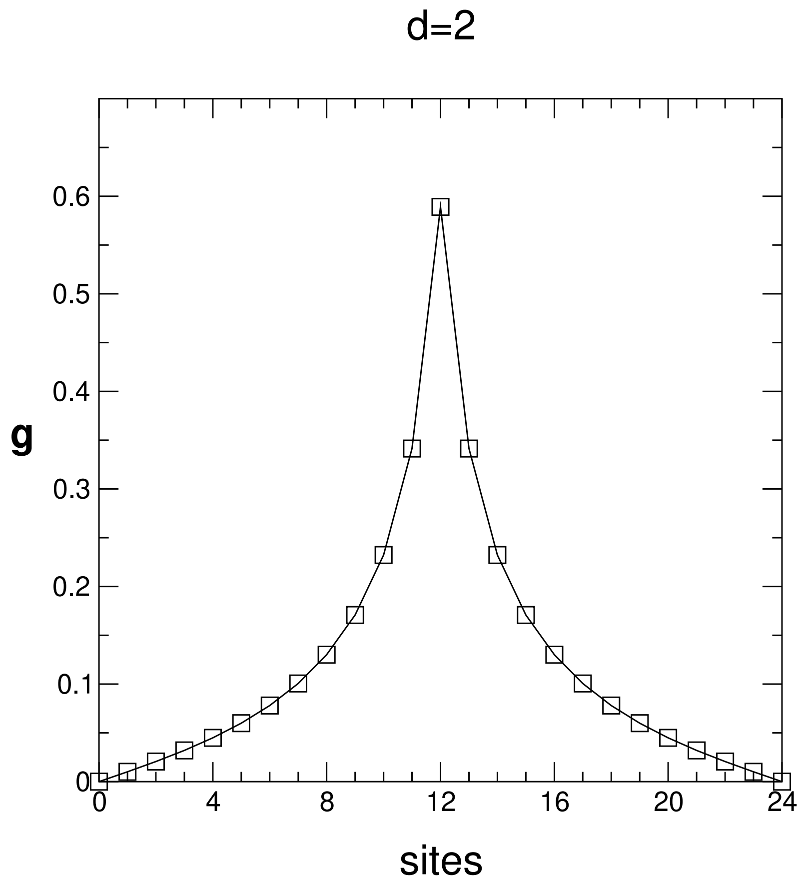


Figure 2.11.2: Green function with fixed boundary conditions for $d = 2$.

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

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

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

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

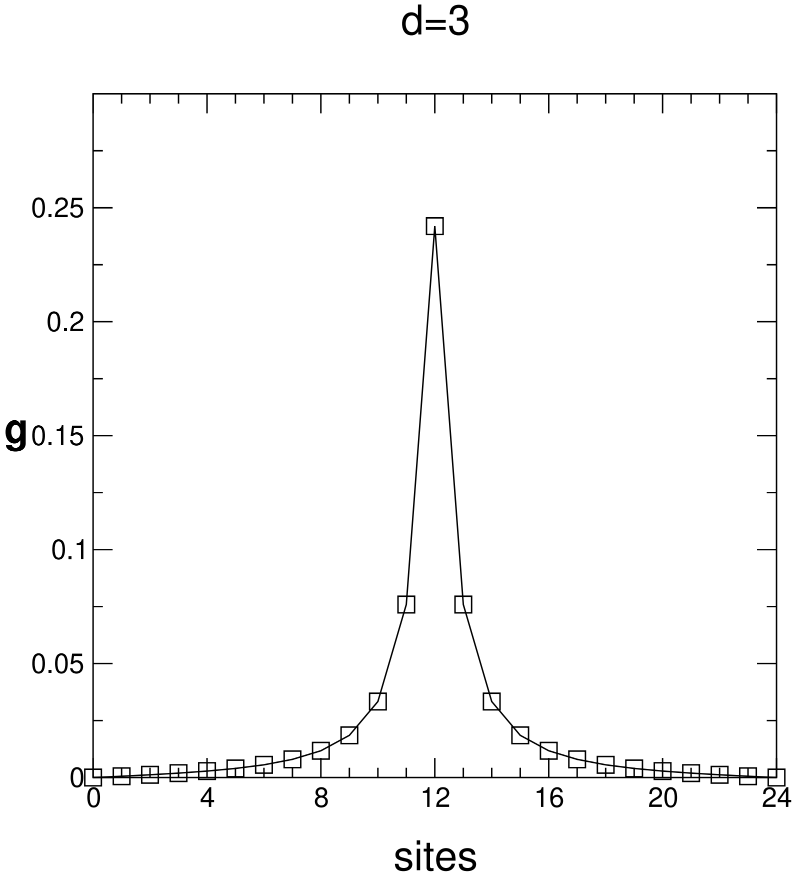


Figure 2.11.3: Green function with fixed boundary conditions for $d = 3$.

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

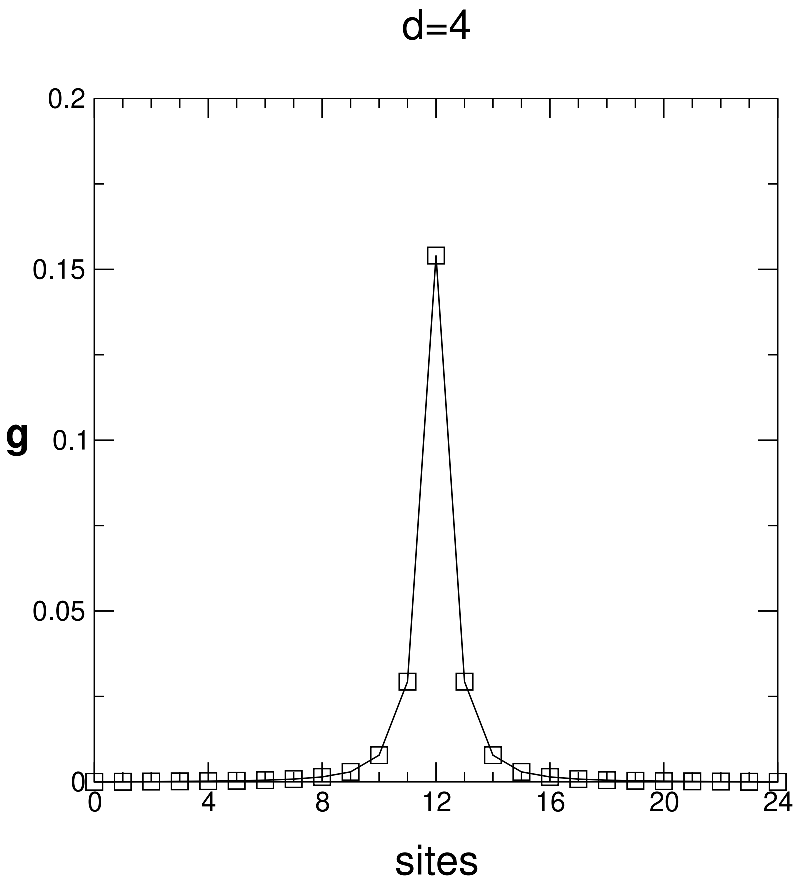


Figure 2.11.4: Green function with fixed boundary conditions for $d = 4$.

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

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

Chapter 3

Quantum Field Theory

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

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

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

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

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

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

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

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

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

where the integration element is

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

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

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

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

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

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

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

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

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

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,

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

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

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

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

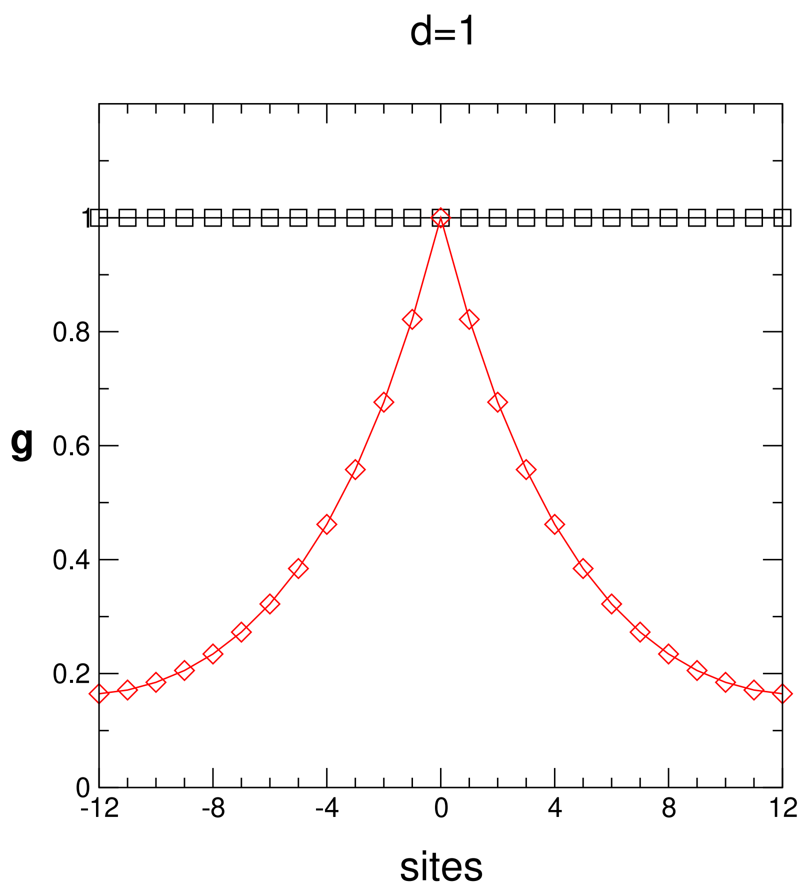


Figure 3.1.1: Periodical two-point correlation functions for $d = 1$.

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

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

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

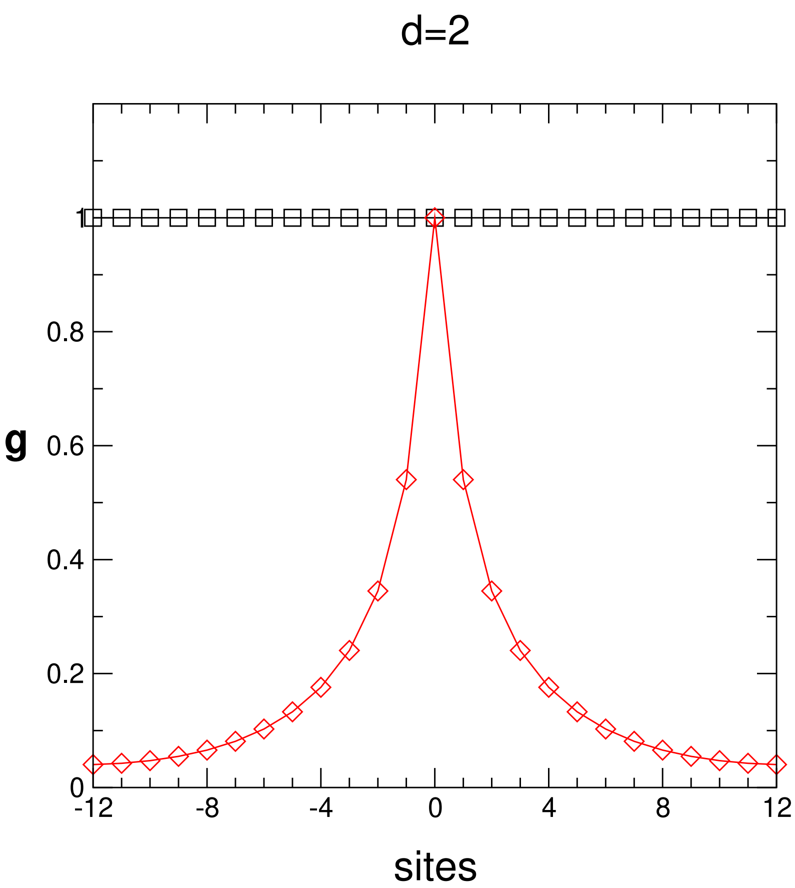


Figure 3.1.2: Periodical two-point correlation functions for $d = 2$.

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

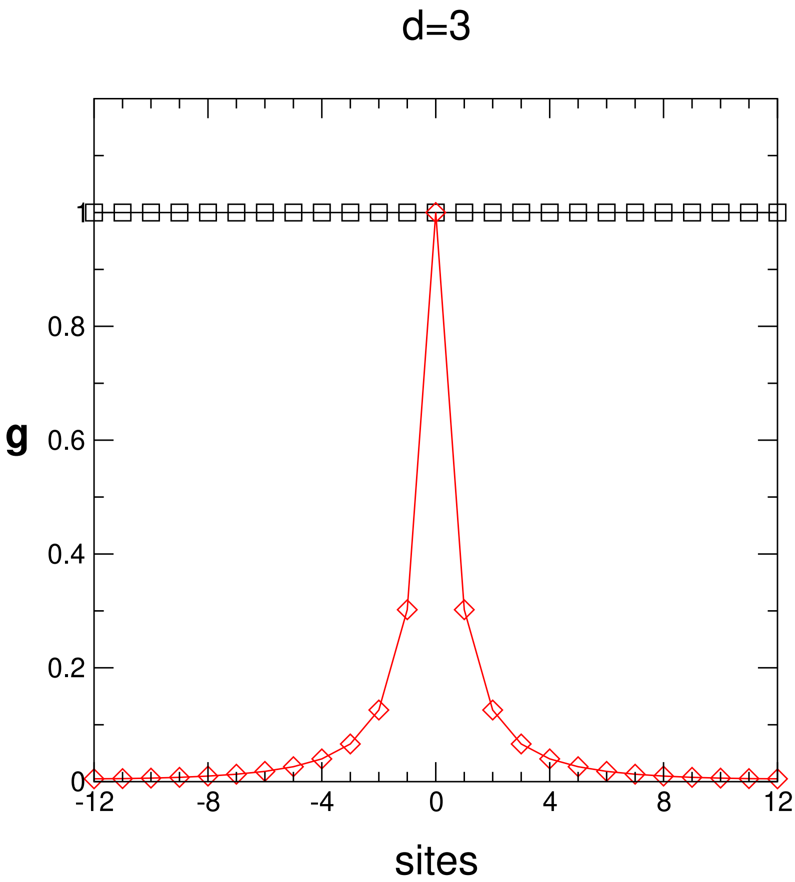


Figure 3.1.3: Periodical two-point correlation functions for $d = 3$.

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

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

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

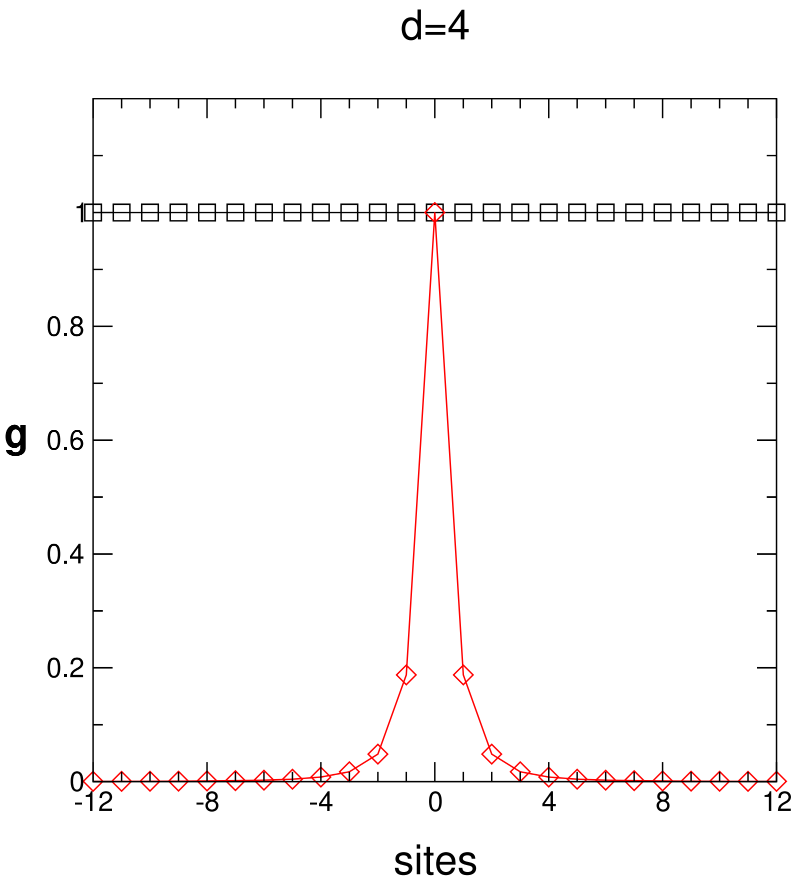


Figure 3.1.4: Periodical two-point correlation functions for $d = 4$.

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

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

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

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

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

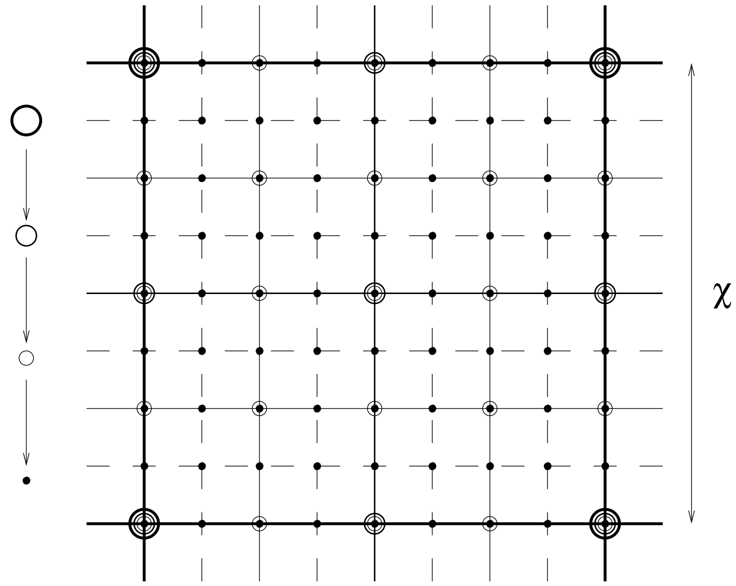


Figure 3.1.5: A sequence of lattices with decreasing lattice spacing.

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

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

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

Problems

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

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

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

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

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

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

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

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

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

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

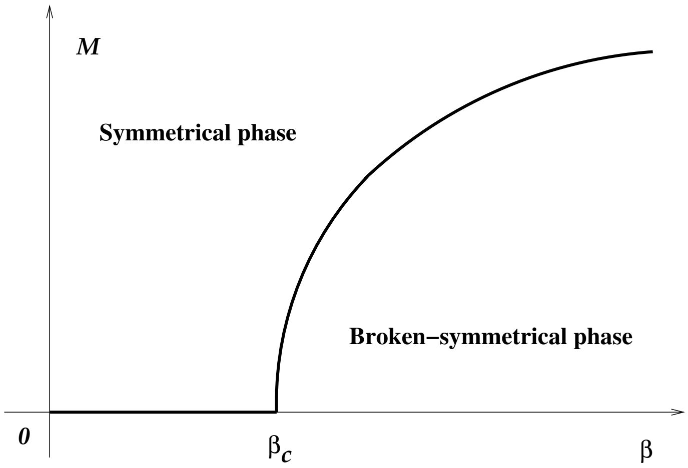


Figure 3.2.1: Qualitative diagram of the magnetization as a function of β.

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

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

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

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

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

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

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

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

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

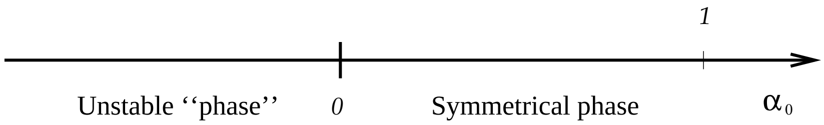


Figure 3.2.2: Critical diagram for the theory of the free field.

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

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

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

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

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

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

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

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

Problems

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

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

so that the original integral is

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

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

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

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

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

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

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

Comparing these two expressions we obtain the result for I_2,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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,

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

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

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

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

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

Once more, we may use the delta functions to obtain

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

as we already discussed above for the periodical case.

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

$n^{-n/2}$, 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.

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

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

where the Dirac delta function appears. Hint: make, at each point along the curve, a transformation of variables from (x, y) to (u, v), where u varies along the tangent to the curve and v varies along the line perpendicular to it, that is, $\mathrm{d}u \propto \mathrm{d}\ell$; remember that $\mathrm{d}f \equiv 0$ along the curve; for simplicity, assume that C is the graph of a function $y(x)$.[2]

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

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

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

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

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

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

[2] Many thanks to Dr. Miguel Bello Gamboa for detecting an error in the first version of this problem, and for correcting it for the author.

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

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 sign of the field, that is, that $S_0[\widetilde{\varphi}] = S_0[-\widetilde{\varphi}]$. Hence, all the same facts that follow from this invariance are true in this case and all the expectation values of the Fourier components of the field in momentum space involving an odd number of factors are zero, that is, for any vectors $\vec{k}_i$ we have

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

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

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

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

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

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

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

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

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

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

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

$$\langle|\widetilde{\varphi}(\vec{k})|^4\rangle = \frac{\displaystyle\int[\mathbf{d}\widetilde{\varphi}]\;|\widetilde{\varphi}(\vec{k})|^4\;e^{-S_0[\widetilde{\varphi}]}}{\displaystyle\int[\mathbf{d}\widetilde{\varphi}]\;e^{-S_0[\widetilde{\varphi}]}},$$

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

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

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

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

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

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

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

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

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

$$= \frac{\left(\dfrac{-\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \prod_{\vec{k}'}\sqrt{\dfrac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}{\prod_{\vec{k}'}\sqrt{\dfrac{2\pi}{N^d[\rho^2(\vec{k}')+\alpha_0]}}}$$

$$= \frac{\left(\dfrac{-\partial}{\partial\{N^d[\rho^2(\vec{k})+\alpha_0]\}}\right)^2 \dfrac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}}{\dfrac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}}$$

$$= \frac{(-1)^2\,(-1)\,(-2)\,\dfrac{1}{\{N^d[\rho^2(\vec{k})+\alpha_0]\}^3}}{\dfrac{1}{N^d[\rho^2(\vec{k})+\alpha_0]}}$$

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

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 is, that the quantum fluctuations superpose linearly and in this way do not affect the linearity of the theory. The propagator itself, the sole correlation function in momentum space that does not factor our in terms of other lower-order functions, describes how objects propagate in this model, which ends up being the *only* physics that it contains.

Problems

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

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

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

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

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

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

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

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

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

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

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

for an arbitrary integer n in either case.

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

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

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),

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

We know that the external source will make $v \neq 0$, unlike what happened before, since it breaks the symmetry by the transformation $\varphi \rightarrow -\varphi$, which we used before to show that the expectation value was zero. We may then rewrite the theory in terms of a new variable, the shifted field φ' given implicitly by $\varphi' = \varphi - v$, where $\langle\varphi'\rangle = 0$ by definition. If j is a function of position then the same should hold for v. We may then rewrite the action in terms of φ', obtaining

$$\begin{aligned}
S_0[\varphi] &= \frac{1}{2}\sum_{\ell}(\Delta_\ell\varphi')^2 + \frac{1}{2}\sum_{\ell}(\Delta_\ell v)^2 + \sum_{\ell}(\Delta_\ell v)(\Delta_\ell\varphi') \\
&\quad + \frac{\alpha_0}{2}\sum_s \varphi'^2(s) + \frac{\alpha_0}{2}\sum_s v^2(s) + \alpha_0\sum_s v(s)\varphi'(s) \\
&\quad - \sum_s j(s)\varphi'(s) - \sum_s j(s)v(s) \\
&= \frac{1}{2}\sum_{\ell}(\Delta_\ell\varphi')^2 + \frac{\alpha_0}{2}\sum_s \varphi'^2(s) \\
&\quad + \sum_{\ell}(\Delta_\ell v)(\Delta_\ell\varphi') + \alpha_0\sum_s v(s)\varphi'(s) - \sum_s j(s)\varphi'(s) \\
&\quad + \frac{1}{2}\sum_{\ell}(\Delta_\ell v)^2 + \frac{\alpha_0}{2}\sum_s v^2(s) - \sum_s j(s)v(s).
\end{aligned}$$

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

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

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

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

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

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

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

so that we may write equation (3.5.1) as

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

where we used the fact that the complex exponentials are eigenvalues of the finite-difference operator and also the orthogonality and completeness relations. Note that, once more, this must be true for all the configurations $\widetilde{\varphi}'(\vec{k})$ of the field, functions which are as arbitrary in momentum space as the functions $\varphi'(\vec{n})$ are arbitrary in position space. It follows therefore, exactly as before, that it is necessary that the contents of the bracket vanish,

$$\tilde{v}(\vec{k})\left[\rho^2(\vec{k})+\alpha_0\right]-\widetilde{\jmath}(\vec{k})=0,$$

which is the version in momentum space of the equation for v that one obtains from equation (3.5.2),

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

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

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

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

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

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

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

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

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

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

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

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

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

and, therefore, that it is independent of both j and the lattice position where the expectation values are calculated.

3.6 Functional Generators on the Lattice

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

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

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

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

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

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

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

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 which time Z will be gone from the picture.

We will consider, then, the functional derivatives of Z with respect to $j(\vec{n})$, that is, the variations of Z when we vary j at a single point $\vec{n}$. On the lattice functional differentiation is no more than partial differentiation with respect to the variables related to the degrees of freedom of the system. There is one $j(\vec{n})$ for each degree of freedom φ of the system, and each value of $j(\vec{n})$ at the various sites is a variable that may be changed independently, so that we have for our functional variations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

so that we may think of W as something like a "renormalized version" of the term in the fundamental action involving the external sources, $\sum_{\vec{n}} j(\vec{n})\varphi(\vec{n})$. Since there is a definite relation between each j and each $\varphi_{(c)}$, we are led to think that it should be possible to write W as a functional of $\varphi_{(c)}$ instead of j. Let us recall that the first functional derivative of W is given by

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

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

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

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

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

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

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

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

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

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

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

and its functional differential by

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

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

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

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

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

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 that the connected three-point function relates to the complete three-point function by

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

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

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

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

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

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

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

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

3.7 Physical Significance of the Effective Action

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

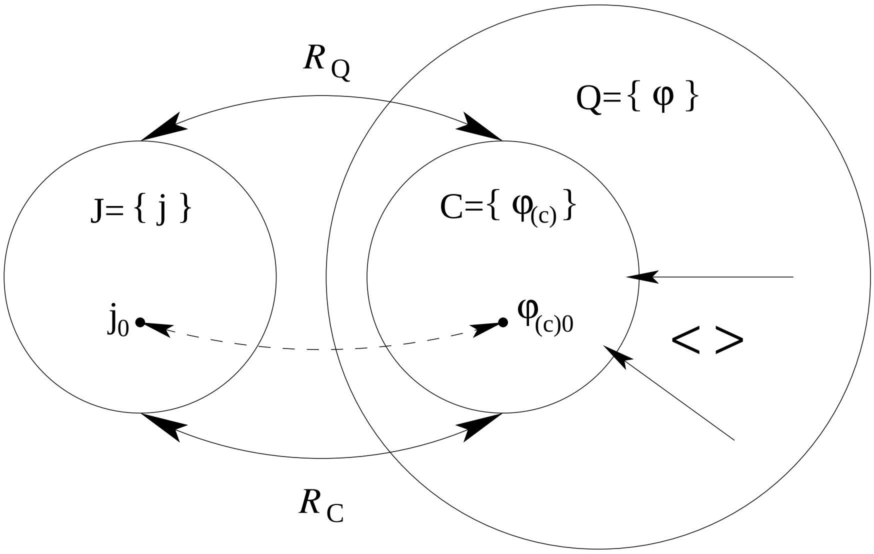


Figure 3.7.1: A diagram of the function spaces involved in the classical and quantum theories.

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

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

We see in this way that, starting from the most general possible set of configurations, the dynamical structure of the quantum theory itself automatically defines the subspace of configurations which is relevant for the corresponding classical theory, eliminating any need of imposing by hand the properties of this space in the classical limit of the theory. By and large, we may think of J and C as copies of the same space, the space where classical field-like objects exist. After all, an external source is no more than a representation of an expectation value within some other model or some other part of a more general model, representing a part of the physical world 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 the second term of the equation above the external source is kept fixed at a given function $j_0(\vec{n})$ while $\varphi_{(c)}$ varies, but in the first term we should calculate the variation of Γ that comes from its definition. Hence, when we calculate the variation of Γ, the $j[\varphi_{(c)}]$ that appears in the definition, being a functional of $\varphi_{(c)}$, does *not* remain fixed but rather varies with $\varphi_{(c)}$ according to the functional relation established between them by the quantum theory.

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

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

so that, using the definition of Γ, we obtain

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

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

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

from which it follows that

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

from which it follows that

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

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

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

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

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

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

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

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

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

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

$$\left(-\sum_{\mu}\partial_{\mu}^{2}+m_{0}^{2}\right)G_{(c)}(x_1-x_2)=\delta^{d}(x_1-x_2).$$

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

Problems

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

$$\widetilde{\varphi}_{(c)}(\vec{k})=\frac{\widetilde{\jmath}(\vec{k})}{\rho^{2}(\vec{k})+\alpha_0}.$$

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

$$\frac{\mathfrak{d}^{2}\Gamma[\varphi_{(c)}]}{\mathfrak{d}\varphi_{(c)}(n_1)\mathfrak{d}\varphi_{(c)}(n_2)},$$

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

Chapter 4

Correlation Structure

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

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

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

4.1 Structure of the Two-Point Function

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

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

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

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

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

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

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

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

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

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

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

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

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

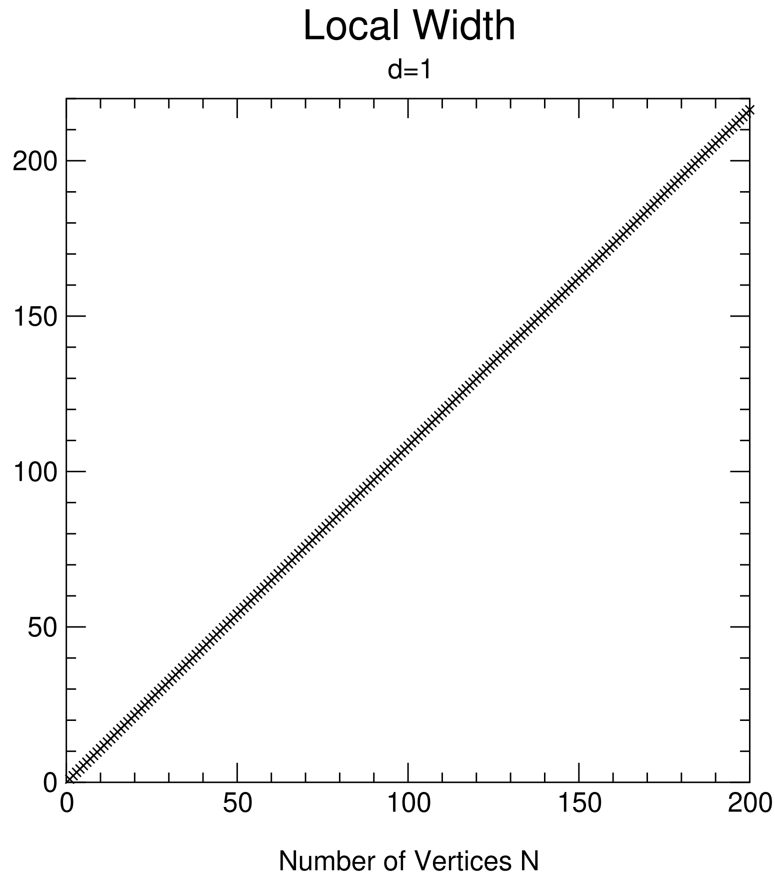


Figure 4.1.1: Behavior of the squared local width σ^2 with N in the case $d = 1$.

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

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

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

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

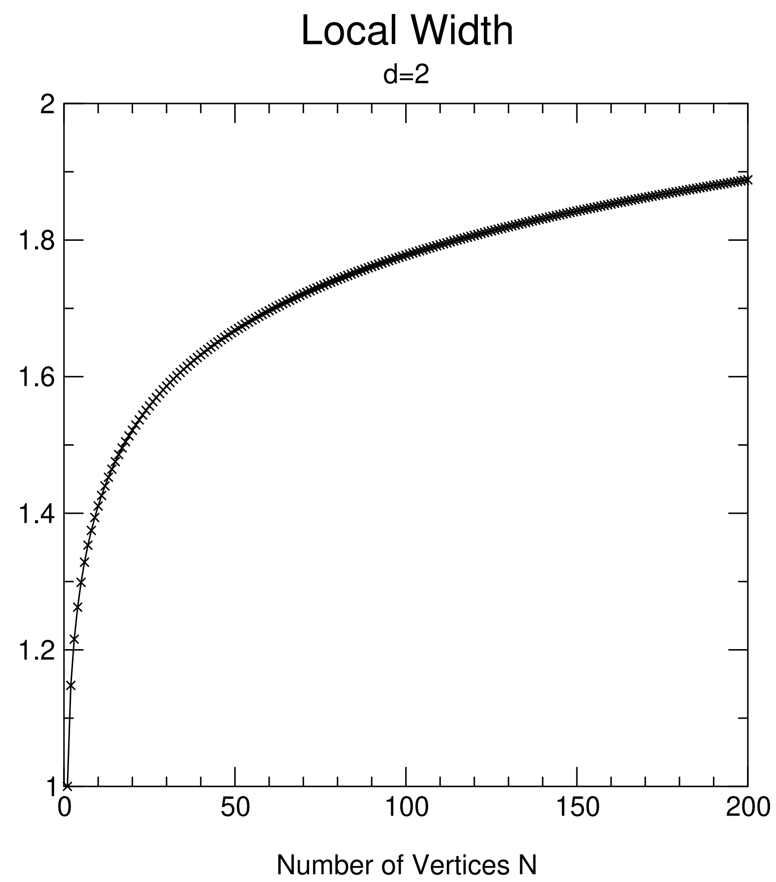


Figure 4.1.2: Behavior of the squared local width σ^2 with N in the case $d = 2$.

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

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

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

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

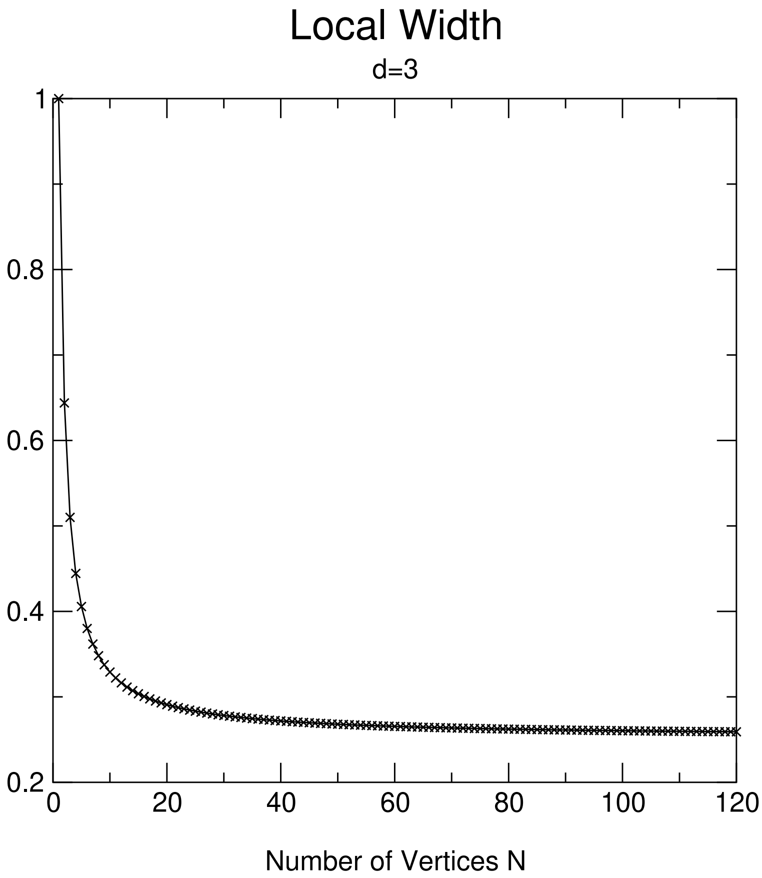


Figure 4.1.3: Behavior of the squared local width σ^2 with N in the case $d = 3$.

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

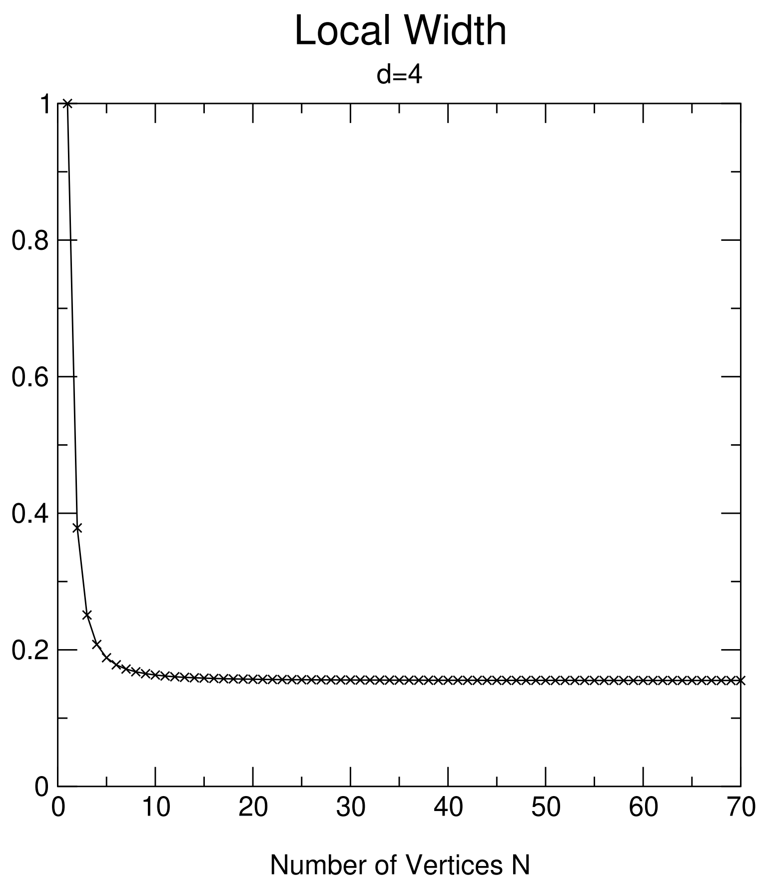


Figure 4.1.4: Behavior of the squared local width σ^2 with N in the case $d = 4$.

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

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

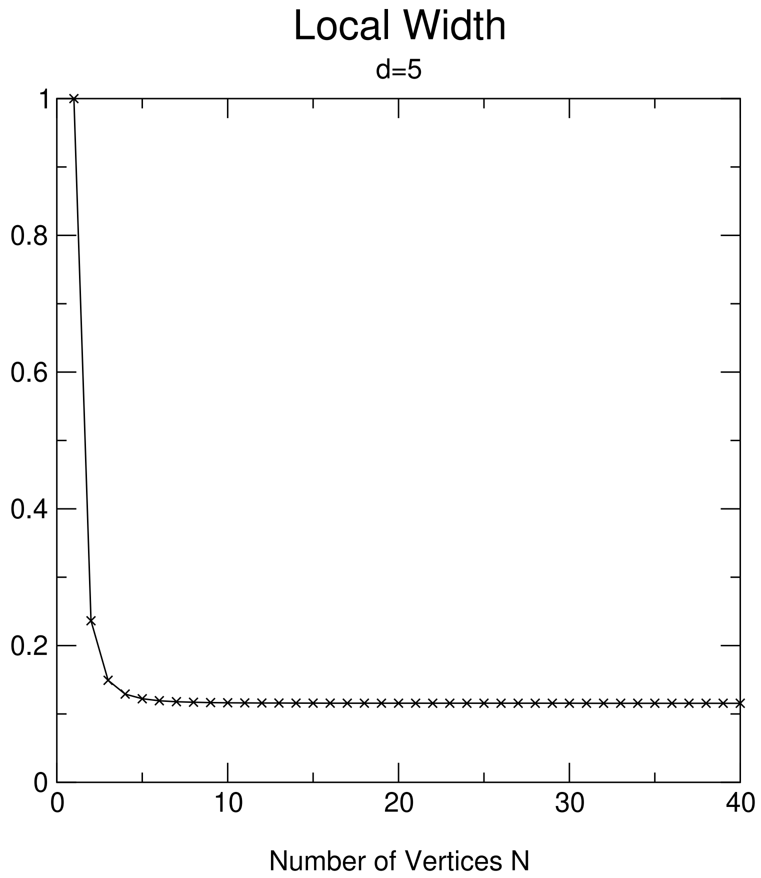


Figure 4.1.5: Behavior of the squared local width σ^2 with N in the case $d = 5$.

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

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

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

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

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

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

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

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

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

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

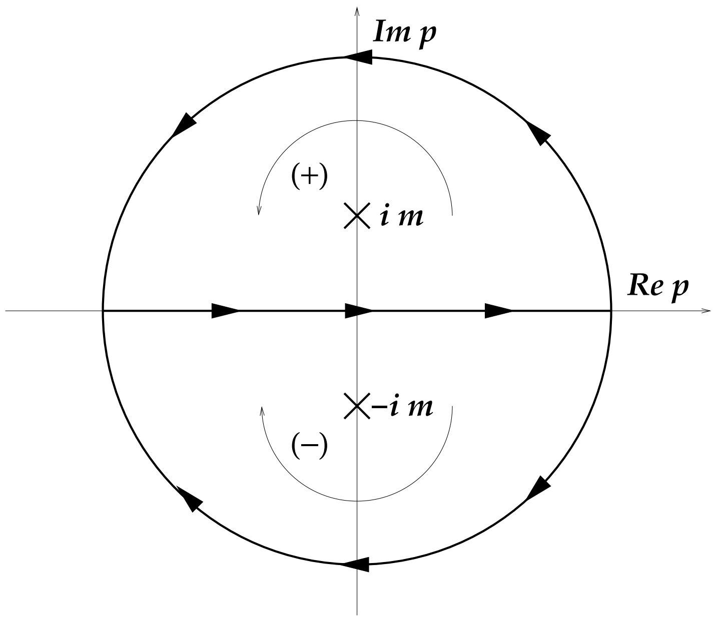


Figure 4.1.6: Integration contours in the complex p plane.

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

$$G(x>0)=\frac{1}{2\pi}(-2\pi\imath)\frac{e^{-m_0x}}{-2\imath m_0}=\frac{e^{-m_0x}}{2m_0}.$$

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

$$G(x<0)=\frac{1}{2\pi}(2\pi\imath)\frac{e^{m_0x}}{2\imath m_0}=\frac{e^{m_0x}}{2m_0}.$$

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

$$G(r)=\frac{e^{-m_0r}}{2m_0}.$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \mathfrak{f}(r) &= \begin{cases} 1 & \text{if} \quad r = 0 \\ 0 & \text{if} \quad r \neq 0 \end{cases}, \\ g(r) &= \begin{cases} \sigma^2 & \text{if} \quad r = 0 \\ 0 & \text{if} \quad r \neq 0 \end{cases}. \end{aligned}$$

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

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

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

Problems

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

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.

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

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

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

4.2 Discontinuity of the Configurations

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

Let us cite a few examples, so that the reader can judge the importance of the topic: the discontinuity of the field configurations is the basic phenomenon responsible for the appearance of divergent quantities in the perturbative approach to the theory; it causes different finite-differencing schemes on the lattice, which are equivalent in the classical theory, not to be so in the quantum theory; it changes in 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 the fields may be examined by first taking the lattice spacing to zero, while ε is kept constant in relation to the correlation length of the theory, and only after that making ε tend to zero within the continuous space that results from the first limit. This might be the more natural way to take the limit in order to establish a notion of continuity for fields defined on a lattice, but it is not the most relevant way in the context of the definition of the theory in terms of functional integrals on the lattice.

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

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

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

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

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

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

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

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

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

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

The most important thing is that we arrive at the inevitable conclusion that S_0 typically diverges and therefore that the statistical weights $\exp(-S_0)$ typically go to zero very fast in the continuum limit. It is necessary to emphasize that this is the *minimum* possible value for these weights, very different from the *maximum* possible value that it assumes for the classical solution, which shows that typically the dominant configurations of the quantum theory are *very distant* from the classical solution, if we use the action as a measure of this distance. This fact may 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 $\Delta_\mu\varphi(\vec{x}) \to 0$.

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

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

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

4.2.3. Calculate the d-dimensional sum in momentum space

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

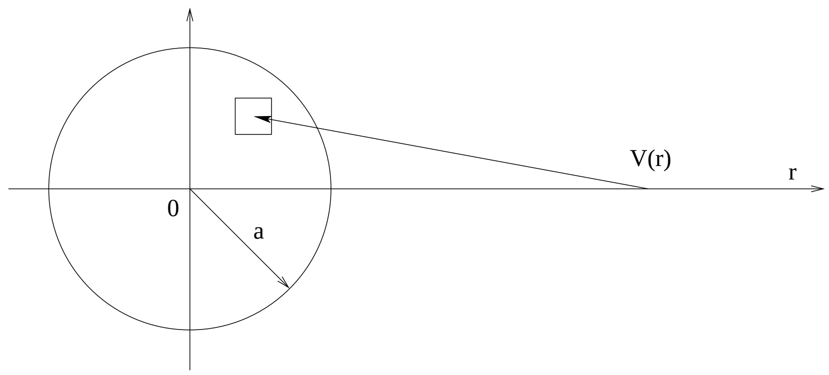


Figure 4.3.1: The problem of the calculation of the gravitational potential of a homogeneous spherical body.

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

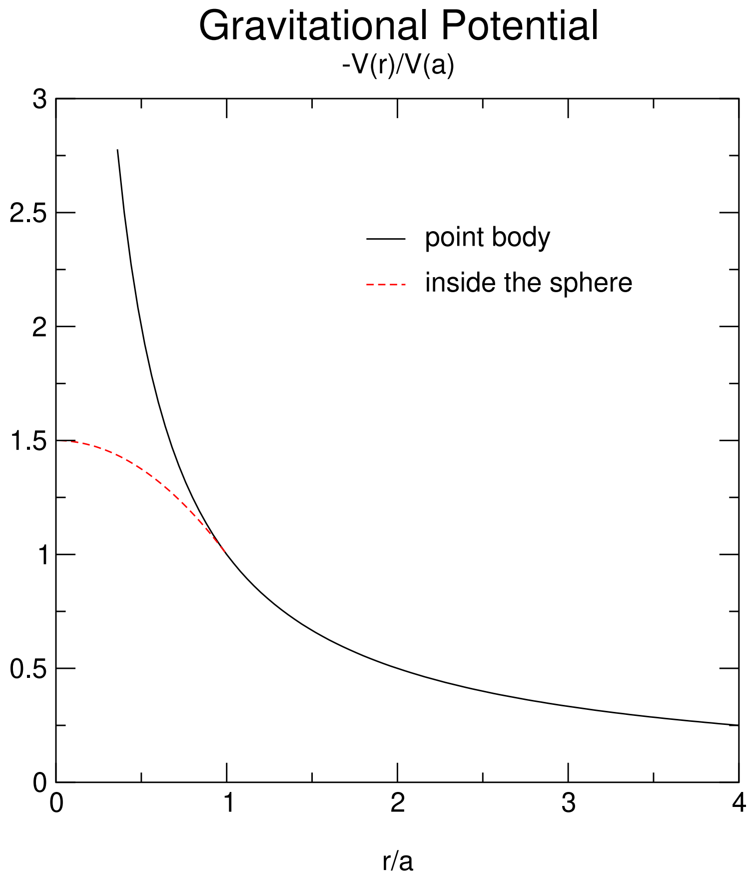


Figure 4.3.2: The gravitational potentials of the point body and of the extended spherical body, showing the smoothing of the singularity.

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

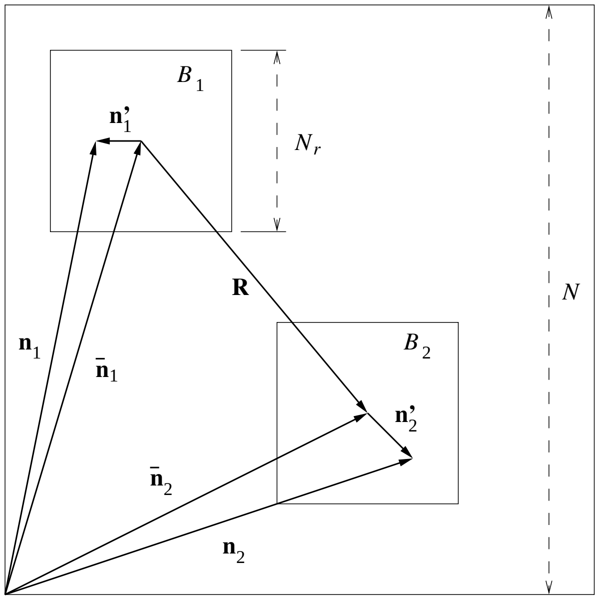


Figure 4.3.3: A cubical lattice with identical cubical blocks.

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

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

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

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

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

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

so that we obtain for the block propagator

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

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

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

from which it follows that

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

so that we may write for the block propagator

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

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

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

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,

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

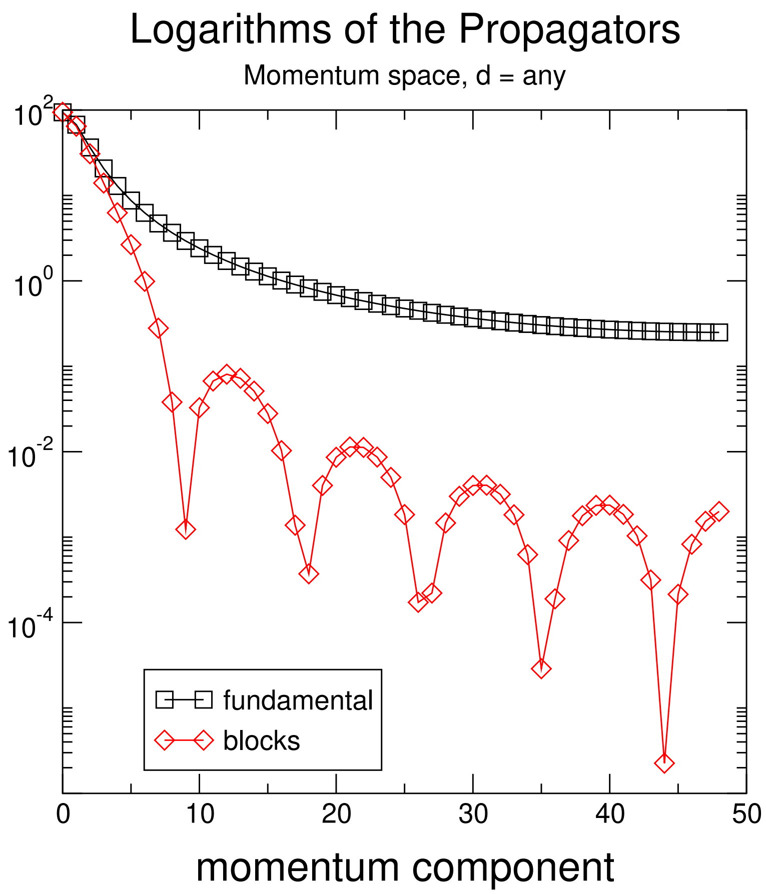


Figure 4.3.4: Logarithms of the fundamental and block propagators in momentum space.

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

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

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

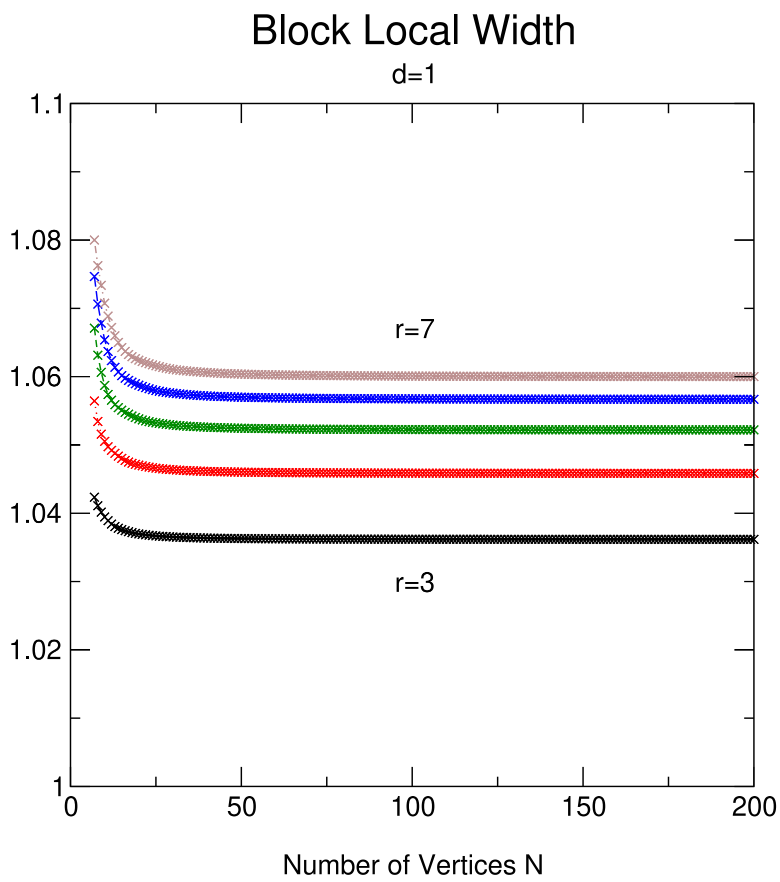


Figure 4.3.5: Behavior of the local block width as a function of N, for $d = 1$.

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

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

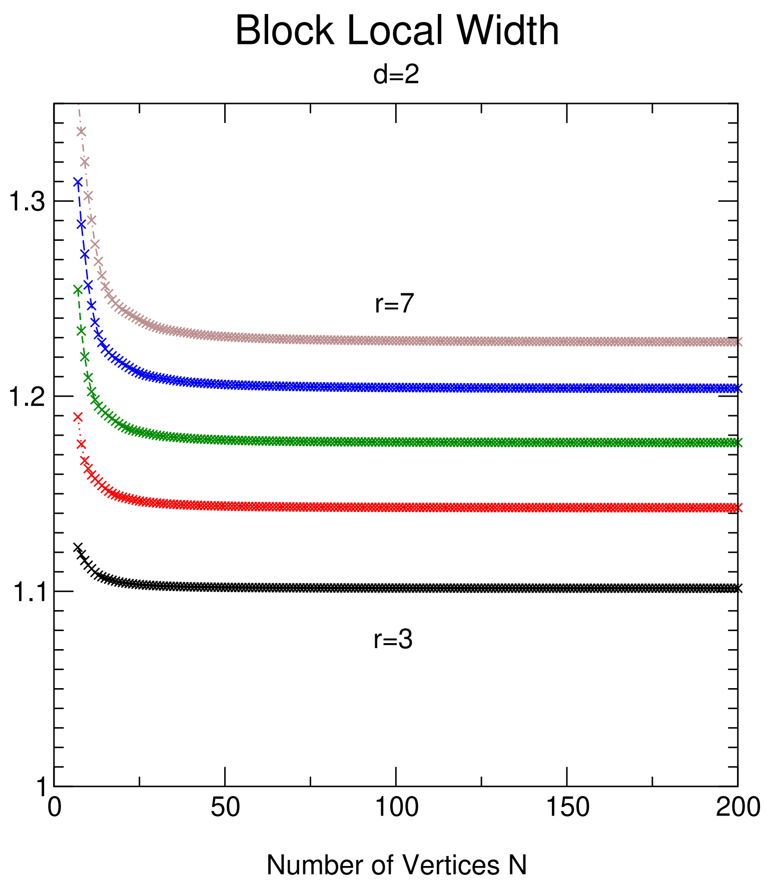


Figure 4.3.6: Behavior of the local block width as a function of N, for $d = 2$.

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

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

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

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

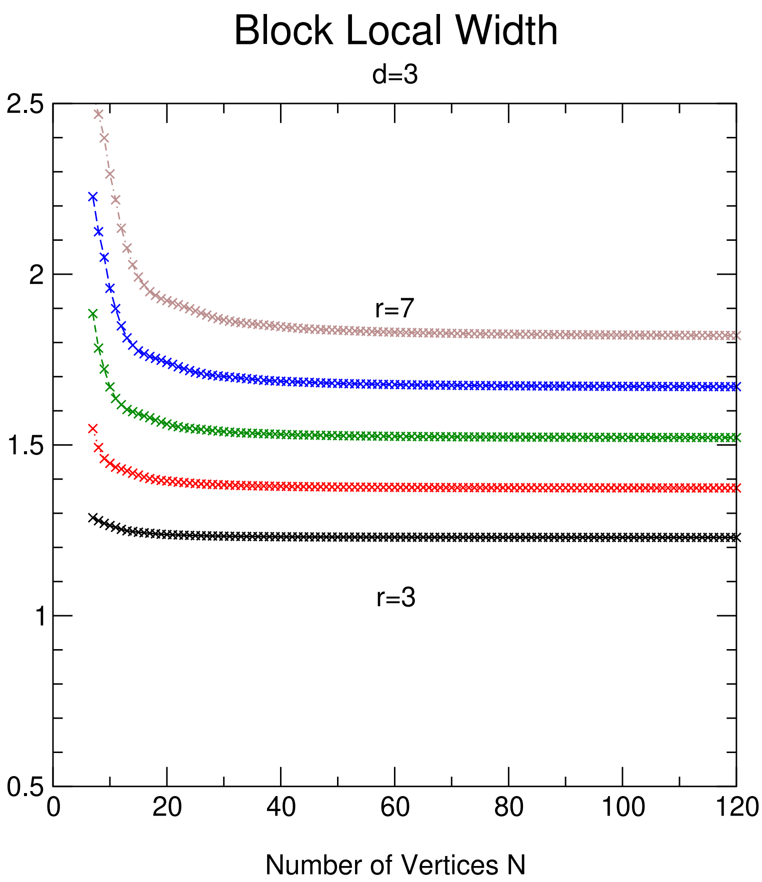


Figure 4.3.7: Behavior of the local block width as a function of N, for $d = 3$.

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

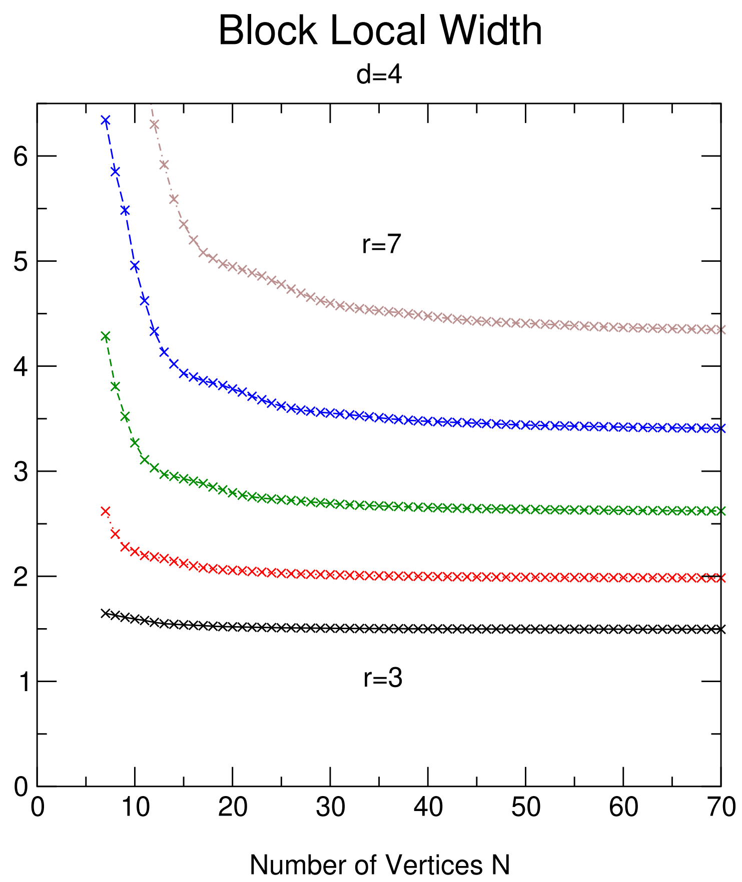


Figure 4.3.8: Behavior of the local block width as a function of N, for $d = 4$.

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

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

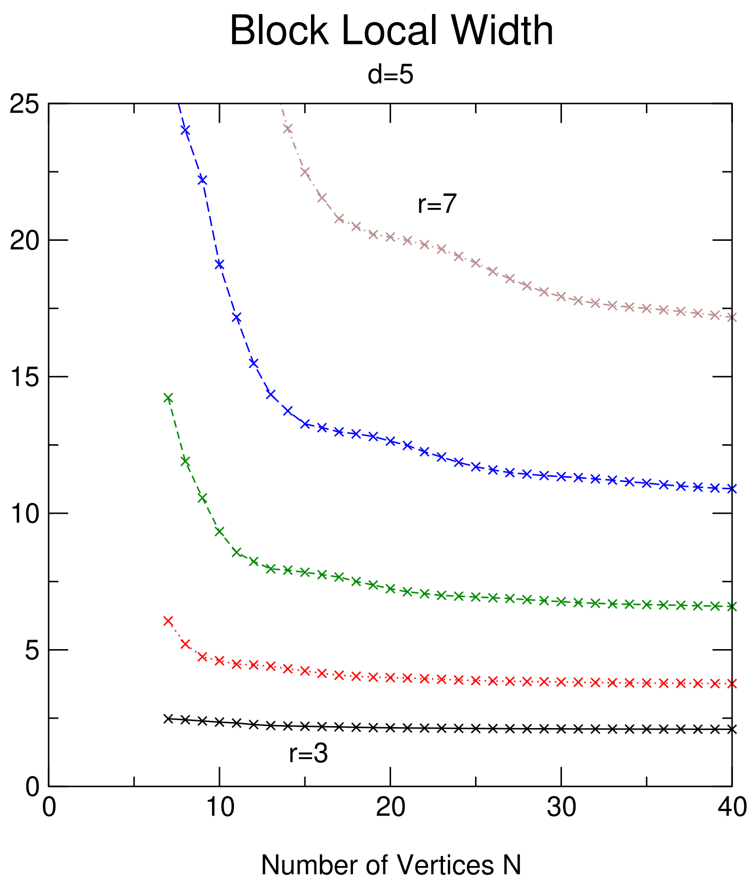


Figure 4.3.9: Behavior of the local block width as a function of N, for $d = 5$.

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

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

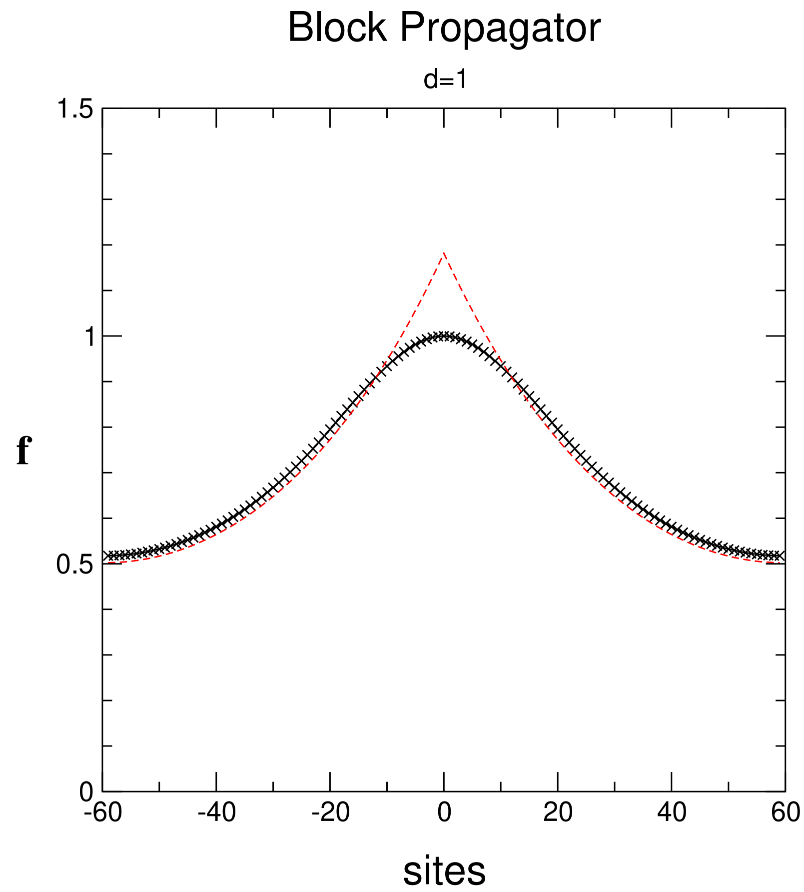


Figure 4.3.10: Block propagator in position space, for $d = 1$.

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

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

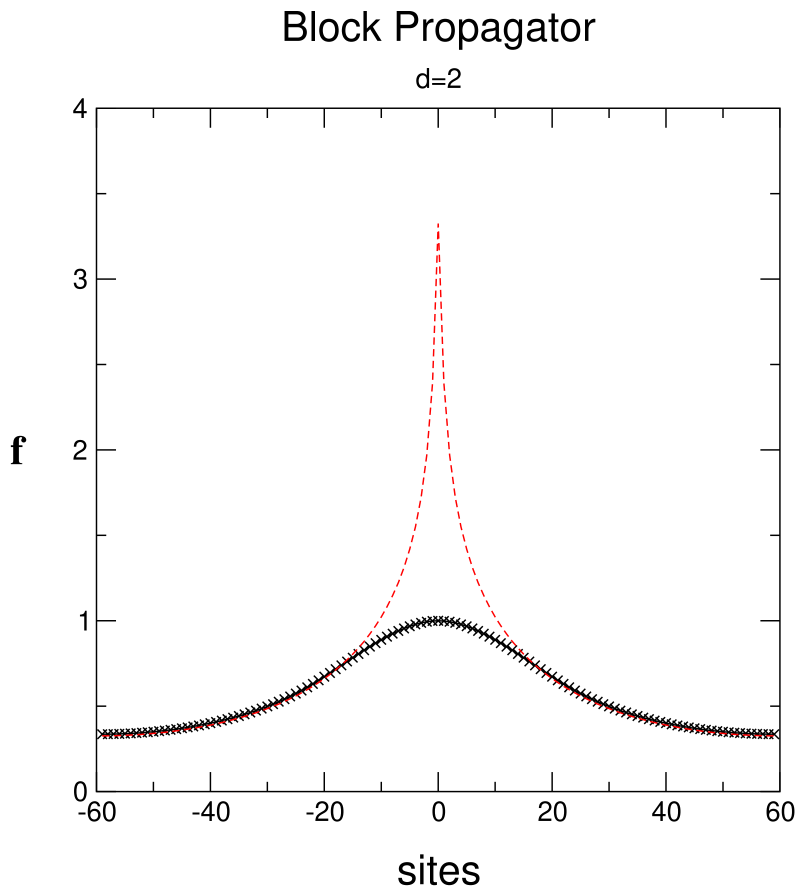


Figure 4.3.11: Block propagator in position space, for $d = 2$.

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

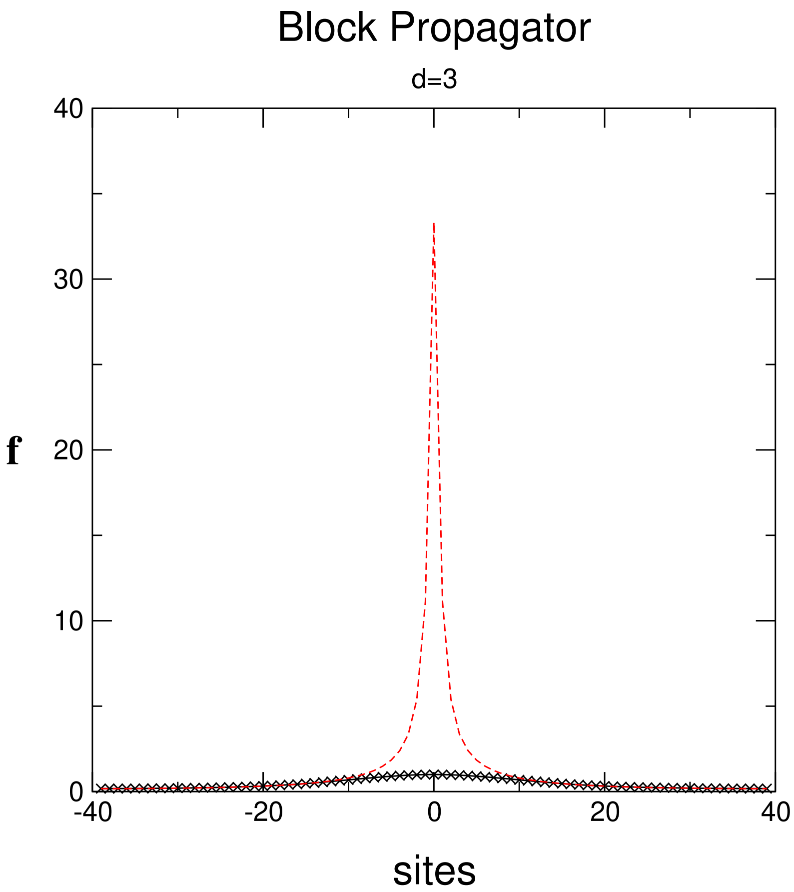


Figure 4.3.12: Block propagator in position space, for $d = 3$.

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

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

Problems

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

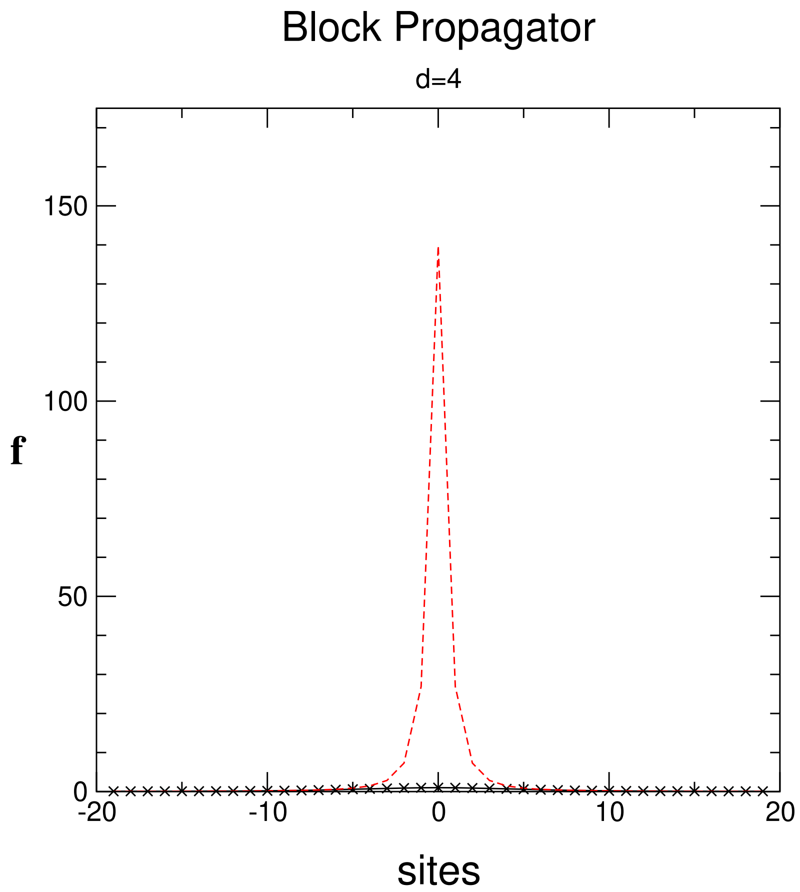


Figure 4.3.13: Block propagator in position space, for $d = 4$.

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.

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

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

Chapter 5

The Concept of Energy

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

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

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

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

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

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

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

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

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

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

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

$\Delta_0\varphi$, 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

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

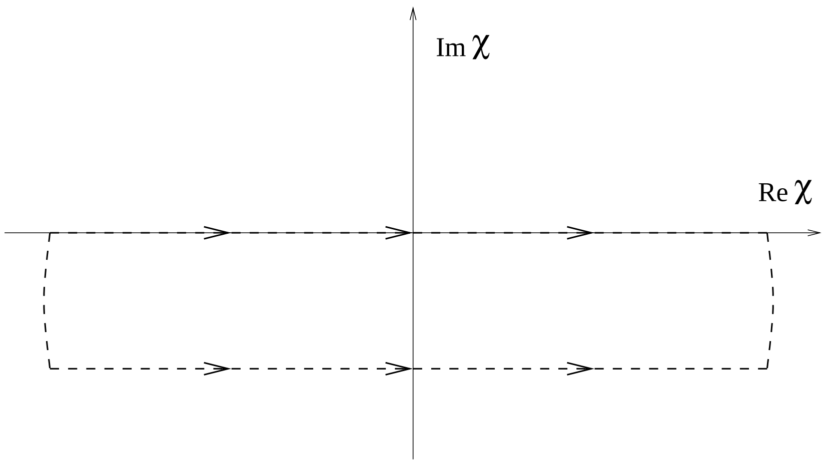
We may then complete the square on $\bar{\pi}$ in the exponent of the second exponential, obtaining

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

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.



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

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

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

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

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

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

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

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

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

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

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

so that we have

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

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

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

Doing the Gaussian integrations in the first term we obtain

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

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

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

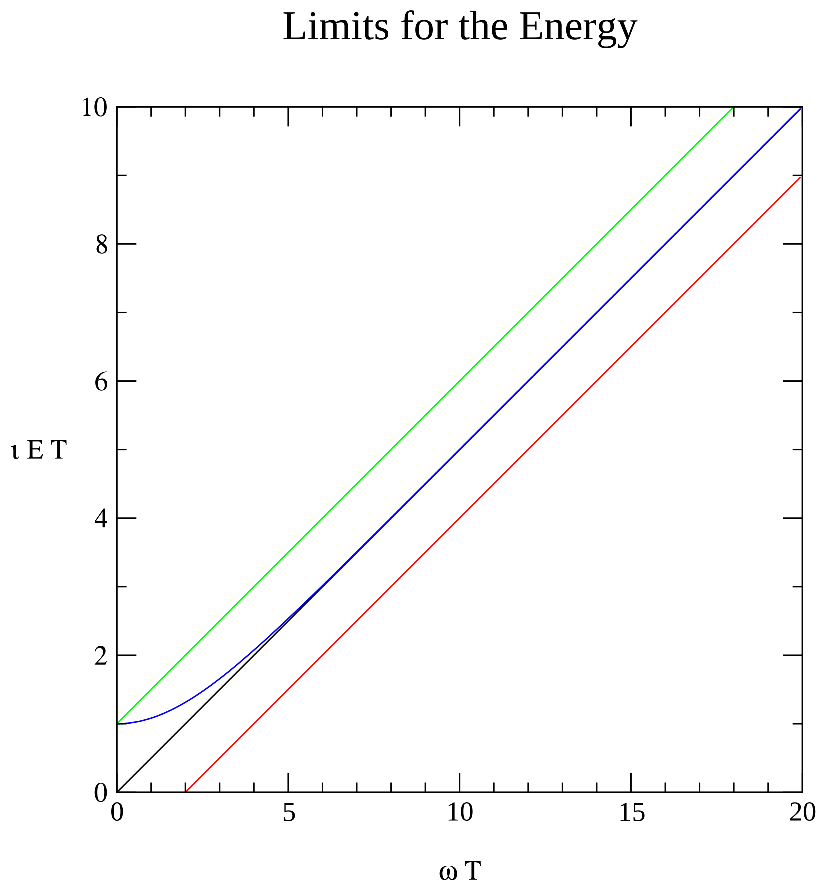


Figure 5.1.1: The energy as a function of the variable ωT. The curved line corresponds to the numerical result for $N_T = 1000$. The central straight line corresponds to the continuum limit in an infinite temporal box. The other straight lines correspond to the upper and lower bounds which are mentioned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

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

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

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

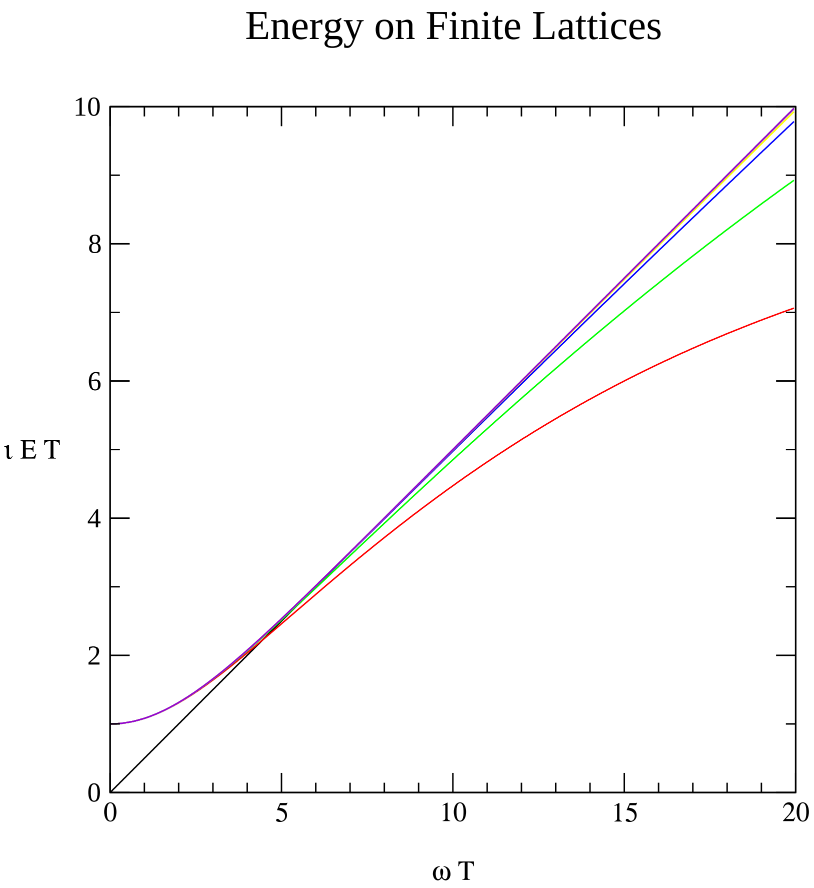


Figure 5.1.2: The energy as a function of the variable ωT. The straight line corresponds to the continuum limit in an infinite temporal box, that is, to the case $N_T \to \infty$ and $T \to \infty$. The curved lines correspond to the numerical results in progressively larger lattices, from $N_T = 10$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

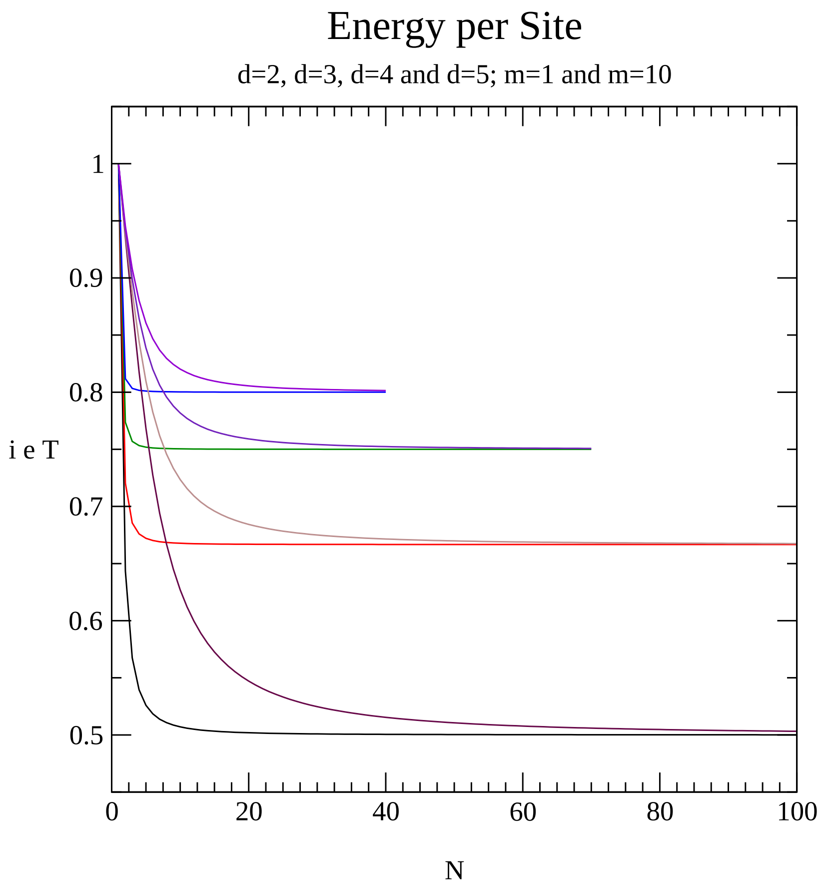


Figure 5.1.3: The energy per site as a function of N in the symmetrical case $N_T = N_L = N$. Each pair of curves corresponds to a different dimension d, converging to the value $(d-1)/d$ in the limit $N \to \infty$. In each pair the curve that converges faster is the one that corresponds to $m_0 = 1$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.1.4. Repeat the analysis made in problems 5.1.2 and 5.1.3 and determine upper and lower bounds for the sum Σ in the case in which N_T is odd, in which the limits of k_0 are $k_m = -(N_T - 1)/2$ and $k_M = (N_T - 1)/2$. Write the corresponding inequalities for $\imath E$ and verify that they are compatible with the inequalities obtained for the case of even N_T.

5.1.5. 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.

5.2 Energy and States of Particles

In possession of the concept of energy within the lattice formalism, we will now discuss in considerable more detail the concept of state. This discussion will lead us to the construction within this formalism of states with a given number of particles and, therefore, to the concept of particle itself. This is a central concept within the structure of the theory, which is directly connected with the fundamental issues of the observation of physical phenomena and of the process of measurement.

Up to now we have been defining and developing a formalism that allows us to define and calculate, at least in principle, any observables within any given model of quantum field theory. We have been doing this through the use of a statistical model in which we define a certain statistical distribution of probabilities that applies to each and every one of the possible configurations of the fields. This distribution is the Boltzmann distribution, which can be expressed in terms of the action functional S of a given model as

$$|0\rangle \sim \frac{[\mathrm{d}\varphi]\ e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ e^{-S[\varphi]}},$$

or, if we wish to use the canonical formalism, as

$$|0\rangle \sim \frac{[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}}{\displaystyle\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}}.$$

The symbolism of Dirac "bras" and "kets" that we use here expresses the fact that our interpretation of the structure that we are building is that this statistical distribution is a representation of the vacuum state of the theory, for this particular model.

It is a difficult task to define a-priori what the vacuum might be. The classical idea that it is a situation in which there is total absence of any physical content is not very useful in the context of the quantum theory, due to the concept of uncertainty that is inherent to such a theory. We will simply say that this state defines completely the physical situation in the region of space-time where it is realized, and accept its introduction as part of the definition of the quantum theory. We will also see that it is a state that contains no particles, that is, no observable amount of energy. This does not mean that there is nothing in it, because there is the field, which fluctuates permanently in a rather violent way. One might say that the vacuum is the state that contains nothing but the minimum mount of uncertainty which is inherent to the quantum theory.

This idea which we introduced above, that physical states are connected with certain statistical distributions, immediately suggest the generalization of its application to other stated besides the vacuum. Strictly speaking this is not necessary for the measurement of observables, since we can measure any observables using only the vacuum state. This is a remarkable characteristic of this structure of ours, it is 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,

$$|1,\vec{k}\rangle \sim \frac{[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{-S[\varphi]}},$$

or, in terms of the canonical formalism,

$$|1,\vec{k}\rangle \sim \frac{[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}}{\displaystyle\int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^2 e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}},$$

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.

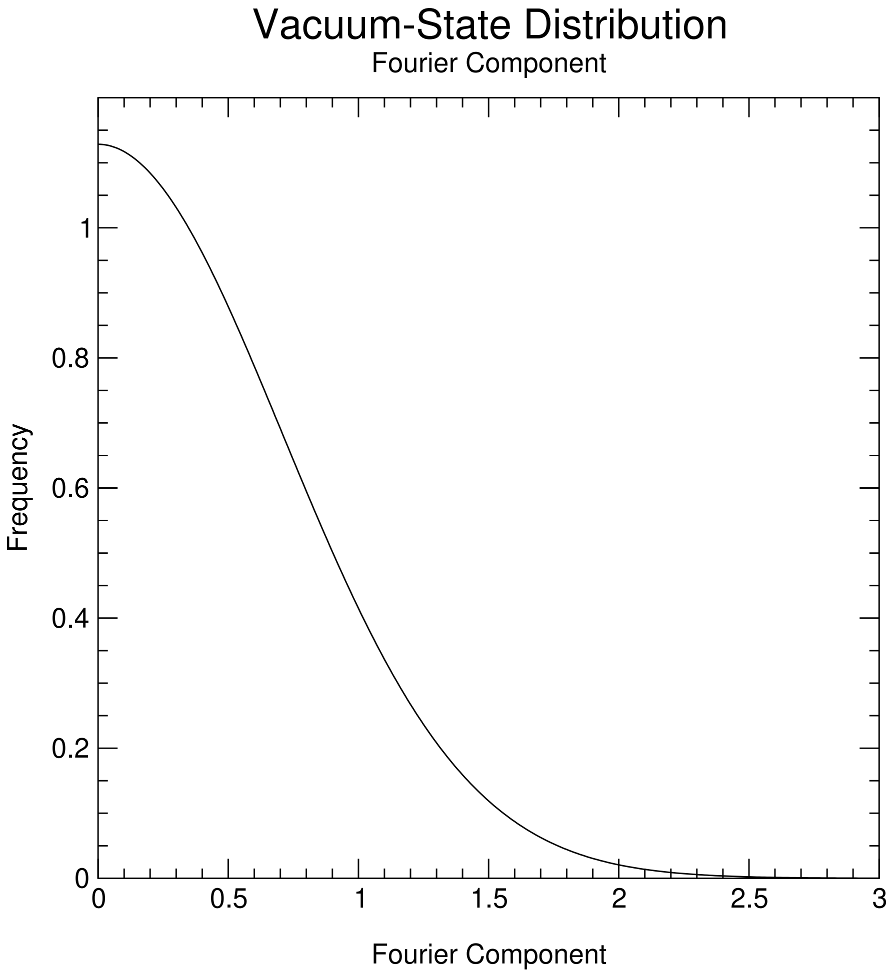


Figure 5.2.1: Qualitative diagram of the probability distribution $\exp(-x^2)$ of the Fourier components of the field in the vacuum state, showing the point of maximum at 0.

Before we begin to examine some properties of this new distribution let us emphasize here that, while we are proposing a relation between states of the quantum theory of fields and statistical distributions of the fields, we are absolutely *not* stating that *any* such statistical distribution is related to a physical state of the theory. There are many distributions that are clearly not related to physical states, such as, for example, any "delta-functional" distribution, that attributes the probability 1 to a certain configuration and the probability 0 to all others, because this would translate into a physical situation in which the fundamental field does not fluctuate at all, which is a classical, not a quantum situation. We will postpone to a future opportunity a more detailed discussion of the conditions that the distributions must satisfy in order to be associated to states, and will limit ourselves here only to the comment that such conditions are related to the principle of uncertainty and to the issues of observation and measurement. Our difficulties with the "ab-initio" definition of the vacuum will have to be resolved in the context of this future discussion, possibly

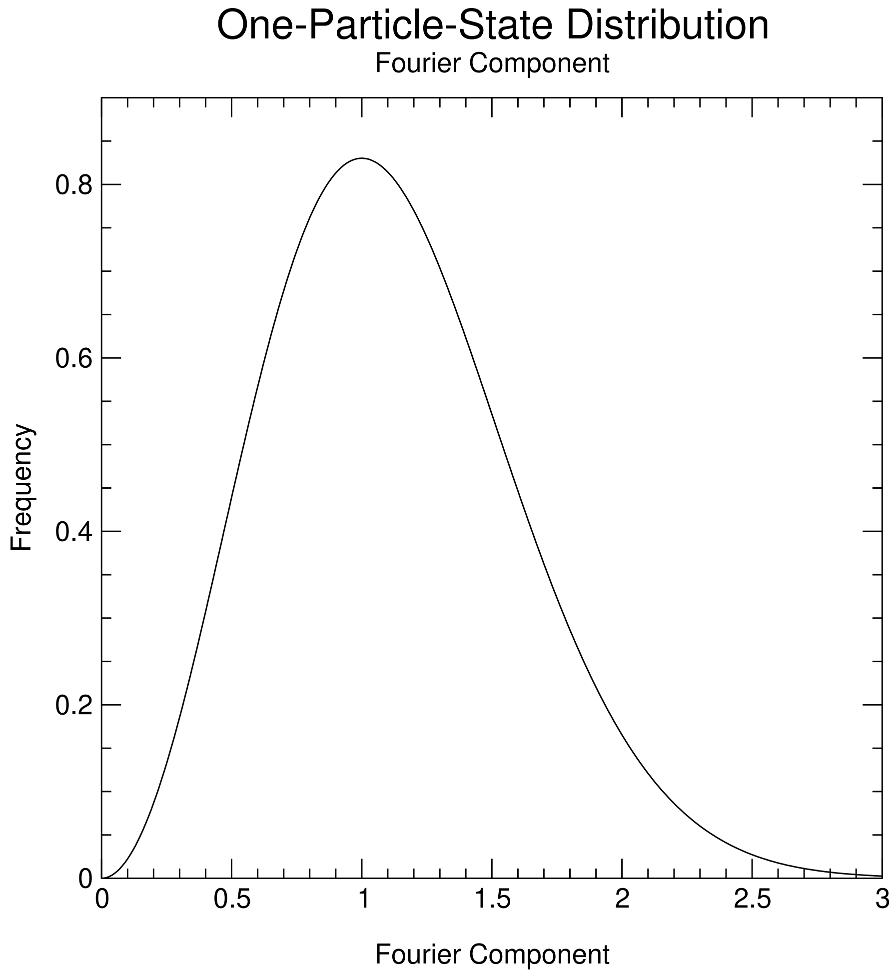


Figure 5.2.2: Qualitative diagram of the probability distribution $x^2 \exp(-x^2)$ of the Fourier component of the field that is singled out in the one-particle state with a given momentum vector $\vec{k}$, showing the point of maximum at 1.

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 the configurations that have a larger component of plane wave with momentum $\vec{k}$.

In order to calculate the energy of this new state, we will use the canonical definition and the form of the dimensionless Hamiltonian defined in section 5.1,

$$\mathbf{H} = -\frac{\imath}{2}\sum_{\mathbf{x}}\left[\bar{\pi}^2 + \sum_i(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

With these ingredients we obtain (problem 5.2.1) for the expectation value of the Hamiltonian in the state of one particle with momentum $\vec{k}$,

$$\langle\mathbf{H}\rangle_{1,\vec{k}} = -\frac{\imath}{2}N_L^{d-1} + \frac{\displaystyle\int[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2\mathbf{H}'e^{-S[\varphi]}}{\displaystyle\int[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^2e^{-S[\varphi]}},$$

where $\mathbf{H}'$ is, as before, the expression of $\mathbf{H}$ with $\bar{\pi}$ substituted by $\imath\Delta_0\varphi$, showing once more that the difference between the canonical definition and the initial definition is just a constant that diverges in the continuum limit. Repeating procedures used before in section 5.1 we may write explicitly for the energy

$$\begin{aligned}\imath E_{1,\vec{k}}T &= \frac{N_TN_L^{d-1}}{2} \\ &+\frac{N_TN_L^{d-1}}{2}\,\frac{\displaystyle\int[\mathrm{d}\widetilde{\varphi}]\ e^{-S[\widetilde{\varphi}]}|\widetilde{\varphi}_{\vec{k}}|^2\sum_{\vec{q}}\left[-\rho_0^2(\vec{q})+\sum_i\rho_i^2(\vec{q})+\alpha_0\right]|\widetilde{\varphi}_{\vec{q}}|^2}{\displaystyle\int[\mathrm{d}\widetilde{\varphi}]\ |\widetilde{\varphi}_{\vec{k}}|^2e^{-S[\widetilde{\varphi}]}},\end{aligned}$$

where we recall that we have for $S[\widetilde{\varphi}]$ written in momentum space

$$S[\widetilde{\varphi}] = \frac{N_TN_L^{d-1}}{2}\sum_{\vec{k}}(\rho_{\vec{k}}^2+\alpha_0)|\widetilde{\varphi}_{\vec{k}}|^2,$$

with

$$\rho_{\vec{k}}^2 = 4\sin^2\left(\frac{k_0\pi}{N_T}\right) + \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right).$$

For the terms of the sum over the momenta $\vec{q}$ such that $\vec{q}\neq\pm\vec{k}$ the calculation proceeds as in the case of the calculation of the energy of the vacuum, but for $\vec{q}=\pm\vec{k}$ there are differences, because in this case we have the expectation value of a larger power of the Fourier component $\widetilde{\varphi}_{\vec{k}}$ of the fields. Taking into account the symmetries by exchange of the sign of $\vec{q}$ in the sum, we may write

$$\begin{aligned}\imath E_{1,\vec{k}}T &= \frac{N_TN_L^{d-1}}{2} + \frac{1}{2}\sum_{\vec{q}\neq\pm\vec{k}}\frac{-\rho_0^2(\vec{q})+\sum_i\rho_i^2(\vec{q})+\alpha_0}{\rho_{\vec{q}}^2+\alpha_0} \\ &\quad +N_TN_L^{d-1}\left[-\rho_0^2(\vec{k})+\sum_i\rho_i^2(\vec{k})+\alpha_0\right]\frac{\langle|\widetilde{\varphi}_{\vec{k}}|^4\rangle_0}{\langle|\widetilde{\varphi}_{\vec{k}}|^2\rangle_0},\end{aligned}$$

where we already used in the second term the result

$$\langle|\widetilde{\varphi}_{\vec{k}}|^2\rangle_0 = \frac{1}{N_T N_L^{d-1}} \frac{1}{\rho_{\vec{k}}^2 + \alpha_0}.$$

For the other expectation value, which appears in the third term, we have

$$\langle|\widetilde{\varphi}_{\vec{k}}|^4\rangle_0 = \frac{2}{\left(N_T N_L^{d-1}\right)^2} \frac{1}{\left(\rho_{\vec{k}}^2 + \alpha_0\right)^2},$$

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 $\Delta E = \Delta \mathcal{E}/a = N_T \Delta \mathcal{E}/T$.

As we will see later on, we may extend the definition of our states to arbitrary numbers of particles but, before we do that, let us discuss the physical meaning of the expression we obtained for the energy in the continuum limit. Our definition of the one-particle state is in fact the definition of a collection of states, one for each d-dimensional mode $\vec{k}$ existing on the lattice, each one of them having its energy given in terms of $\vec{k}$ by the expression in equation (5.2.1). If we write the version of this result in Minkowski space, thus *de-Euclideanizing* the result, we obtain

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{\rho_0^2(\vec{k}) + \sum_i \rho_i^2(\vec{k}) + \alpha_0}{-\rho_0^2(\vec{k}) + \sum_i \rho_i^2(\vec{k}) + \alpha_0}.$$

There are, in fact, two limits to discuss here, the continuum limit in which we make $N \to \infty$, and the $T \to \infty$ limit in which we make the box infinite in the temporal direction. We will discuss the first limit in the symmetrical case, making $N_T = N_L = N \to \infty$ while we keep T finite, leaving for later on the discussion of other ways to take this limit. In this case we may multiply both the denominator and the numerator by N^2/L^2, take the limit and write the result as

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{p_0^2(\vec{k}) + \mathbf{p}^2(\vec{k}) + m_0^2}{-p_0^2(\vec{k}) + \mathbf{p}^2(\vec{k}) + m_0^2},$$

where $m_0^2 = \alpha_0 N^2/L^2$ and the $(d-1)$-dimensional momentum $\mathbf{p}$ is defined by

$$\mathbf{p}_{\vec{k}}^2 = \lim_{N\to\infty} \frac{N^2}{L^2} \sum_i \rho_i^2(\vec{k}) = \lim_{N\to\infty} \frac{4N^2}{L^2} \sum_i \sin^2\left(\frac{k_i \pi}{N}\right) = \sum_i \left(\frac{2\pi k_i}{L}\right)^2.$$

Let us consider now the limit $T \to \infty$, with L either kept fixed or not. Since T appears in the denominator, our expression for the energy of a particle goes to zero, unless the momentum-dependent expression in the denominator vanishes in the limit. This takes us to the *on-shell condition*, that selects a subset of all possible d-dimensional modes. In order to see this we may rewrite the expression as

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{p_0^2(\vec{k}) + \mathbf{p}_{\vec{k}}^2 + m_0^2}{\left[-p_0(\vec{k}) + \sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}\right]\left[p_0(\vec{k}) + \sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}\right]}.$$

Observe that we can obtain a finite and non-vanishing limit only so long as in the limit one of these two relations holds,

$$p_0(\vec{k}) = \sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2} \quad \text{or} \quad p_0(\vec{k}) = -\sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}.$$

We thus obtain the on-shell condition that relates the energy, the momentum and the rest mass of a relativistic particle. We see also that we may have some limits in which the energy is positive as well as other limits in which it is negative, as mentioned in section 5.1. Besides the two possibilities presented by the two factors in the denominator, in each case it is possible to take the limit in which p_0 approaches

$\pm\sqrt{\mathbf{p}^2 + m_0^2}$ 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

$$\Delta E_{1,\vec{k}} = \frac{-1}{A}\sqrt{\mathbf{p}_{\vec{k}}^2 + m_0^2}.$$

We see therefore that, in order for the expectation value of the energy to coincide numerically with the temporal component of the vector $\vec{k}$, we should impose that the $T \to \infty$ limit be such that $A = -1$. Note that this arbitrariness in the value of A is equivalent to the arbitrariness in the choice of units for the energy.

It is interesting to discuss here the case $d = 1$ and thus verify that we obtain the correct results for the harmonic oscillator in quantum mechanics. In this case the on-shell condition within a finite temporal box reduces, already making $A = -1$, to

$$p_0 = \frac{1}{T} + m_0,$$

that is, except for the infrared effects due to the finite size of the temporal box, the energy parameter p_0 reduces to the mass parameter m_0. Since in this case we do not have the components p_i, this relation determines completely p_0 and, therefore, k_0. If we recall that we have $\alpha_0 = m_0^2 a^2$ and that this same parameter α_0 relates to the angular frequency ω of the harmonic oscillator by $\alpha_0 = \omega^2 a^2$, we see that we have $m_0 = \omega$, so that we may write

$$p_0 = \omega + \frac{1}{T} = \omega \left(1 + \frac{1}{\omega T} \right).$$

We may now substitute this value for p_0 in the expression of the expectation value of the Hamiltonian, obtaining, after some manipulation and keeping only the first-order corrections in $1/T$, in the limit of very large T,

$$\Delta E_1 = \omega \left(1 + \frac{1}{2\omega T} \right),$$

showing that this quantity also suffers infrared deviations, is a way similar to p_0. With a slightly different choice for A, making $A = -1+1/(2\omega T)$ rather than $A = -1$, we can make p_0 and ΔE_1 approach their limits in exactly the same way. In any case, in the $T \to \infty$ limit we have the result

$$\Delta E_1 = \omega,$$

which is the correct result for the difference between the energies of the first excited state and of the fundamental state of a one-dimensional harmonic oscillator in quantum mechanics.

We may now extend our definition of particle states to arbitrary numbers of identical particles. The state of n particles with momentum $\vec{k}$ can be defined by means of the distribution

$$|n, \vec{k}\rangle \sim \frac{[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{-S[\varphi]}},$$

or, in terms of the canonical formalism,

$$|n,\vec{k}\rangle \sim \frac{[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}}{\displaystyle\int[\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\ |\widetilde{\varphi}_{\vec{k}}|^{2n} e^{\imath\sum_s[\bar{\pi}\Delta_0\varphi-\mathcal{H}(\varphi,\bar{\pi})]}}.$$

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

$$\langle S \rangle_0 = \frac{N_T N_L^{d-1}}{2}.$$

One might interpret this result as one half the number of degrees of freedom of the d-dimensional lattice, but this is of no direct physical importance. What is most interesting to us is the calculation of the expectation value of S on the state of one particle with momentum $\vec{k}$, which can easily be done (problem 5.2.3), resulting in

$$\langle S \rangle_{1,\vec{k}} = \frac{N_T N_L^{d-1}}{2} + 1,$$

and, in general, on a state of n particles with momentum $\vec{k}$

$$\langle S \rangle_{n,\vec{k}} = \frac{N_T N_L^{d-1}}{2} + n,$$

Hence, the observable

$$\mathcal{N} = S - \langle S \rangle_0$$

gives us the number of particles of a given state. This can be extended to states for arbitrary numbers of particles with various different momenta, in which case it gives us the total number of particles (problem 5.2.4). Note that this observable is not sensitive to whether or not the particles correspond to modes that satisfy the on-shell condition.

It is interesting to note here that the definition of this observable is quite general and does not depend on any particularity of our simple model here. In fact, it is possible to verify numerically that the observable $\mathcal{N}$ gives us the number of particles even in non-linear models such as, for example, the $\lambda\varphi^4$ model. Not only one verifies that the expectation value of this observable is always proportional to the number n of particles, whatever the values of the parameters of the model may be, but one also verifies that the value of the increment $\Delta\langle\mathcal{N}\rangle$ between the states of n and $n+1$ particles approaches the value 1 in the immediacy of the critical region in the space of parameters of the model, indicating that this increment tends to 1 in the continuum limit. The existing numerical results, still of a somewhat limited quality due to the limitations of the available resources, can be found in [3].

In a linear model such as our standard example here it is possible to define, additionally, observables that function like projection operators, returning the number of particles with a given momentum $\vec{k}$ that exist on the state. The definition of these observables is simple,

$$\mathcal{N}_{\vec{k}} = \frac{1}{2}\left[N_T N_L^{d-1}\left(\rho_{\vec{k}}^2 + \alpha_0\right)|\widetilde{\varphi}_{\vec{k}}|^2 - 1\right].$$

It is easy to verify (problem 5.2.6) that we have for this observable

$$\langle \mathcal{N}_{\vec{k}} \rangle_{n,\vec{k}} = n,$$

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,

$$|n_1, \vec{k}_1; n_2, \vec{k}_2\rangle \sim \frac{[\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}_1}|^{2n_1} |\widetilde{\varphi}_{\vec{k}_2}|^{2n_2} e^{-S[\varphi]}}{\displaystyle\int [\mathrm{d}\varphi]\ |\widetilde{\varphi}_{\vec{k}_1}|^{2n_1} |\widetilde{\varphi}_{\vec{k}_2}|^{2n_2} e^{-S[\varphi]}}.$$

5.2.5. Calculate the expectation value of the Hamiltonian $\Delta\mathbf{H}$ on the state having n_1 particles with momentum $\vec{k}_1$ and n_2 particles with momentum $\vec{k}_2$ considered in problem 5.2.4. Show in this way that the energy is additive, that is, that the total energy of the state is the sum of the energies of the particles that it contains.

5.2.6. Calculate the expectation value of the observable $\mathcal{N}_{\vec{k}}$ on a state having n particles with momentum $\vec{q}$. Consider in separate the cases in which $\vec{q} \neq \pm\vec{k}$ and the case in which $\vec{q} = \vec{k}$.

5.3 Relation with Hilbert Spaces

In possession of the concept of energy and having constructed the states of particles within the structure of our theory, we will now examine another concept which is of central importance in the traditional formalism, the concept of the eigenstates of an observable. In the traditional formalism the observables are represented by Hermitian operators in a Hilbert space and the physical states are represented by vectors in this space. In that formalism the eigenstates of an observable are the eigenvectors of the corresponding operator. Our first problem here is to determine how to characterize the property of a state being or not being an eigenstate of an observable.

In order to build this characterization of the concept of eigenstate in our formalism, it is necessary to think in terms of expectation values, as it is in terms of the direct definition of these values that our formalism is built. Let us start by recalling that, if a state $|e\rangle$ is an eigenstate of an observable $\mathcal{O}$ with eigenvalue ω, then we have in the traditional formalism

$$\mathcal{O}_{\rm op}|e\rangle = \omega|e\rangle,$$

where $\mathcal{O}_{\rm op}$ is an operator and ω a number. In terms of expectation values we can write this in the form

$$\langle e|\mathcal{O}_{\rm op}|e\rangle = \omega,$$

where we used the fact that the states are normalized, $\langle e|e\rangle = 1$. As a consequence of the relations above we also have

$$\mathcal{O}_{\rm op}^2|e\rangle = \mathcal{O}_{\rm op}\omega|e\rangle = \omega\mathcal{O}_{\rm op}|e\rangle = \omega^2|e\rangle,$$

so that we may write a relation between expectation values,

$$\langle e|\mathcal{O}_{\rm op}^2|e\rangle = \omega^2\langle e|e\rangle = \omega^2,$$

or, in other words,

$$\langle e|\mathcal{O}_{\rm op}^2|e\rangle = \langle e|\mathcal{O}_{\rm op}|e\rangle^2.$$

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,

$$\begin{aligned}
\langle \mathcal{N}^2\rangle - \langle \mathcal{N}\rangle^2 &= \langle (S^2 - 2S\langle S\rangle_0 + \langle S\rangle_0^2)\rangle - (\langle S\rangle - \langle S\rangle_0)^2 \\
&= \langle S^2\rangle - 2\langle S\rangle\langle S\rangle_0 + \langle S\rangle_0^2 - \langle S\rangle^2 + 2\langle S\rangle\langle S\rangle_0 - \langle S\rangle_0^2 \\
&= \langle S^2\rangle - \langle S\rangle^2,
\end{aligned}$$

for any state in which we may be measuring the dispersion. This is a general fact which is important for us: the addition of a constant to an observable, be it finite or divergent in the limit, does not change the dispersion of the observable. In order to calculate the dispersion of S on the vacuum, we first obtain (problem 5.3.2) the results

$$\langle S\rangle_0 = \frac{N_T N_L^{d-1}}{2},$$

and

$$\langle S^2\rangle_0 = \left(\frac{N_T N_L^{d-1}}{2}\right)^2 + \frac{N_T N_L^{d-1}}{2},$$

so that we have for the dispersion

$$\langle S^2\rangle_0 - \langle S\rangle_0^2 = \frac{N_T N_L^{d-1}}{2},$$

that is, we have

$$\sigma_{\mathcal{N}} = \sigma_S = \sqrt{\frac{N_T N_L^{d-1}}{2}},$$

which, instead of vanishing in the continuum limit, diverges, thus showing that the vacuum is *not* an eigenstate of the observable number-of-particles. Note that this dispersion is small by comparison with the value of $\langle S\rangle_0 = N_T N_L^{d-1}/2$, so that we have

$$\frac{\sqrt{\langle S^2\rangle_0 - \langle S\rangle_0^2}}{\langle S\rangle_0} = \sqrt{\frac{2}{N_T N_L^{d-1}}} \longrightarrow 0,$$

that is, the relative dispersion goes to zero in the continuum limit, but the dispersion itself is not small by comparison to the finite value of $\langle\mathcal{N}\rangle_0$. Hence, the observable $\mathcal{N}$ gives us the correct number of particles in each state, including the value 0 for the vacuum, but the vacuum is not an eigenstate of this observable.

With a little more work we can repeat these calculations for the states of n particles with momentum $\vec{k}$ which we introduced in section 5.2 (problem 5.3.3). In this case we obtain the preliminary results

$$\langle S\rangle_{n,\vec{k}} = \frac{N_T N_L^{d-1}}{2} + n,$$

and

$$\langle S^2\rangle_{n,\vec{k}} = \left(\frac{N_T N_L^{d-1}}{2}\right)^2 + N_T N_L^{d-1}\left(n+\frac{1}{2}\right) + \left(n+\frac{1}{2}\right)^2 - \frac{1}{4},$$

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

$$\Delta E = \Delta\mathcal{E}/a = N_T\Delta\mathcal{E}/T.$$

We can calculate the expectation values of $\mathbf{H}^2$ and $(\Delta\mathbf{H})^2$ both by the canonical definition and by the usual definition. Since these observables depend on $\bar{\pi}$ the results of these two calculations will be different. In any case, since $\Delta\mathbf{H}$ and $\mathbf{H}$ are related by the addition of a constant quantity, we know beforehand that both will have the same dispersion. Because of this, we may calculate directly the dispersion of $\mathbf{H}$. Besides the question of using the canonical definition or the usual definition, it is also necessary to consider in detail the question of the temporal average, which we used before to facilitate the calculations. To take this average is equivalent to defining an average Hamiltonian over a temporal block, which we denote as

$$\mathbf{H}_b = \frac{1}{N_T}\sum_t \mathbf{H}.$$

As we observed before, the invariance of the lattice model by discrete temporal translation implies that $\mathbf{H}_b$ and $\mathbf{H}$ have the same expectation value, but these are two conceptually different observables. The observable $\mathbf{H}$ corresponds to the measurement of the energy at a perfectly well-defined instant of time, while the observable $\mathbf{H}_b$ constitutes a type of block variable and we should expect that its fluctuations will be smaller than those of $\mathbf{H}$, due to the average over the temporal block. Since the dispersions of the observables are a measure of the average magnitude of the fluctuations that they undergo, the dispersions will be different. We may, in fact, predict that the dispersion of $\mathbf{H}_b$ will be smaller than that of $\mathbf{H}$, as it is characteristic for block variables.

We see therefore that we have several calculations to do, including two possibilities for the definition of the observable and two possibilities for the definition of the averages. We will present here the calculation of the dispersion of $\mathbf{H}_b$, which is simpler and sufficient for our purposes, leaving the case of $\mathbf{H}$ for the problems of this section (problems 5.3.5, 5.3.6 and 5.3.7). Besides, we will start with the canonical definition of the averages, showing, first of all, the relation of the result obtained by means of this definition with that obtained by means of the usual definition. Let us recall that the Hamiltonian density is given by

$$\mathcal{H} = -\frac{\imath}{2}\left[\bar{\pi}^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right],$$

where summation over i is implicit, so that we have the Hamiltonian

$$\mathbf{H} = \sum_{\mathbf{x}} \mathcal{H} = -\frac{\imath}{2}\sum_{\mathbf{x}}\left[\bar{\pi}^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

Calculating the temporal average of this quantity we obtain the blocked Hamiltonian

$$\mathbf{H}_b = \frac{1}{N_T}\sum_t \mathbf{H} = \frac{1}{N_T}\sum_{\vec{x}} \mathcal{H} = -\frac{\imath}{2N_T}\sum_{\vec{x}}\left[\bar{\pi}^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right].$$

We will now calculate the dispersion of $\mathbf{H}_b$, which involves the calculation of the expectation values of $\langle\mathbf{H}_b\rangle$ and $\langle\mathbf{H}_b^2\rangle$. We will do the calculation starting by the 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

$$\begin{aligned}
\langle \mathbf{H}_b \rangle^2 \;\; = \;\; -\frac{1}{4N_T^2} \Bigg[& \left(N_L^{d-1} N_T\right)^2 + 2N_L^{d-1} N_T \sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \\
& + \left(\sum_{\vec{k}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0}\right)\left(\sum_{\vec{q}} \frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0}\right)\Bigg], \qquad (5.3.1)
\end{aligned}$$

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

$$e^{\imath \sum_s (\bar{\pi}\Delta_0\varphi - \mathcal{H})} = e^{-\frac{1}{2}\sum_s (\bar{\pi}^2 - 2\imath\bar{\pi}\Delta_0\varphi)} e^{-\frac{1}{2}\sum_s \left[(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]}$$

we make the shift

$$\chi = \bar{\pi} - \imath\Delta_0\varphi \Longrightarrow \bar{\pi}^2 - 2\imath\bar{\pi}\Delta_0\varphi = \chi^2 + (\Delta_0\varphi)^2,$$

so that we may write, reconstituting the complete form of the action in the exponent,

$$\begin{aligned}\langle \mathbf{H}_b^2 \rangle \;=\; & -\frac{1}{4N_T^2 Z}\sum_{\vec{x}}\sum_{\vec{y}}\int [\mathrm{d}\varphi][\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2}\; e^{-S} \\ & \times \Big\{ (\chi + \imath\Delta_0\varphi)^2_{\vec{x}}(\chi + \imath\Delta_0\varphi)^2_{\vec{y}} + 2(\chi + \imath\Delta_0\varphi)^2_{\vec{x}}\left[(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]_{\vec{y}} \\ & \qquad + \left[(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]_{\vec{x}}\left[(\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]_{\vec{y}} \Big\},\end{aligned}$$

where S is the action and

$$Z = \int [\mathrm{d}\varphi][\mathrm{d}\bar{\pi}]\; e^{\imath\sum_s(\bar{\pi}\Delta_0\varphi - \mathcal{H})} = \int [\mathrm{d}\varphi][\mathrm{d}\chi]\; e^{-\frac{1}{2}\sum_s \chi^2}\; e^{-S}$$

is the denominator that normalizes the expectation values. We may now expand the terms inside the brackets, collecting powers of χ, making exchanges of $\vec{x}$ and $\vec{y}$, and recalling that terms with odd powers of χ at a given site vanish due to the symmetry of the integration, in order to arrive at the expression

$$\begin{aligned}\langle \mathbf{H}_b^2 \rangle \;=\; & -\frac{1}{4N_T^2 Z}\sum_{\vec{x}}\sum_{\vec{y}}\int [\mathrm{d}\varphi][\mathrm{d}\chi]\; e^{-S}\; e^{-\frac{1}{2}\sum_s \chi^2} \\ & \times \left[\chi^2_{\vec{x}}\chi^2_{\vec{y}} + 4\imath\chi^2_{\vec{x}}\mathcal{H}'_{\vec{y}} - 4\delta^d_{\vec{x},\vec{y}}\chi^2_{\vec{x}}(\Delta_0\varphi)^2_{\vec{x}} - 4\mathcal{H}'_{\vec{x}}\mathcal{H}'_{\vec{y}}\right],\end{aligned}$$

where

$$\mathcal{H}' = -\frac{\imath}{2}\left[-(\Delta_0\varphi)^2 + (\Delta_i\varphi)^2 + \alpha_0\varphi^2\right]$$

is, as usual, the Hamiltonian density with $\bar{\pi}$ substituted by $\imath\Delta_0\varphi$. We may now use the known results

$$\frac{\displaystyle\int d\chi\; \chi^2\; e^{-\frac{1}{2}\chi^2}}{\displaystyle\int d\chi\; e^{-\frac{1}{2}\chi^2}} = 1 \qquad \text{and} \qquad \frac{\displaystyle\int d\chi\; \chi^4\; e^{-\frac{1}{2}\chi^2}}{\displaystyle\int d\chi\; e^{-\frac{1}{2}\chi^2}} = 3,$$

as well as the result, which can be easily obtained,

$$\sum_{\vec{x}}\langle(\Delta_0\varphi)^2\rangle = \sum_{\vec{k}}\frac{\rho_0^2}{\rho^2 + \alpha_0},$$

in order to do the integrations and write

$$\langle \mathbf{H}_b^2 \rangle = -\frac{1}{4}N_L^{2(d-1)} - \frac{1}{2}\frac{N_L^{d-1}}{N_T} - \imath N_L^{d-1}\langle \mathbf{H}'_b \rangle + \frac{1}{N_T^2}\sum_{\vec{k}}\frac{\rho_0^2}{\rho^2 + \alpha_0} + \langle {\mathbf{H}'_b}^2 \rangle,$$

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 $\mathbf{H}_b$

$$-\sigma_{\mathbf{H}_b}^2 = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2 = \langle {\mathbf{H}_b'}^2 \rangle - \langle \mathbf{H}_b' \rangle^2 - \frac{1}{2}\frac{N_L^{d-1}}{N_T} + \frac{1}{N_T^2}\sum_{\vec{k}} \frac{\rho_0^2}{\rho^2 + \alpha_0}.$$

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

$$-\sigma_{\mathbf{H}_b}^2 = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2 = \langle {\mathbf{H}_b'}^2 \rangle - \langle \mathbf{H}_b' \rangle^2 - \frac{\imath}{N_T}\langle \mathbf{H}_b' \rangle = -\sigma_{\mathbf{H}_b'}^2 - \frac{\imath}{N_T}\langle \mathbf{H}_b' \rangle,$$

that is,

$$\sigma_{\mathbf{H}_b}^2 = \sigma_{\mathbf{H}_b'}^2 + \frac{\imath}{N_T}\langle \mathbf{H}_b' \rangle.$$

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 ${\mathbf{H}_b'}^2$

$$\langle {\mathbf{H}_b'}^2 \rangle = -\frac{N_L^{2(d-1)}}{4}\sum_{\vec{k}}\sum_{\vec{q}} (-\rho_0^2 + \rho_i^2 + \alpha_0)_{\vec{k}} (-\rho_0^2 + \rho_i^2 + \alpha_0)_{\vec{q}} \langle |\widetilde{\varphi}_{\vec{k}}|^2 |\widetilde{\varphi}_{\vec{q}}|^2 \rangle.$$

In order to calculate the indicated expectation values it is necessary to consider in detail and separately the cases in which $\vec{k} = \pm\vec{q}$ and the cases in which $\vec{k} \neq \pm\vec{q}$. In addition to this it is necessary to recall that the expectation values of products of four fields have different behaviors when the Fourier components are real, in comparison to the case in which they have non-vanishing imaginary parts. For simplicity of the argument, let us consider explicitly the case in which N is odd, in which the only real Fourier component is the zero mode, $\vec{k} = \vec{0}$. As usual in this type of calculation, once the answer is obtained in terms of complete sums over the modes in momentum space, we may lift the restriction that N be odd without affecting the validity of the answer. Under these conditions we have the following four mutually exclusive possibilities:

$$\vec{k} = \vec{q} = \vec{0}, \qquad \vec{k} = \vec{q} \neq \vec{0}, \qquad \vec{k} = -\vec{q} \neq \vec{0}, \qquad \vec{k} \neq \pm\vec{q}.$$

Each pair $(\vec{k}, \vec{q})$ which is possible is exclusively in one of these four categories, while the union of the four exhausts all the possibilities for the pairs. With this we can write for our expectation value

$$\begin{aligned}\langle \mathbf{H}_b'^{\,2} \rangle \;=\; & -\frac{N_L^{2(d-1)}}{4} \Bigg[\alpha_0^2 \langle |\widetilde{\varphi}_{\vec{k}=\vec{0}}|^4 \rangle + 2 \sum_{\vec{k}\neq\vec{0}} (-\rho_0^2 + \rho_i^2 + \alpha_0)^2 \langle |\widetilde{\varphi}|^4 \rangle \\ & + \sum_{\vec{k}\neq\pm\vec{q}} (-\rho_0^2 + \rho_i^2 + \alpha_0)_{\vec{k}} (-\rho_0^2 + \rho_i^2 + \alpha_0)_{\vec{q}} \langle |\widetilde{\varphi}_{\vec{k}}|^2 |\widetilde{\varphi}_{\vec{q}}|^2 \rangle \Bigg].\end{aligned}$$

The expectation values involving different momenta can be factored and, in addition to this, we can use the known results

$$\begin{aligned}\langle |\widetilde{\varphi}_{\vec{k}=\vec{0}}|^4 \rangle &= 3 \langle |\widetilde{\varphi}_{\vec{k}=\vec{0}}|^2 \rangle, \\ \langle |\widetilde{\varphi}_{\vec{k}\neq\vec{0}}|^4 \rangle &= 2 \langle |\widetilde{\varphi}_{\vec{k}\neq\vec{0}}|^2 \rangle, \\ \langle |\widetilde{\varphi}_{\vec{k}}|^2 \rangle &= \frac{1}{N_L^{d-1} N_T} \frac{1}{\rho^2 + \alpha_0},\end{aligned}$$

to write

$$\begin{aligned}\langle \mathbf{H}_b'^{\,2} \rangle \;=\; & -\frac{1}{4N_T^2} \Bigg[3 + 4 \sum_{\vec{k}\neq\vec{0}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 \\ & + \sum_{\vec{k}\neq\pm\vec{q}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)_{\vec{q}} \Bigg].\end{aligned}$$

One of the three units in the first term and two of the four units in the second term may now be joined with the third term in order to complete the sum that appears in this last one, resulting in

$$\begin{aligned}\langle {\mathbf{H}_b'}^2 \rangle &= -\frac{1}{4N_T^2}\left[2 + 2\sum_{\vec{k}\neq\vec{0}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)^2\right.\\ &\qquad \left. + \sum_{\vec{k}}\sum_{\vec{q}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)_{\vec{k}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)_{\vec{q}}\right].\end{aligned}$$

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 $\mathbf{H}_b'$

$$-\sigma_{\mathbf{H}_b'}^2 = \langle {\mathbf{H}_b'}^2 \rangle - \langle \mathbf{H}_b' \rangle^2 = -\frac{1}{2N_T^2}\sum_{\vec{k}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)^2,$$

and, consequently, for the dispersion of $\mathbf{H}_b$

$$-\sigma_{\mathbf{H}_b}^2 = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2 = -\frac{1}{2N_T^2}\sum_{\vec{k}}\left(\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}\right)^2 - \frac{1}{2N_T^2}\sum_{\vec{k}}\frac{-\rho_0^2+\rho_i^2+\alpha_0}{\rho^2+\alpha_0}.$$

We may join the two sums that appear in this expression into a single sum, thus obtaining

$$-\sigma_{\mathbf{H}_b}^2 = \langle \mathbf{H}_b^2 \rangle - \langle \mathbf{H}_b \rangle^2 = -\frac{1}{N_T^2}\sum_{\vec{k}}\frac{(\rho_i^2+\alpha_0)(-\rho_0^2+\rho_i^2+\alpha_0)}{(\rho^2+\alpha_0)^2},$$

that is,

$$\sigma_{\mathbf{H}_b}^2 = \frac{1}{N_T^2}\mathcal{S}_{\mathbf{H}_b},$$

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

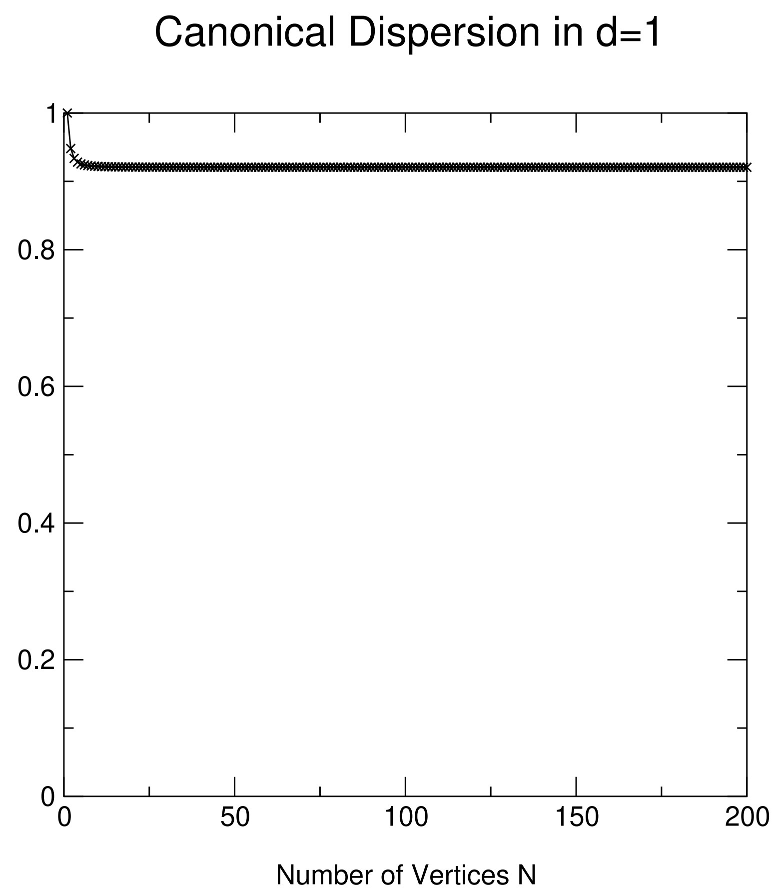


Figure 5.3.1: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, in the case $d = 1$.

that the positive terms predominate in the only factor which is not manifestly positive, the second factor in the numerator of the sum. This is due to the fact that there is an implicit sum over i in ρ_i^2, so that we have $d - 1$ positive terms and only 1 negative term in the sum of the ρ's. Since the possible values for each ρ_i and for each ρ_0 are the same, we arrive at the conclusion that the sums are predominantly positive for sufficiently large dimensions d. The only case which raises some doubt, if we recall that $\alpha_0 \to 0$ in the continuum limit, is the case $d = 2$, but in this case it is possible to rewrite the sum in a manifestly positive form (problem 5.3.8).

The issue now is to determine how these sums behave in the continuum limit. Since the term that is being added is homogeneous of order zero on the ρ's, and therefore typically of the order of 1, it is to be expected that the sums behave as $N_L^{d-1} N_T$ or, in the symmetrical limit, as N^d, which is the number of terms in the sum. One exception should be the case $d = 1$, in which all the ρ_i's disappear and the situation changes qualitatively. We can easily evaluate these sums numerically in the symmetrical case, obtaining what is seen in the figures from 5.3.1 to 5.3.5. In

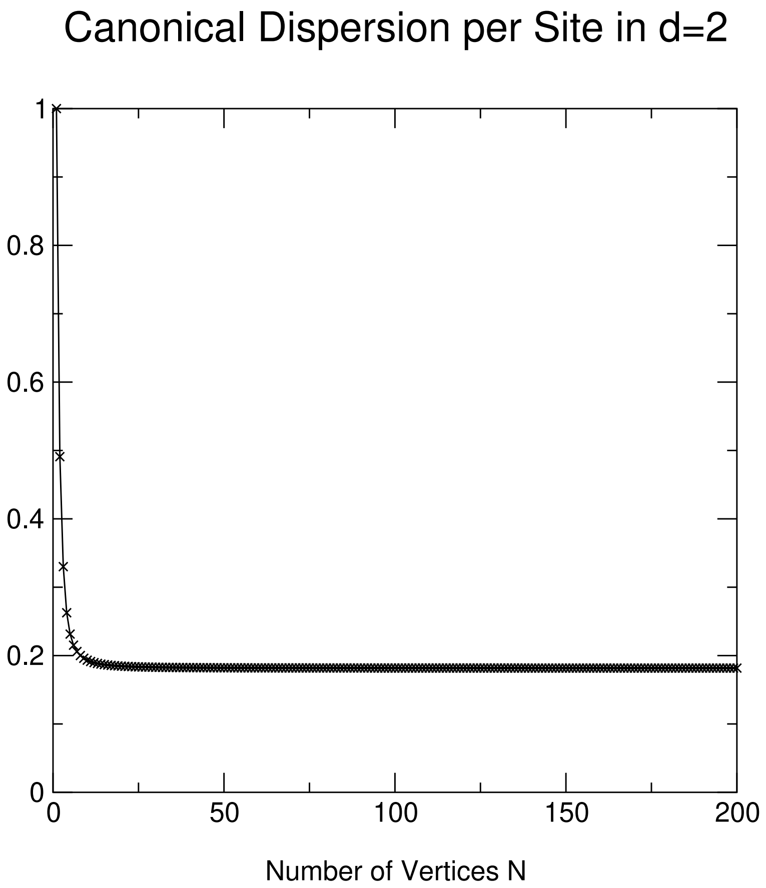


Figure 5.3.2: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 2$.

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

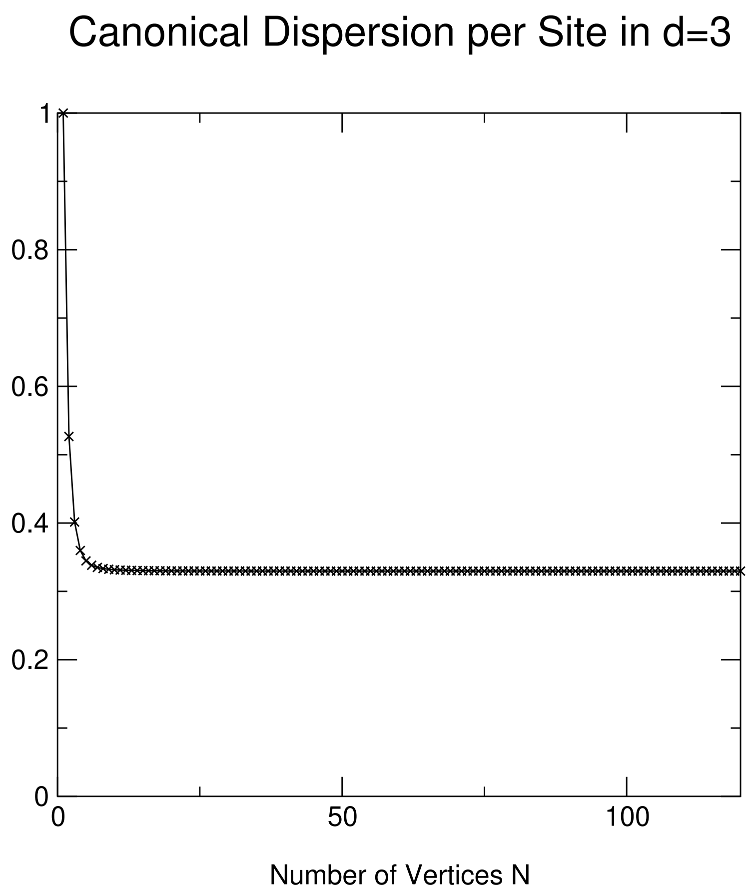


Figure 5.3.3: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 3$.

this particular case we can verify that this result is still obtained if we use the non-blocked Hamiltonian H instead of H_b, but is a much weaker form, since we are forced to adopt a particular way to take the limits for the dispersion to vanish in the limit (problem 5.3.9).

To complete the discussion we may also examine the corresponding results for $\mathbf{H}_b'$, that is, calculated according to the usual definition of the expectation values, instead of the canonical definition. In this case the result can be written as

$$\sigma^2_{\mathbf{H}_b'} = \frac{1}{N_T^2} \mathcal{S}_{\mathbf{H}_b'},$$

where the sum is defined by

$$\mathcal{S}_{\mathbf{H}_b'} = \frac{1}{2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 .$$

The results of the numerical evaluation of the sums $\mathcal{S}_{\mathbf{H}_b'}$, in the case of the symmetrical limit, can be seen in the figures from 5.3.6 to 5.3.10. The only case in which

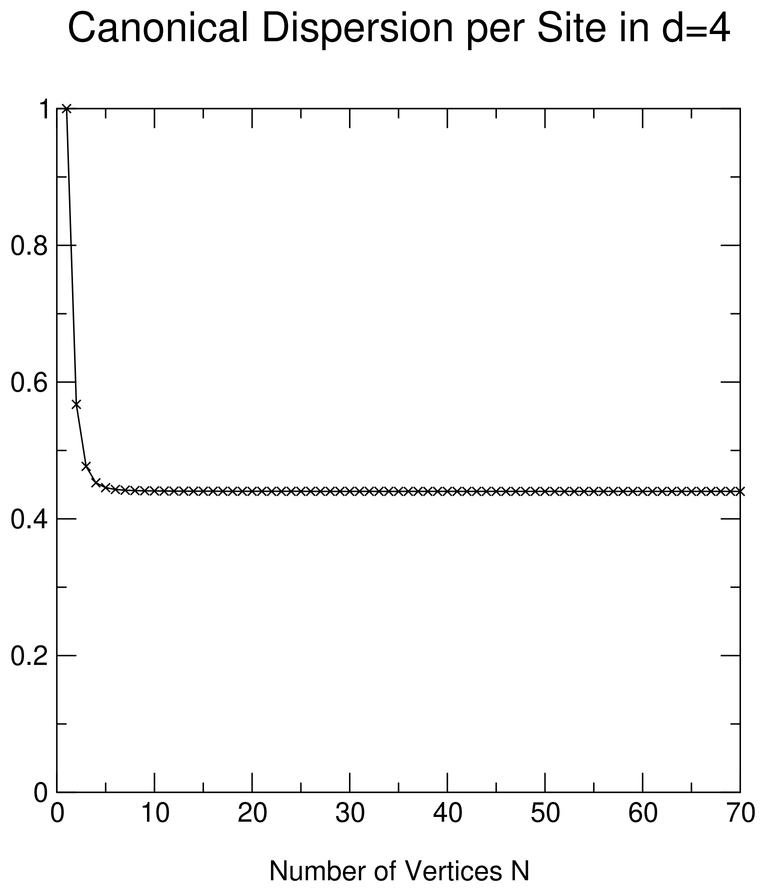


Figure 5.3.4: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 4$.

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

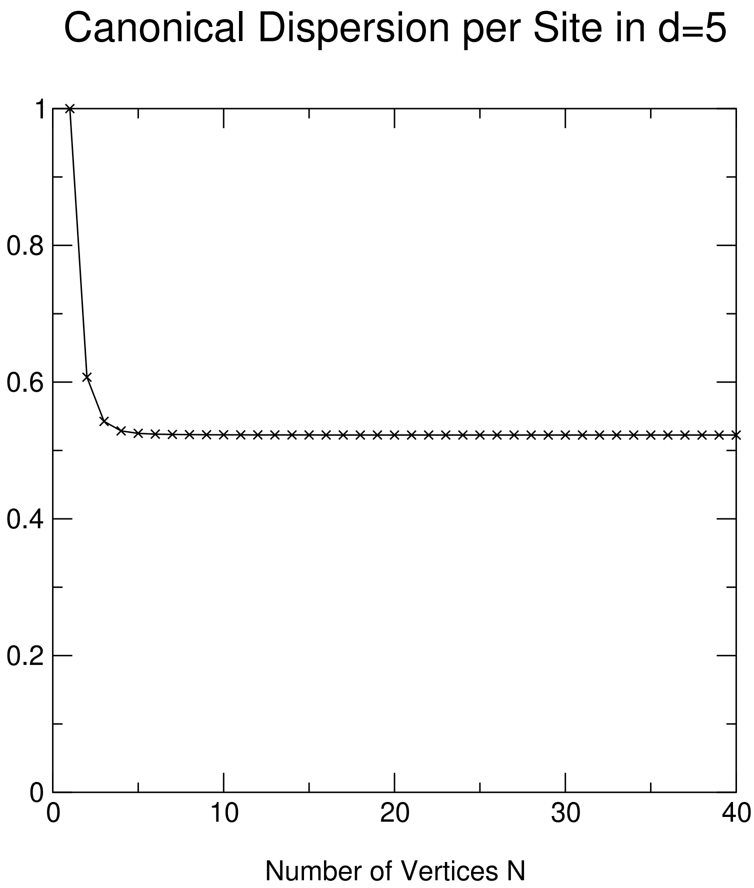


Figure 5.3.5: The sum $\mathcal{S}_{\mathbf{H}_b}$ that appears in the expression of the dispersion of $\mathbf{H}_b$, calculated according to the canonical definition of the expectation values, divided by N^d, in the case $d = 5$.

forced to use if we try to employ the non-blocked Hamiltonian H with the canonical definition of the expectation values (problem 5.3.9). Limits of this type will be discussed in detail in a little while, for the case of the quantum theory of fields. On the other hand, if we try to use the non-blocked Hamiltonian H and the non-canonical definition of the expectation values, then we verify that it is not possible to make the dispersion go to zero in the limit even in the case of quantum mechanics (problem 5.3.10).

In order to discuss in a more direct way the physical significance of these results, it is necessary to first translate these dimensionless results in terms of the dimensionfull physical energy, as we did above for the case of quantum mechanics. We will use in this discussion the results obtained according to the canonical definition of the expectation values. The dispersion $\Sigma^2_{\mathbf{H}_b} = \sigma^2_{\mathbf{H}_b}/a^2$ of the dimensionfull energy is given by

$$\Sigma^2_{\mathbf{H}_b} = \frac{1}{T^2}\mathcal{S}_{\mathbf{H}_b},$$

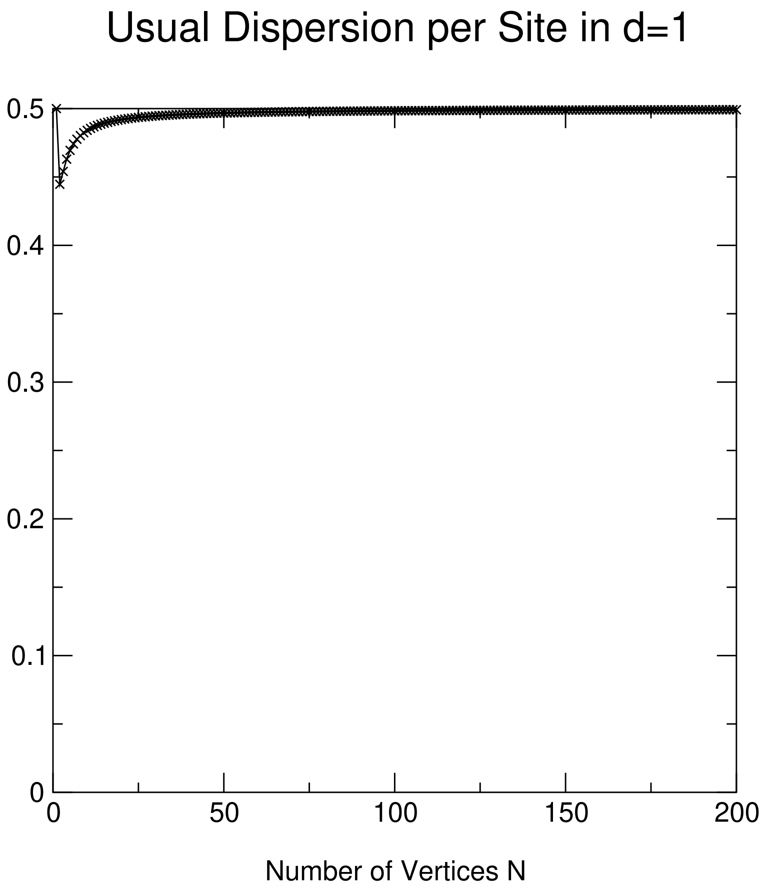


Figure 5.3.6: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 1$.

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

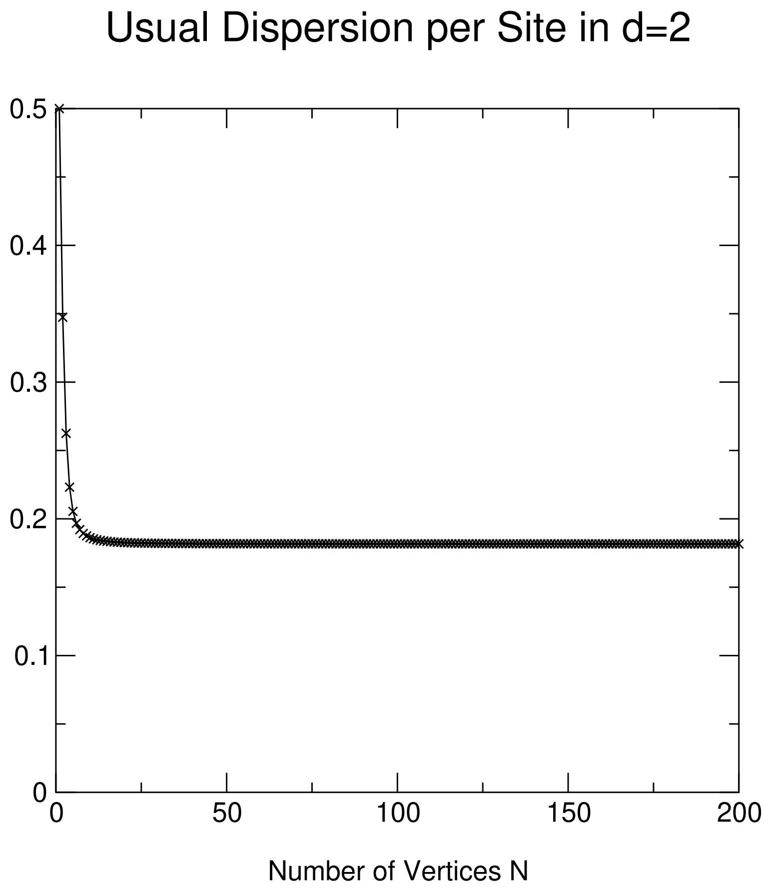


Figure 5.3.7: The sum $\mathcal{S}_{\mathbf{H}_b'}$ that appears in the expression of the dispersion of $\mathbf{H}_b'$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 2$.

$$\Sigma^2_{\mathbf{H}_b} \sim \frac{1}{a^2}.$$

For larger dimensions the situation gets progressively worse. So long as we limit ourselves to taking the continuum limit in the symmetrical way, the situation seems to be that the concept of eigenstate and, ultimately, the concept of Hilbert space, only apply to the case of quantum mechanics, and not to the case of the quantum theory of fields.

We will therefore examine what happens if we take the continuum limit in a non-symmetrical way, which obviously only makes sense for $d \geq 2$. The most extreme case in this context is to take first the limit $N_T \to \infty$ with fixed N_L, as in the case of quantum mechanics, and only after that take the limit $N_L \to \infty$. The effect of this procedure is to first reduce the system to the quantum mechanics of an arbitrary but finite number of degrees of freedom, and only after that make the number of degrees of freedom increase without limit. In this case all the sums $\mathcal{S}_{\mathbf{H}_b}$ and $\mathcal{S}_{\mathbf{H}_b'}$

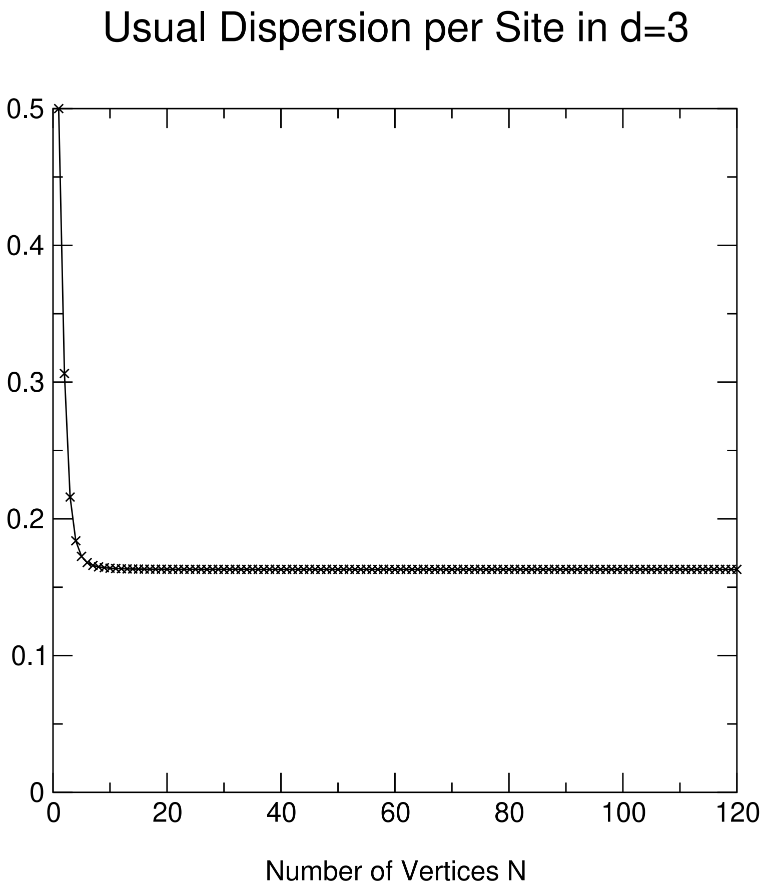


Figure 5.3.8: The sum $\mathcal{S}_{\mathbf{H}'_b}$ that appears in the expression of the dispersion of $\mathbf{H}'_b$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 3$.

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

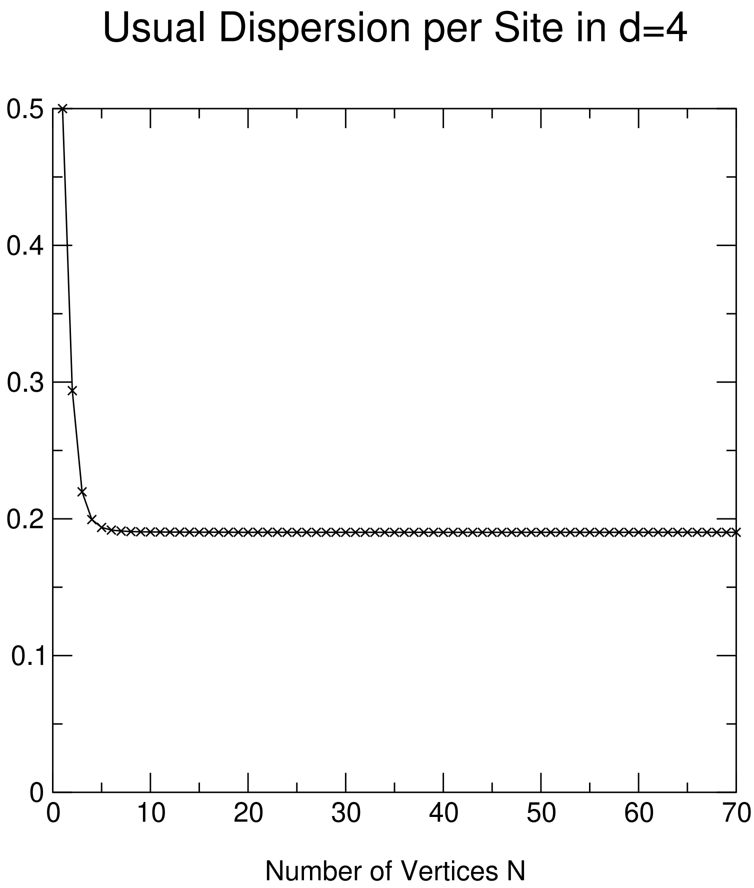


Figure 5.3.9: The sum $\mathcal{S}_{\mathbf{H}_b'}$ that appears in the expression of the dispersion of $\mathbf{H}_b'$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 4$.

$$t(\vec{k}) \longrightarrow \left[\frac{-(2\pi k_0)^2 + N_T^2 \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right) + (N_T/N_L)^2 m_0^2 L^2}{(2\pi k_0)^2 + N_T^2 \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right) + (N_T/N_L)^2 m_0^2 L^2} \right]^2 .$$

Now, since $1/N_L$ does not go to zero, the sine function that appears in the second terms in the numerator and in the denominator does not become small, so that these terms diverge like N_T^2, as do the third terms. Hence, the only difference between the numerator and the denominator, which is the sign of the first term, tends to disappear, so that we obtain, in the limit $N_T \to \infty$ with fixed N_L and finite T,

$$\mathcal{S}_{\mathbf{H}_b'} \longrightarrow \sum_{\vec{k}} 1 = N_L^{d-1} N_T .$$

The same is true if we make $T \to \infty$ together with $N_T \to \infty$, since T has to increase slower than N_T in order to guarantee that $a \to 0$, that is, that we have in fact a

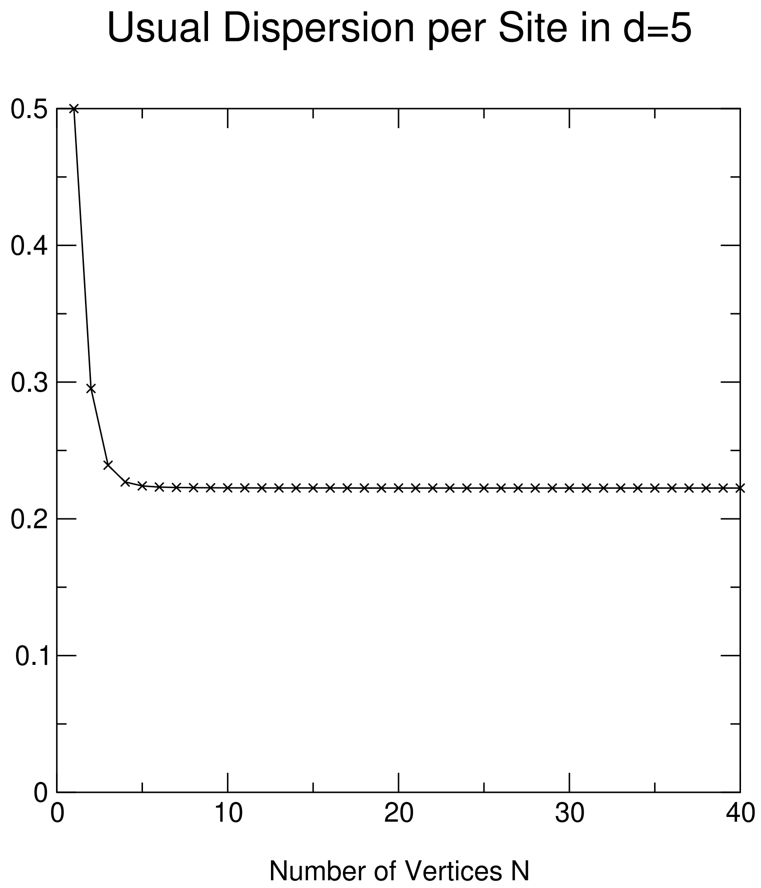


Figure 5.3.10: The sum $\mathcal{S}_{\mathbf{H}_b'}$ that appears in the expression of the dispersion of $\mathbf{H}_b'$, that is, the dispersion of $\mathbf{H}_b$ calculated according to the usual definition of the expectation values, divided by N^d, in the case $d = 5$.

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 sums behave as

$$\mathcal{S}_{\mathbf{H}_b}, \mathcal{S}_{\mathbf{H}'_b} \longrightarrow C(d) N_L^{d-1} N_T,$$

with, in each dimension, some positive constant $C(d)$, smaller than and of the order of 1. However, in order to check these facts beyond any doubt, it is necessary to evaluate numerically these sums in this type of asymmetrical limit (problem 5.3.15).

Let us observe that in this type of limit we have for the dimensionfull dispersions, both for $\Sigma_{\mathbf{H}_b}$ and for $\Sigma_{\mathbf{H}'_b}$, in dimensions $d \geq 2$, the behavior

$$\Sigma^2_{\mathbf{H}_b} \sim N_L^{d-1} \frac{N_T}{T^2}.$$

This allows us to make the dispersion vanish in the limit, it suffices to make T go to infinity sufficiently fast as a function of N_T, in order to compensate the increase of N_T. We can do this by relating T to some finite temporal length $\mathcal{T}$ (something like a mean life) by means of

$$T = N_T^p \mathcal{T}.$$

There are limits for the possible values of the power p. In order for T to go to infinity in the limit, we must have $p > 0$. On the other hand, we must remember that $T = N_T a$ and that there is also the need to make a go to zero in the limit, so that it be in fact a continuum limit. Combining this condition with the equation above we obtain

$$T = N_T a = N_T^p \mathcal{T} \Longrightarrow \mathcal{T} = N_T^{1-p} a,$$

so that in order that we have $\mathcal{T}$ finite with $a \to 0$ it is necessary that $1 - p > 0$, that is, that $p < 1$. Joining these two conditions we see that p must be inside the open interval $(0, 1)$. Writing now the dispersion $\Sigma_{\mathbf{H}_b}$ in this type of limit we obtain

$$\Sigma^2_{\mathbf{H}_b} \sim N_L^{d-1} \frac{N_T}{\mathcal{T}^2 N_T^{2p}} = \frac{N_L^{d-1}}{\mathcal{T}^2} N_T^{1-2p}.$$

In order for this to vanish in the limit we must have $1 - 2p < 0$, that is, $p > 1/2$. This set of conditions over p can be satisfied by values of p in the open interval $(1/2, 1)$, for example $p = 3/4$.

As another way to define asymmetrical limits, we can also generalize the symmetrical limits to the case in which both N_L and N_T increase in the limit, but with N_T increasing faster than N_L, thus establishing an asymmetry. We will call this type of limit the "simultaneous asymmetrical limits". It suffices to establish between these two quantities a relation of the type

$$N_L = N_T^q.$$

In order for N_L to increase slower than N_T, but so that both still increase simultaneously, we must have $0 < q < 1$. Observe that the terms of the sums still have 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

$$\Delta E_{1,\vec{k}} = \frac{-1}{T}\,\frac{4\sin^2\left(\frac{k_0\pi}{N_T}\right) + \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right) + \alpha_0}{-4\sin^2\left(\frac{k_0\pi}{N_T}\right) + \sum_i 4\sin^2\left(\frac{k_i\pi}{N_L}\right) + \alpha_0}.$$

We may now multiply the numerator and the denominator by N_T^2 and take the limit $N_T \to \infty$ with $N_L = N_T^q$ and $q > 0$. Note that, since in this case the momentum $\vec{k}$ is fixed and finite, we can approximate all the sine functions by their arguments without introducing any imprecision of thought. When we do this we obtain

$$\Delta E_{1,\vec{k}} \sim \frac{-1}{T}\,\frac{(2\pi k_0)^2 + N_T^{2(1-q)}\sum_i (2\pi k_i)^2 + N_T^{2(1-q)} m_0^2 L^2}{-(2\pi k_0)^2 + N_T^{2(1-q)}\sum_i (2\pi k_i)^2 + N_T^{2(1-q)} m_0^2 L^2}.$$

Since k_0, k_i and m_0 are finite and $q \neq 1$, in the limit in which $N_T \to \infty$ with $T \to \infty$ the first term becomes negligible by comparison with the other two, both in the numerator and in the denominator, so that we are left with the relation

$$\Delta E_{1,\vec{k}} = \lim_{T\to\infty} \frac{1}{T},$$

which goes to zero. Since the energy of the corresponding state of n particles is n times this result, we see that the energies of all the particle states collapse to zero in this type of limit. In other words, none of the states has energy different from the energy of the vacuum state in the continuum limit, whatever the momentum-space mode it is related to. Another way to say this is that, in this type of limit, there are no physical states left except the vacuum, once the limit is taken. One is left with an empty theory.

The fundamental reason causing this behavior can be identified as the underlying relativistic invariance of the theory. It is this invariance that implies the form of the action and therefore the form of the terms in the results for the energy, with the sum of ρ_0^2 and of the ρ_i^2, all with coefficients 1. The terms $(\Delta_0\varphi)^2$, $(\Delta_i\varphi)^2$ and $\alpha_0\varphi^2$ in the action lead directly to the terms ρ_0^2, ρ_i^2 and α_0 contained in our results. In the ultimate analysis, the relativistic invariance requires that the continuum limit be taken in a symmetrical way.

Note that this does not mean that the box inside which we are defining our model has to be exactly cubical. We may have a fixed proportionality relation between N_T and N_L, such as $N_T = CN_L$ with some constant C, meaning that the temporal size T and the spacial size L of the box may not be the same. However, it is necessary that the continuum limit be taken in a symmetrical way, that is, that N_T and N_L increase with the same speed in the limit. So long as the lattice spacing a remains the same in all the directions of the lattice there is no change in the form of the action and therefore no change in our results here. In other words, the requirement of symmetry in the continuum limit is a characteristic related to the ultraviolet regime, not to the infrared regime of the theory.

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 quantum-mechanical system of coupled harmonic oscillators with finite couplings, which is to make $\beta_0 \to 0$, also implies that $\nu \to 0$, that is, leads to the total absence of wave propagation in the continuum limit in Minkowski space.

Note that recovering the balance between the three terms of the sums in our results for the energy, which leads to the on-shell condition, also implies making $\beta_0 \to 0$ in this asymmetrical limit. This analysis can be extended to the case of the simultaneous asymmetrical limits, with the same basic results. Any trial at recovering the on-shell condition in these limits implies the absence of wave propagation in the continuous limit in Minkowski space. With the introduction of β_0 the numerator and the denominator that appear in our results acquire the form

$$\pm 4 \sin^2\left(\frac{k_0 \pi}{N_T}\right) + \beta_0 \sum_i 4 \sin^2\left(\frac{k_i \pi}{N_L}\right) + \alpha_0,$$

so that in order to compensate the factor $(N_T/N_L)^{2(1-q)}$ that appears in the second terms when we multiply both the numerator and the denominator by N_T^2 we must make $\beta_0 \to 0$ in the limit, which is equivalent, from the point of view of quantum mechanics, to making finite the couplings between sites and, from the point of view of quantum field theory, to the absence of wave propagation in the continuum limit in Minkowski space.

We end this section with the interesting historical observation that this is not the first time that the existence of a useful Hilbert space for quantum field theory is submitted for discussion. In a very interesting (but difficult to find) little book titled "Lectures on Quantum Field Theory" [4] no lesser a figure than Dirac gave us his views about the state of the subject. In this book one finds the following two statements, that we take the liberty of quoting here:

> The interactions that are physically important in quantum field theory are so violent that they will knock any Schrödinger state vector out of Hilbert space in the shortest possible time interval.
>
> [The Schrödinger picture] is thrown out by the interactions which physicists are interested in being so violent in the high frequencies, and it doesn't seem to be possible to get interactions satisfying relativity which do not have this violent behaviour in the high frequencies.

These statements are by no means exactly the same that we are led by our results to make here, since Dirac is talking about interactions between fields and the Schrödinger picture of quantum mechanics, but the reference to the lack of usefulness of the Hilbert space, because the dynamics of the theory does not allow it to permanently contain the states, and the reference to relativistic invariance as being in conflict with the usual Hilbert space structure, are both, at the very least, extremely interesting and suggestive.

Problems

5.3.1. 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

$$\sigma_H^2 = \sigma_{H'}^2 + \imath\langle \mathbf{H}'\rangle.$$

5.3.6. Calculate, according to the usual (non-canonical) definition of the expectation values, using the Fourier components of the fields, the dimensionless dispersion $\sigma_{H'}^2 = \langle \mathbf{H}' \rangle^2 - \langle \mathbf{H}'^2 \rangle$, of the non-blocked Hamiltonian, obtaining

$$\begin{aligned}\sigma_{H'}^2 &= \frac{1}{2N_T^2} + \frac{1}{N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 \\ &+ \frac{1}{2N_T^2} \sum_{\mathbf{k}} \sum_{k_0} \sum_{q_0} \frac{\left| -e^{-\imath\pi \frac{k_0 - q_0}{N_T}} \rho_0(k_0)\rho_0(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0 \right|^2}{\left[\rho_0^2(k_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0\right] \left[\rho_0^2(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0\right]}.\end{aligned}$$

5.3.7. Combine the results of problems 5.3.5 and 5.3.6 and calculate completely the dispersion $\sigma_H^2 = \langle \mathbf{H} \rangle^2 - \langle \mathbf{H}^2 \rangle$, obtaining

$$\begin{aligned}\sigma_H^2 &= \frac{1}{2N_T^2} + \frac{1}{2N_T} \sum_{\vec{k}} \frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} + \frac{1}{N_T^2} \sum_{\vec{k}} \left(\frac{-\rho_0^2 + \sum_i \rho_i^2 + \alpha_0}{\rho^2 + \alpha_0} \right)^2 \\ &+ \frac{1}{2N_T^2} \sum_{\mathbf{k}} \sum_{k_0} \sum_{q_0} \frac{\left| -e^{-\imath\pi \frac{k_0 - q_0}{N_T}} \rho_0(k_0)\rho_0(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0 \right|^2}{\left[\rho_0^2(k_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0\right] \left[\rho_0^2(q_0) + \sum_i \rho_i^2(\mathbf{k}) + \alpha_0\right]}.\end{aligned}$$

Compare your result with the dispersion of the blocked Hamiltonian $\mathbf{H}_b$ and show that $\sigma_H^2 > \sigma_{H_b}^2$, as expected.

5.3.8. Show that the sum $\mathcal{S}_{H_b}^2$ in dimension $d = 2$,

$$\mathcal{S}_{H_b} = \sum_{\vec{k}} \frac{(\rho_1^2 + \alpha_0)(-\rho_0^2 + \rho_1^2 + \alpha_0)}{(\rho_0^2 + \rho_1^2 + \alpha_0)^2},$$

can be written as a manifestly positive quantity in the case of the symmetrical limit, in which $N_L = N_T = N$. Use the possibility of interchanging, in this symmetrical case, the variables k_0 and k_1 within the sum.

5.3.9. Write the dispersion σ_H of the non-blocked Hamiltonian in the $d = 1$ case of quantum mechanics. Evaluate the behavior in the $N_T \to \infty$ limit of the sums that appear in this result. In order to do this, consider the expressions in the limit $\alpha_0 \to 0$, which is the most relevant for us because α_0 in fact vanishes in the continuum limit. Note that in this limit you must treat separately the terms with $k_0 = 0$ and/or $q_0 = 0$. Use your results to show that the corresponding dimensionfull dispersion behaves in the limit as

$$\Sigma_H^2 \sim \frac{-N_T}{T^2}.$$

Find out how to define limits in which $N_T \to \infty$ and $T \to \infty$ simultaneously so as to guarantee that this dimensionfull dispersion vanishes in the limit.

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

$$\Sigma_{H'}^2 \sim \frac{N_T^2}{T^2},$$

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 $\sigma_{H_b}^2$. Also do the same for the sums $\mathcal{S}_{H_b'}$ that appear in the expression of $\sigma_{H_b'}^2$. Use your programs to reproduce the graphs which are shown in the text.

5.3.12. Calculate in detail the quantity $\langle H_b'^2 \rangle$ 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 $\sigma_{H_b}^2$. Also do the same for the sums $\mathcal{S}_{H_b'}$ that appear in the expression $\sigma_{H_b'}^2$. 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.

Chapter 6

Conclusions and Outlook

In this last chapter we discuss what conclusions can be drawn from the work done so far and presented in this book, describe some things that will be discussed in the next volume of the series, and finally talk about the future possibilities for research in the context of the ideas presented here. In the first section we present a fairly complete analysis of the final situation we are faced with after the development presented in the previous chapters. In the second section we propose a basic idea about one of the main problems that remains open within the theoretical structure we are building; it should be noted here that the material found in that section is of a rather speculative character. We will close this book with a short description of some other things that have been done, of some of the open problems and of some possibilities for further research in the area.

6.1 Analysis of the Situation

Let us consider what has been successfully obtained within the formalism presented in the previous chapters. First of all, in chapter 2 we obtained a complete and correct realization of the classical theory of fields using the lattice and the continuum limit from it. In addition to this, as was shown along chapters from 3 to 5, the same formalism in the quantum case for dimension $d = 1$ succeeded in producing a complete and correct realization of non-relativistic quantum mechanics. In the case of dimensions $d \geq 2$ we can go so far as to say that the formalism can be used to produce a fairly complete and constructive mathematical definition of the quantum theory of fields.

The definition of the Gaussian model on the Euclidean lattice results in the correct set of correlation functions for that simple model. A closer examination of the structure of the two-point function, which is the only non-trivial function of the model, revealed some rather surprising aspects of its behavior, but these issues were completely resolved by the introduction of block variables, leading to a completely satisfactory physical interpretation of the correlation functions of the theory. While it is a widely accepted position that all the observables in quantum field theory must be averages over spacial regions or blocks, the same does not seem to be so clear with 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 in momentum space than in position space. Elementary particles are therefore extended objects, not point-like objects. From a conceptual point of view the particles should really be identified with exchanges of packets of energy between external sources and the quantum field within the cavity. These exchanges do not happen in a sharply localized way, but over the whole extent of the cavity. In the non-relativistic limit, in which one makes $T \to \infty$ while keeping L finite, this association of relativistic particles with the d-dimensional cavity is mapped onto a corresponding association of the physical particles with the modes of the $(d-1)$-dimensional cavity that is left after the limit. This is a direct consequence of the non-relativistic limit of the on-shell condition, which establishes the expected values for the energy of the particles in terms of the momenta of the modes of the $(d-1)$-dimensional cavity.

We see, therefore, that the construction of the theory on the lattice is successful in many respects. There remains, however, one main issue to be dealt with, because we arrived at the unexpected result that neither the vacuum state nor any of the particle states are eigenstates of the blocked Hamiltonian observable, which is in sharp contrast with the situation in the case of non-relativistic quantum mechanics, in which we do find that the vacuum is an eigenstate of the blocked Hamiltonian. Due to this the construction does not lead to the usual structure of states and operators in a Hilbert space, as one might have expected it would do. Since there is a well-known formalism due to Osterwalder and Schrader [6] dealing precisely with the construction of a Hilbert space structure starting from the lattice structure, we must now compare our results with those of that formalism.

It is the examination of the asymmetrical continuum limits discussed in section 5.3, which first reduce the structure of the theory to the quantum mechanics of a finite number of coupled degrees of freedom, and only after that may let the number of degrees of freedom tend to infinity, that leads us to make contact with the Osterwalder-Schrader formalism. In this formalism the authors establish necessary and sufficient conditions for the construction of a positive-norm Hilbert space from the discrete structure defined on a lattice. When one examines the development of the argument in that formalism, one observes that it implicitly assumes that $N_T = \infty$ from the very beginning, so that the applicability of its conclusions to lattice systems such as the ones discussed in this book is limited to those that result from the asymmetrical limits.

Although the condition that $N_T = \infty$ is not explicit within the hypothesis of the formalism, it is implied by the operations that are performed during the development of the argument. One of the basic hypothesis of that formalism, which is given explicitly, is that the lattice must be separable into two disjoint sets by means of the definition of a $(d-1)$-dimensional boundary surface, which defines a moment in time. This eliminates the possibility of the use of periodical boundary conditions in the temporal direction of the lattice, as we have done regularly in this book. In addition to this, during the development one requires the possibility of performing temporal translations under which the system should be invariant. Without periodical boundary conditions this is only possible if the lattice is infinite in the temporal 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 the electromagnetic field, are excitations of the modes of oscillation of the electromagnetic field within the cavity. The photons are clearly identified with packets of energy that are exchanged between an external source, in this case the atom, and the modes of oscillation of the field within the cavity.

The only way in which it seems possible to keep the symmetry between the temporal and spacial directions and still be within the hypothesis of the Osterwalder-Schrader formalism is to start with lattices that are infinite in all directions. Starting with both N_T and N_L infinite would be compatible with the aforementioned hypothesis of that formalism, but is equivalent to giving up the constructive definition of the theory by a limiting process from finite and discrete mathematical systems. We regard this as philosophically unacceptable, since adopting such a definition would rule out any truly constructive analysis of the structure of the theory. Note that it would also rule out any type of finite computational simulation as a calculational tool for the theory.

It seems to us that there is no reasonable way out of this situation, and that we must accept the fact that the traditional Hilbert-space formalism is not an appropriate tool for the description of relativistic quantum theory at the most fundamental level. A constructive definition which could include such a formalism at the fundamental level is, it would seem, still to be exhibited. As we will see in our continued explorations in the next volume, the usual perturbative theory can be formulated entirely on the lattice, without any reference to Hilbert spaces, and hence all the calculations that can be made in that formalism can also be performed within the lattice formalism, possibly with some quantitative differences, so that not much is lost in the perturbative front. In fact, something is gained, due to a much clearer and more solid insight into the mathematical structure of the theory.

Note that the loss of the usual Hilbert-space formalism is not really a physical loss, but rather a mathematical one. The fundamental physical principle underlying the quantum theory, the principle of uncertainty, is not lost. In fact, one can say that the exact opposite is true, and that quantum field theory contains a higher degree of uncertainty than non-relativistic quantum mechanics, as was argued by Landau and Peierls a long time ago [8]. This is reflected in the violent fluctuations undergone by the fundamental field, leading to its being typically a completely discontinuous function, and also causing the Hilbert-space formalism to cease to be an appropriate tool for the description of the structure of the theory. It is possible, however, that the Hilbert-space structure can be recovered as an approximation, under certain conditions. For example, this is certainly to be expected in the non-relativistic limit of the theory.

One situation in which one would expect that an approximate Hilbert-space structure can be implemented would be for an effective theory using block variables and an energy cutoff. This is made reasonable due to the fact that the behavior we see in quantum field theory is clearly related to the large fluctuations of the fields, and these become much smaller for the block variables. As we saw in section 4.3, the larger the blocks, the smaller the fluctuations undergone by the block variables, so that large blocks are associated to the classical limit of the theory. If in some specific 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

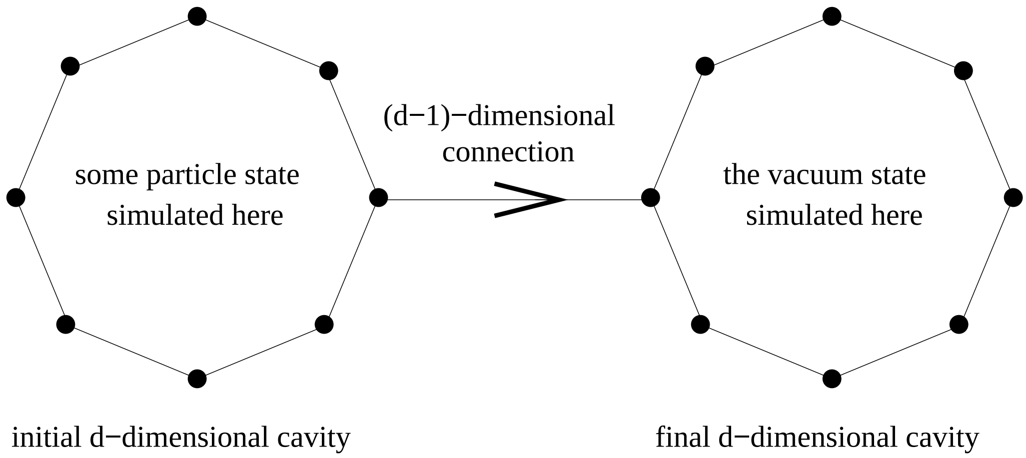


Figure 6.2.1: The lattice model proposed as a representation of the temporal evolution of blocked quantities.

boundary conditions we will adopt periodical boundary conditions for each lattice. Note that there is no problem involved with the use of the periodical boundary condition in the temporal direction within each box, because this internal temporal variable does not represent temporal evolution. The middle arrow represents the interface between the two lattices, connecting a $(d-1)$-dimensional spacial section of the left lattice with a corresponding spacial section of the right one.

The $(d-1)$-dimensional surface interfacing the two boxes will become an arrow of time, establishing a temporal ordering between the two boxes, in the following way: the initial box will contain a full realization of some state of particles, that is, a stochastic simulation of the corresponding statistical distribution; one then takes the field that results from this distribution, on the chosen $(d-1)$-dimensional space-like surface perpendicular to the temporal variable of that box, and copies it dynamically into a corresponding space-like surface of the final box; within the second box one builds a direct stochastic realization of the statistical distribution of another physical state, typically the vacuum state, at all sites except for this $(d-1)$-dimensional space-like surface, which will function as a dynamical boundary condition for the rest of the lattice within the second box.

If the state in the first box is, say, a one-particle state with momentum $\vec{k}$, then the second box will be subject to the effect of a $(d-1)$-dimensional surface containing a section of that first ensemble. This will affect the distribution within the second box, which will no longer be simply the vacuum. In this way the physical situation within the first box can propagate into the second box, along what we may call Monte-Carlo time, in a type of diffusion process, leading eventually to an equilibrium situation which represents the physical propagation of the state. The physical propagation is expressed as the difference between what we implemented directly in the second box (the vacuum state) and what eventually turns up within it as a consequence of the influence of the first box (in this example, possibly a one-particle state). Note that the cause-and-effect relationship is only from the first box to the second box, 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

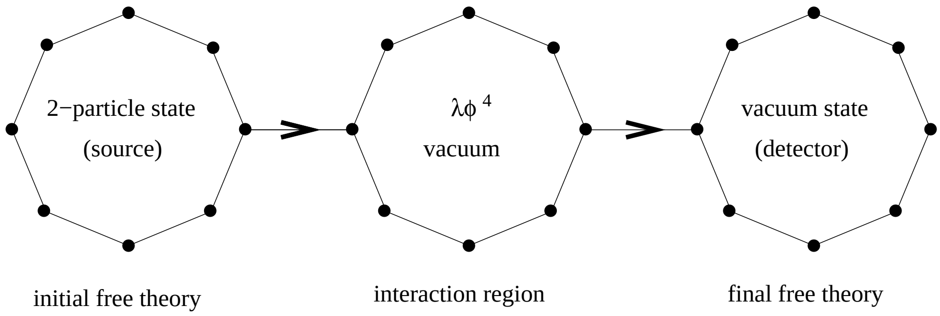


Figure 6.2.2: The lattice model proposed as a representation of a scattering process.

vectors pointing more directly through the $(d-1)$-dimensional interface. However, definite answers to any of the many questions one could ask about this idea will have to wait for the results of further research, probably involving some large-scale stochastic simulations of the proposed system.

If this idea turns out to work, then one can readily imagine other uses for it, for example the direct representation of scattering processes, as illustrated in figure 6.2.2. Here we have three consecutive boxes, the initial one holding an initial state of two particles, say with momenta $\vec{k}_1$ and $\vec{k}_2$. The middle box is an interaction region, where an interaction such as one finds in the $\lambda\phi^4$ polynomial model is turned on, and the parameters of the model are tuned so that the physical mass of its particles is equal to the physical mass of the incoming free particles. The third box contains the free vacuum and is a detection region, where one will look to find out what particles with which momenta show up. This would be a discrete realization of the scattering structure which is usually represented by asymptotic "in" and "out" fields and states in the traditional approach to the subject.

One can go further on with ideas like this, for example proposing the definition of thermal states, by starting with a state containing some set of many particles, and propagating it through a large number of consecutive interaction regions, until the set of particles finds a true thermal equilibrium distribution, that is, a distribution of particles that no longer changes when it passes through an interaction region. For practical reasons one could adopt the following alternative approach: instead of a long series of interaction regions, use only one interaction region and add to the system a feedback mechanism from the third box to the first box, that modifies the initial distribution of particles so that it converges to the final distribution of particles which is detected in the third box. In any case, one can see that there is plenty of field for exploration and further research in this subject.

6.3 Problems and Possibilities

The facts about the theory found in the explorations described in this book have some important consequences on the treatment of some other models, namely the non-linear models of scalar fields usually referred to as the polynomial models and 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.

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