Part One

Introduction to Classical and Quantum Field Theory. Tai-Kai Ng

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Introduction

1.1
What is a Field Theory?

Field theory deals with objects which form a *medium*, for example objects like water, air, solids, magnets, electromagnetic fields, or even our universe. A common feature of these objects is that they are all composed of a large number of microscopic constituents. The goal of field theory is to study the *thermodynamics* and *dynamical* properties of these media.

1.1.1
Mathematical Description

To describe these objects, we have to introduce variables that are functions of space and time. These variables can be real or complex scalars, vectors, tensors, and so on. For example, to describe the motion of air (or fluid), we have to introduce the variables $\rho(\vec{x}, t)$ and $\vec{j}(\vec{x}, t)$, which are the mass and current density of air (or fluid) molecules, respectively. To describe magnets, we introduce the magnetization density $\vec{M}(\vec{x}, t)$, which is a vector variable describing the magnitude and direction of magnetization at point $\vec{x}$ inside the magnet at time t.

Question
How about vacuum (or our universe)? Can you think of any *continuous* physical quantities that can describe different states of the vacuum?

Answer
Yes, electromagnetic and gravitational fields, density of stars (galaxies), and so on.

In physics, the properties of the media are characterized by two important ingredients, the thermodynamic and dynamical properties of the media. Examples of thermodynamic properties include

– How density and pressure of air change with temperature, volume, and so on.

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– How magnetization of a magnet changes with temperature, external magnetic field, and so on.

An important concept coming from thermodynamics is *phases and phase transitions* – that the same physical medium can behave in qualitatively different ways (different phases) under different conditions, and that the medium can evolve from one phase to another when some thermodynamic parameters change. For example, water can evolve from the solid to the liquid phase when the temperature rises, and the physical properties of the two phases are qualitatively different. We shall see later that we can ask similar questions even for our vacuum. For example, how will the dynamics of an electromagnetic field change if our vacuum evolves to a different phase?

In studying dynamics we typically ask the question of how the variables describing a medium will evolve with time with an initial condition or under external, time-dependent force. These are the situations we encounter when we want to investigate a medium with our experimental probes.

Question

What do we need to study the thermodynamics of a field theory?

According to Gibbs, the (equilibrium) thermodynamics of any physical system is determined by the *partition function*

$$Z = \int e^{-\frac{H[\phi]}{k_B T}} D\phi,$$

where H is the Hamiltonian (energy) function, T is the temperature, and $\phi_{i,j,\ldots}(\vec{x})$ are the variables characterizing the medium. The integral sign $\int \ldots D\phi$ is a shorthand notation meaning that we have to sum over all configurations of the field ϕ. Note that to evaluate the partition function we need to know how the energy of the system depends on the field configurations $H[\phi(\vec{x})]$. In quantum systems the situation is complicated by the fact that different variables may not commute with each other. The simplest way to get out of this trouble is to replace the sum over all configurations ϕ by a sum over all eigenstates φ_n. We shall discuss concrete examples later in the book.

Question

Can you give us some examples of $H[\phi(\vec{x})]$?

$$\text{Ising model for magnet: } H[S_i] = -J \sum_{\langle i \cdot j \rangle} S_i S_j \quad (S_i = \pm 1).$$

$$\text{(Classical) Heisenberg model: } H[\vec{S}_i] = -J \sum_{\langle i \cdot j \rangle} \vec{S}_i \cdot \vec{S}_j \quad (\vec{S} = \text{unit vector}).$$

Can you think of other examples?

The computation of the partition function of a classical field system is in general a very complicated problem. We shall look into this subject more carefully in the second part of this chapter. Let us discuss the question of dynamics first.

Question

What is required to understand the dynamics of a field theory?

In classical field theory we need to solve equations of motion of the fields typically of the form $\frac{\partial}{\partial t}\phi(\vec{x},t) = F\big[\phi(\vec{x}',t')\big], \ldots,$ and so on. A well-known example of equations of motion of a classical field theory are the Maxwell equations

$$\nabla\cdot\vec{E} = \frac{\rho}{\varepsilon_0}, \quad \nabla\cdot\vec{B} = 0, \quad \nabla\times\vec{B} = \mu_0\vec{J} + \frac{1}{c^2}\frac{\partial\vec{E}}{\partial t}, \quad \nabla\times\vec{E} + \frac{\partial\vec{B}}{\partial t} = 0.$$

Another well-known example is the Navier–Stokes equation. We also have equations for elastic waves in solids, surface waves in water, and so on. Equations of motion in quantum field theories have a different meaning because the field variables become operators. We shall explore the quantum situation in later chapters.

Summarizing, for classical field theory we need mathematical tools to (i) evaluate the partition function and (ii) solve the equations of motion. Both of these tasks can be achieved rigorously only if the system is *linear*. In general it is impossible to accomplish these two tasks and approximate methods have to be used. We shall review the basic mathematical techniques needed for the above problems in the following.

1.2
Basic Mathematical Tools in (Classical) Field Theory

1.2.1
Solution of Field Equations of Motion

First, we shall consider linear systems where the above mathematical tasks can be solved exactly in principle.

For linear equations of motion, we can write the equations in a general form

$$\widehat{L}\left(\frac{\partial}{\partial t}, \nabla\right)\psi(\vec{x},t) = 0, \tag{1.1a}$$

where $\widehat{L}$ is in general an $N\times N$ Hermitian matrix operator and ψ is an N-dimensional vector function. An example is the Maxwell equation where $\psi \to \vec{E}, \vec{B}$ are field vectors each with three components. Many equations of motion involving vectorial fields can be written in matrix form.

Examples of $\widehat{L}$:

$$\widehat{L} = \frac{\partial^2}{\partial t^2} - c^2\nabla^2 \text{ (wave equation)}, \quad \widehat{L} = i\frac{\partial}{\partial t} - \widehat{H} \text{ (Schrödinger equation)}.$$

Note that the above equations can be viewed as eigenvalue equations with zero eigenvalue, that is

$$\widehat{L}\left(\frac{\partial}{\partial t}, \nabla\right)\psi_0(\vec{x},t) = (0)\cdot\psi_0(\vec{x},t). \tag{1.1b}$$

Very often, we also need to solve the equations with an external driving force. In this case we have equations of the form

$$\widehat{L}\left(\frac{\partial}{\partial t}, \nabla\right)\psi(\vec{x}, t) = f(\vec{x}, t), \tag{1.2}$$

where $f(\vec{x}, t)$ is a vector function with the same dimension as ψ.

A general strategy to solve this kind of problem is the eigenfunction expansion method plus Green's functions. We shall treat space and time on equal footings in the following general discussion.

1.2.1.1 Eigenfunction Expansion Method

In the theory of differential equations a very important and useful result is the completeness and orthonormality of the set of eigenfunctions that satisfies an eigenvalue equation $H\psi_n = \lambda_n\psi_n$, where H is any Hermitian differential operator operating in space and time and the λ_n are the corresponding eigenvalues.

It can be proved that the eigenstates ψ_n form a complete set, that is any (continuous, differentiable) function which is defined in the (Hilbert) space where H operates can be written as

$$f(\vec{x}t) = \sum_n a_n\psi_n(\vec{x}t), \tag{1.3a}$$

where a_n are complex, numerical coefficients that can be determined from another important property of the ψ: the orthonormality of eigenstates with different eigenvalues, that is

$$\int_V \psi_n^*(\vec{x}t)\psi_m(\vec{x}t)\mathrm{d}^d x\,\mathrm{d}t = \delta_{nm}. \tag{1.3b}$$

With Equation (1.3a) it can be shown easily that

$$a_n = \int_V f(\vec{x}t)\psi_n^*(\vec{x}t)\mathrm{d}^d x\,\mathrm{d}t. \tag{1.3c}$$

Degeneracy In many cases the eigenstates are degenerate, that is there is more than one eigenstate with the same eigenvalue. In this case let $\{\{\psi_m'^{(n)}\}\}$ be a complete set of eigenstates with eigenvalue λ_n; then, a result from linear algebra tells us that we can always construct a set of orthonormal states $\{\psi_m^{(n)}\}$ from $\{\psi_m'^{(n)}\}$ and from completeness any function $g_n(\vec{x}t)$ that satisfies $\widehat{L}g_n(\vec{x}t) = \lambda_n g_n(\vec{x}t)$ can be written as

$$g_n(\vec{x}t) = \sum_m a_m^{(n)}\psi_m^{(n)}(\vec{x}t), \tag{1.4a}$$

where

$$\begin{aligned} &\int_V \psi_m^{(n)^*}(\vec{x}t)\psi_{m'}^{(n)}(\vec{x}t)\mathrm{d}^d x\,\mathrm{d}t = \delta_{mm'} \quad \text{and} \\ &a_m^{(n)} = \int_V g_n(\vec{x}t)\psi_m^{(n)^*}(\vec{x}t)\mathrm{d}^d x\,\mathrm{d}t. \end{aligned} \tag{1.4b}$$

One should keep in mind that the set $\{\psi_m^{(n)}\}$ is not unique. A different set can be constructed if a different procedure is used to construct the orthonormal set. However, Equation (1.4(a), (b)) remains correct; the only difference is that the coefficients $a_m^{(n)} = \int_V f(\vec{x}t)\psi_m^{(n)^*}(\vec{x}t)\mathrm{d}^d x\,\mathrm{d}t$ will become different when the set $\{\psi_m^{(n)}\}$ changes.

Homework Q1

Consider the solutions of the free-particle Schrödinger equation in three dimensions,

$$-\frac{\hbar^2}{2m}\nabla^2\varphi_\varepsilon = \varepsilon\varphi_\varepsilon,$$

with eigenvalue $\varepsilon > 0$. Construct two different orthonormal sets of eigenstates $\{\varphi_m^{(1)}\}$, $\{\varphi_m^{(2)}\}$ with the same eigenvalue ε. Expand the function $\cos(\vec{k}.\vec{x})$ $\left(\frac{\hbar^2\vec{k}^2}{2m} = \varepsilon\right)$ in the two sets of eigenstates and evaluate the corresponding coefficients $a_m^{(n)} = \int_V \cos(\vec{k}.\vec{x})\varphi_m^{(n)^*}(\vec{x})\mathrm{d}^d x$.

The above result can be applied readily to Equation (1.1b) and the general solution of the equation can be written as

$$\psi_0(\vec{x}t) = \sum_m a_m^{(0)}\psi_m^{(0)}(\vec{x}t),$$

where $\{\psi_m^{(0)}\}$ is a chosen orthonormal set of solutions. Note that the $a_m^{(0)}$ are completely arbitrary and an infinite number of possible solutions exists in general. The coefficients $a_m^{(0)}$ are fixed by initial and boundary conditions, which determine the solution uniquely.

1.2.1.2 Eigenfunction Expansions for Green's Functions

For any linear differential operator $\widehat{L}$, we can introduce a corresponding Green's function through

$$\widehat{L}G(\vec{x}t, \vec{x}'t') = \delta(\vec{x} - \vec{x}')\delta(t - t')\,\widehat{I}\,, \tag{1.5a}$$

where $\widehat{I}$ is an $N \times N$-dimensional identity matrix.

With the Green's function determined, the solution of the equation $\widehat{L}\left(\frac{\partial}{\partial t}, \nabla\right)\psi(\vec{x}, t) = f(\vec{x}, t)$ can be written as

$$\psi(\vec{x}, t) = \psi_0(\vec{x}, t) + \int \mathrm{d}^d x'\mathrm{d}t' G(\vec{x}t, \vec{x}'t')f(\vec{x}', t'), \tag{1.5b}$$

as can be seen by direct substitution.

Note that, in the language of linear algebra, the Green's function is nothing but the inverse operator of $\widehat{L}$, that is $\widehat{G} = \widehat{L}^{-1}$ and $\widehat{L}\widehat{G} = \widehat{I}$. A formal solution of the Green's function can be found using a general method based on completeness and orthogonality.

Let $\psi_n(\vec{x}t)$ be the complete set of eigenstates for the linear operator L, that is $\widehat{L}\psi_n(\vec{x}t) = \lambda_n\psi_n(\vec{x}t)$. To obtain the Green's function defined by

$$\widehat{L}\left(\frac{\partial}{\partial t}, \nabla_x\right)G(\vec{x}t, \vec{x}'t') = \delta(\vec{x} - \vec{x}')\delta(t - t'),$$

we expand $G(\vec{x}t,\vec{x}'t')=\sum_n a_n(\vec{x}'t')\psi_n(\vec{x}t)$ and, from completeness, $\delta(\vec{x}-\vec{x}')\delta(t-t')=\sum_n \psi_n^*(\vec{x}'t')\psi_n(\vec{x}t)$. Therefore,

$$\widehat{L}\left(\frac{\partial}{\partial t},\nabla_x\right)G(\vec{x}t,\vec{x}'t')=\sum_n \lambda_n a_n(\vec{x}'t')\psi_n(\vec{x}t)=\sum_n \psi_n^*(\vec{x}'t')\psi_n(\vec{x}t),$$

which leads to $a_n(\vec{x}'t')=\frac{\psi_n^*(\vec{x}'t')}{\lambda_n}$

or

$$G(\vec{x}t,\vec{x}'t')=\sum_n \frac{\psi_n^*(\vec{x}'t')\psi_n(\vec{x}t)}{\lambda_n}. \tag{1.6}$$

Therefore, the Green's function can be determined if we can evaluate the above sum over all eigenstates. This is in general a very difficult task and alternative methods are often used when we want to evaluate the Green's function explicitly. However, the expansion form (1.6) for the Green's function is very useful for formal manipulations, as we shall see later.

Homework Q2

Determine the Green's function of the differential operator $a\frac{\partial}{\partial t}+D\frac{\partial^2}{\partial x^2}$ in one dimension. D is a real number and a can be either real or imaginary. Consider both situations.

(Hint: you have to fix the boundary condition to determine the Green's function uniquely. There are different possible boundary conditions. Choose one which you think is physically meaningful.)

1.2.1.3 A Variant of the Above Method: Initial Condition Problem

Note that time and space are treated on equal footings in the above general discussion. However, in facing real problems we often have to treat space and time separately. This is often reflected in the initial condition problem: what is $\psi(\vec{x},t)$ if we know $\psi(\vec{x},0)$ (plus some time-derivative terms)?

To illustrate this, we shall first consider the Schrödinger equation

$$\widehat{L}=i\frac{\partial}{\partial t}-\widehat{H}(\vec{x}). \tag{1.7a}$$

The key feature of the Schrödinger equation is that the operator $\widehat{L}$ can be written in a separable form $\widehat{L}=L_0(t)+\widehat{H}(\vec{x})$ where the time and space coordinates enter in different pieces in $\widehat{L}$. For this particular form the eigenstates can be written as

$$\psi_n(\vec{x}t)=\phi_n(\vec{x})\chi_m(t), \tag{1.7b}$$

where

$$\widehat{H}\phi_n(\vec{x})=\lambda_n\phi_n(\vec{x}),\ L_0\chi_m(t)=-\omega_m\chi_m(t), \tag{1.7c}$$

and

$$\widehat{L}\,\psi_n(\vec{x}t) = (\lambda_n - \omega_m)\psi_n(\vec{x}t). \tag{1.7d}$$

Moreover, the eigenstates ϕ_n and χ_m form complete and orthonormal sets by themselves, that is

$$f(\vec{x}) = \sum_n a_n\phi_n(\vec{x}) \text{ for any function } f(\vec{x}) \text{ and } \int_V \phi_n^*(\vec{x})\phi_m(\vec{x}t)\mathrm{d}^d x = \delta_{nm}$$

and

$$g(t) = \sum_n b_n\chi_n(t) \text{ for any function } g(t) \text{ and } \int \chi_n^*(t)\chi_m(t)\mathrm{d}t = \delta_{nm}.$$

Therefore, any solution of the equation

$$\widehat{L}\,\psi(\vec{x}t) = (0)\psi_n(\vec{x}t)$$

can be written as

$$\begin{aligned} &\sum_{n,m} \delta_{\lambda_n\omega_m} a_{nm}\chi_m(0)\phi_n(\vec{x}) \\ &\text{and } \ \psi(\vec{x}0) = \sum_{n,m} \delta_{\lambda_n\omega_m} a_{nm}\chi_m(0)\phi_n(\vec{x}). \end{aligned} \tag{1.8a}$$

Using the orthonormality condition, we obtain

$$\sum_m \delta_{\lambda_n\omega_m} a_{nm}\chi_m(0) = \int \mathrm{d}^d x\phi_n^*(\vec{x})\psi(\vec{x},0). \tag{1.8b}$$

Note that, if a_{nm} can be uniquely determined from the above equation, then $\psi(\vec{x}t)$ will be uniquely determined at all times. This becomes possible if there exists only one eigenstate χ_m with eigenvalue $\omega_m = \lambda_n$. This is the case for the Schrödinger operator $L_0 = i\frac{\partial}{\partial t}$, which involves only the first time derivative. In this case $\chi_m(t) = e^{-i\omega_m t}$ is uniquely determined once $\omega_m = \lambda_n$ is fixed.

Homework Q3

Show that in the case $L_0 = -\frac{\partial^2}{\partial t^2}$ the solution $\psi(\vec{x},t)$ is uniquely determined if we know both $\psi(\vec{x},0)$ and $\frac{\mathrm{d}\psi(\vec{x},t)}{\mathrm{d}t}\Big|_{t=0}$.

Homework Q4

In the case of the Schrödinger equation, the eigenstates $\chi_m(t) = e^{-i\omega_m t}$ are known and the sum over χ_m can be performed explicitly when evaluating the Green's function using the expansion method. In this case the Green's function can be written in terms of the eigenvalues λ_n and eigenstates ϕ_n only. Show that in this case the solution of the initial value problem can be represented as $\psi(\vec{x}t) = \int \mathrm{d}^d x' G(\vec{x}t, \vec{x}'0)\psi(\vec{x}',0)$.

1.2.1.4 Comment on Non-Linear Equations of Motion

In general, non-linear equations are unsolvable, in the sense that there is no systematic procedure to obtain all the solutions of the equations. Physicists usually approach non-linear equations from a perturbative picture – we assume that the non-linear term in the equation of motion is 'small' and treat it as a correction to the solution of the linear equation. An order by order expansion of the non-linear term can be obtained if the approach works (converges).

Adiabaticity and Counting Problem An implicit assumption of this approach is that there is a one-to-one correspondence between the solution of the non-linear equation and the solution of the linear equation. This assumption is called the adiabaticity assumption. Physically, the adiabaticity assumption can be viewed in the following way: assume that we start with a solution of the linear equation ϕ_0 which is changing into a different function ϕ when the non-linear term is turning up gradually. If the change is *always continuous* as a function of the magnitude of the non-linear term λ (when λ is either increasing or decreasing), that is $\phi = \phi(\lambda)$ and $\phi(\lambda = 0) = \phi_0$, then there exists always a one-to-one correspondence between ϕ_0 and ϕ and adiabaticity is obeyed.

From a counting point of view this seems reasonable – if the total number of solutions of the linear equation (= size of Hilbert space where the differential operators are defined) is the same as the total number of solutions of the non-linear equation. Unfortunately, this is not always true and the problem is more subtle than this naïve picture. Non-perturbative solutions which have no simple connection to solutions in the corresponding linear equation do exist in non-linear equations. Some of these solutions are particularly *stable* (usually because of topological reasons) and are physically important. They are often called *soliton* solutions. For later purposes let us also introduce the term *instanton* – it is a non-perturbative solution of the non-linear equation of motion if you go to imaginary time – meaning that you replace $t \to it$ in your equation of motion. We shall study some of the important examples of solitions and instantons in Chapter 8.

1.2.2 Evaluation of Partition Function for Quadratic Field Theories

In this section we discuss the general method of evaluating the partition function $Z = \int e^{-\frac{H[\phi]}{k_B T}} D\phi$. Before we proceed to the general formulation, we first consider a simple toy model so that we can have a better feeling for the mathematical meaning of the integral.

We consider a field ϕ defined on a lattice (like the Ising model) with N independent sites. The energy of the system is

$$H[\phi] = \sum_{i=1,\ldots,N} h[\phi_i] = \sum_{i=1,\ldots,N} a\phi_i + b\phi_i^2 + c\phi_i^4. \tag{1.9a}$$

The partition function is therefore

$$Z = \int d\phi_1 d\phi_2 \cdots d\phi_N e^{-\frac{H[\phi]}{k_B T}} = \prod_i \int d\phi_i e^{-\frac{h[\phi_i]}{k_B T}} = z^N, \tag{1.9b}$$

where

$$z = \int_{-\infty}^{\infty} d\phi e^{-\frac{a\phi + b\phi^2 + c\phi^4}{k_B T}}. \tag{1.9c}$$

Note that in this toy model the partition function is just a product of partition functions of individual sites and the evaluation of the partition function becomes a much simpler problem of evaluating a single integral. Our remaining question is thus: can this integral be performed analytically?

The answer is 'yes' only if $b>0$ and $c=0$ (*quadratic or linear field theories*).

In this case we can write $z = \int_{-\infty}^{\infty} d\phi e^{-\left[\frac{b(\phi + a/2b)^2}{k_B T} - \frac{a^2}{4bk_B T}\right]} = e^{\frac{a^2}{4bk_B T}} \sqrt{\frac{\pi k_B T}{b}}$ and the free energy is given by

$$F = -k_B T \ln(Z) = -N\left[\frac{a^2}{4b} + \frac{k_B T}{2} \ln\left(\frac{k_B T}{b}\right)\right]. \tag{1.10}$$

Note that in this case the problem is like evaluating the partition function of *N decoupled classical harmonic oscillators*.

When c is non-zero, the integral $z = \int_{-\infty}^{\infty} d\phi e^{-\frac{a\phi + b\phi^2 + c\phi^4}{k_B T}}$ cannot be evaluated analytically in general. When c is small, we can expand z in a power series of c and evaluate the series term-by-term. This is the spirit of perturbation theory. In the above example, we obtain

$$z(c) = z(0) + cz' + c^2 z'' + \ldots, \tag{1.11}$$

where

$$z(0) = \int_{-\infty}^{\infty} d\phi e^{-\frac{a\phi + b\phi^2}{k_B T}},\ z' = \frac{1}{k_B T} \int_{-\infty}^{\infty} \phi^4 d\phi e^{-\frac{a\phi + b\phi^2}{k_B T}},\ \text{etc.} \tag{1.12}$$

Homework Q5

Treating c as a perturbation, evaluate the first- and second-order corrections in powers of c to the above free energy F.

Question

What is F if the coefficients a and b are site dependent, that is $a \to a_i$, $b \to b_i$?

Answer

$$F = -k_B T \ln(Z) = -\sum_i \left[\frac{a_i^2}{4b_i} + \frac{k_B T}{2} \ln\left(\frac{k_B T}{b_i}\right)\right].$$

Next, we make the problem more realistic by considering a more complicated energy function where different sites are coupled,

$$H[\phi] = \sum_{i,j=1,\ldots,N} b_{ij}\phi_i\phi_j, \quad \text{where } b_{ij} = b(\vec{r}_i - \vec{r}_j). \tag{1.13a}$$

To evaluate the above partition function we try to transform the energy function into the form of independent harmonic oscillators, that is $H[\phi] = \sum_k \lambda_k \phi_k^2$, where we already know how to evaluate the partition function.

The transformation can be readily obtained if we note that the coefficients b_{ij} can be viewed as elements of a matrix B and

$$H[\phi] = \phi^t B \phi, \tag{1.13b}$$

where $\phi = \begin{bmatrix} \phi_1 \\ . \\ . \\ . \\ \phi_N \end{bmatrix}$ is a vector in the Hilbert space spanned by the matrix B. The matrix B can in general be diagonalized by a unitary transformation U,

$$H[\phi] = \phi^t B \phi = (\phi^t U^+)(UBU^+)(U\phi), \tag{1.14a}$$

where

$$(UBU^+)_{kl} = \lambda_k \delta_{kl} \tag{1.14b}$$

is a diagonal matrix, and $U\phi = \bar{\phi} = \begin{pmatrix} \bar{\phi}_1 \\ \bar{\phi}_2 \\ . \\ . \\ \bar{\phi}_N \end{pmatrix}$.

Therefore, $H[\phi] = \sum_k \lambda_k \bar{\phi}_k^2$, and the partition function is now given by the N-dimensional integral $Z = \int d\phi_1 d\phi_2 \cdots d\phi_N e^{-\frac{H[\bar{\phi}]}{k_B T}}$.

There is one more thing we have to be careful of. Note that the energy function is diagonalized in the $\bar{\phi}$ variables but the integral is performed over the ϕ variables. We need a change of integration variables from ϕ to $\bar{\phi}$ to evaluate the integral. For linear transformations, we have

$$Z = \int d\phi_1 d\phi_2 \cdots d\phi_N e^{-\frac{H[\bar{\phi}]}{k_B T}} = \int d\bar{\phi}_1 d\bar{\phi}_2 \cdots d\bar{\phi}_N |\det(U^+)| e^{-\frac{H[\bar{\phi}]}{k_B T}}. \tag{1.15}$$

However, since U is a unitary transformation, $|\det U| = 1$.

$$\text{Therefore, } Z = \int d\bar{\phi}_1 d\bar{\phi}_2 \cdots d\bar{\phi}_N e^{-\frac{H[\bar{\phi}]}{k_B T}} = \prod_k \sqrt{\frac{k_B T}{\lambda_k}} \tag{1.16a}$$

and

$$F = -k_B T \ln(Z) = -\frac{k_B T}{2} \sum_k \ln\left(\frac{k_B T}{\lambda_k}\right). \tag{1.16b}$$

Note that, equivalently, the result can be expressed as

$$F = \frac{k_B T}{2} (\ln(\det B) - \ln(\det(k_B T) I)),$$

which is the form commonly used in the literature.

For the particular form of matrix $b_{ij} = b(|\vec{r}_i - \vec{r}_j|)$, the eigenvectors are $\phi_i(k) = e^{i\vec{k}.\vec{r}_i}$, with eigenvalues given by the Fourier transform $\lambda_k = \sum_i e^{i\vec{k}.\vec{r}_i} b(\vec{r}_i)$. Note that, rigorously speaking, we need $\lambda_k > 0$ for all k for the integrals to converge.

Exercise

Show that for $b_{ij} = b(|\vec{r}_i - \vec{r}_j|)$ the eigenvectors are $\phi_i(k) = e^{i\vec{k}.\vec{r}_i}$, with eigenvalues $\lambda_k = \sum_i e^{i\vec{k}.\vec{r}_i} b(\vec{r}_i)$.

1.2.2.1 Non-Linear Energy Functional

Energy functionals with terms of higher order than ϕ^2 are called non-linear energy functionals and their partition functions cannot be evaluated exactly. A frequently used energy functional is the ϕ^4 model given by

$$H[\phi] = \sum_{i,j=1,\ldots,N} b_{ij} \phi_i \phi_j + c \sum_i \phi_i^4. \tag{1.17}$$

For small c we can evaluate $Z[\phi]$ approximately by expansion in powers of c as in the simple toy model. The evaluation of perturbation series is more complicated than the toy model because we have to make the unitary transformation $\phi \to \bar{\phi}$. There exist at present very elaborate mathematical methods to do the perturbation expansion systematically. We shall give a brief introduction to these techniques in Chapter 5. However, you are encouraged to evaluate the first- and second-order corrections to $Z[\phi]$ using a straightforward expansion method to get a feeling of the perturbation series.

1.2.2.2 Continuum Limit

Having considered partition functions of a quadratic energy functional on a lattice, we now go to the continuum limit and consider an energy functional of the form $H[\phi] = \int \mathrm{d}^d x \phi^+ \widehat{H} \phi$.

An explicit example is

$$H[\phi] = \int \mathrm{d}^d x ((c\nabla\phi)^2 + m^2\phi^2) = \int \mathrm{d}^d x \phi(-c^2\nabla^2 + m^2)\phi. \tag{1.18}$$

Again, we note that we can diagonalize the Hamiltonian to obtain $H[\phi] = \sum_k \lambda_k \bar{\phi}_k^2$, where $\phi_i(k) = e^{i\vec{k}\cdot\vec{r}_i}$ and $\lambda_k = c^2k^2 + m^2$ in this case and

$$F = -k_B T \ln(Z) = -\frac{k_B T}{2} \sum_k \ln\left(\frac{k_B T}{\lambda_k}\right). \tag{1.19a}$$

The difference between lattice models and the continuum case is that, in the lattice models, the dimension of the Hilbert space is N (= number of lattice sites) and we have precisely N eigenvalues and eigenvectors, whereas, in the continuum case, we have an infinite number of eigenstates and the sum over k becomes a continuous integral. In the example we considered, we have

$$F \to -\frac{k_B T}{2}\frac{V}{(2\pi)^d}\int d^d k \, \ln\left(\frac{k_B T}{c^2 k^2 + m^2}\right) \tag{1.19b}$$

and we can define a free-energy density as

$$f = \frac{F}{V} = -\frac{k_B T}{2}\frac{1}{(2\pi)^d}\int d^d k \, \ln\left(\frac{k_B T}{c^2 k^2 + m^2}\right). \tag{1.19c}$$

Note that the integrand diverges at $k \to \infty$ and the free-energy density is infinity! This result is, of course, unphysical. We shall go back to this problem again later, after we discuss the concept of effective field theory (Chapter 7). Note also that the divergence problem is absent in lattice problems where the integral over k is restricted to the first Brillouin zone.

1.2.2.3 **Constraints**

Nowadays we often encounter field theory with constraints. A very good example is the (classical) Heisenberg model: $H[\vec{S}_i] = -J\sum_{\langle i\cdot j\rangle}\vec{S}_i \cdot \vec{S}_j$ where the field variables $\vec{S}$ are unit vectors. How do we handle this situation? To have an idea of how we can handle this kind of constraint let us consider a very simple model with just one spin, $H = -S_z B$, where $\vec{B}$ is an external magnetic field. The partition function is

$$Z = \int dS_x dS_y dS_z \delta(S_x^2 + S_y^2 + S_z^2 - 1) e^{\frac{S_z B}{k_B T}}. \tag{1.20}$$

There are two ways to handle this situation; the first way is to solve the constraint $\vec{S}\cdot\vec{S} = 1$ exactly by writing $S_z = \cos\vartheta$, $S_x = \sin\vartheta\cos\phi$, $S_y = \sin\vartheta\sin\phi$, and

$$Z \to \int d\Omega e^{\frac{\cos\vartheta B}{k_B T}} = \int d\phi \sin\vartheta d\vartheta e^{\frac{\cos\vartheta B}{k_B T}}.$$

The second way is to use the identity $\delta(x) = \frac{1}{2\pi}\int e^{i\lambda x} d\lambda$, and write

$$Z = \int dS_x dS_y dS_z d\lambda e^{i\lambda(S_x^2 + S_y^2 + S_z^2 - 1)} e^{\frac{S_z B}{k_B T}}. \tag{1.21}$$

Note that the partition function now turns into a regular four-dimensional integral and we can employ standard tricks in evaluating integrals to solve the partition function. The first method is readily applicable for one spin but the second method is often used when many spins are present and coupled together and the first method becomes inconvenient. The introduction of λ – called the Lagrange multiplier field – is often more convenient in making systematic approximations. You will see a number of examples of handling constraints later in this book.

A mathematical problem: how do we evaluate the integral $\int dx e^{i\lambda x^2 + bx}$?

Physicist's recipe:

Assume that $\int_{-\infty}^{\infty} d\phi e^{-\left[\frac{b(\phi+a/2b)^{24}}{k_B T} - \frac{a^2}{4bk_B T}\right]} = e^{\frac{a^2}{4bk_B T}} \sqrt{\frac{\pi k_B T}{b}}$ is valid even for $b \to ib$!

To summarize: in this section we have sketched some of the basic mathematical techniques that are used in mathematical analysis of field theories. The techniques we use in more complicated situations are often variants of the above basic techniques. We shall see many examples in later chapters.