2

Path-integral and lattice regularization

In this chapter we introduce the path-integral method for quantum theory, make it precise with the lattice regularization and use it to quantize the scalar field. For a continuum treatment of path integrals in quantum field theory, see for example [8].

2.1 Path integral in quantum mechanics

To see how the path integral works, consider first a simple system with one degree of freedom described by the Lagrange function $L = L(q, \dot{q})$, or the corresponding Hamilton function $H = H(p, q)$,

$$L = \tfrac{1}{2} m\dot{q}^2 - V(q), \quad H = \frac{p^2}{2m} + V(q), \tag{2.1}$$

where p and q are related by $p = \partial L/\partial\dot{q} = m\dot{q}$. In the quantum theory p and q become operators $\hat{p}$ and $\hat{q}$ with $[\hat{q}, \hat{p}] = i\hbar$ (we indicate operators in Hilbert space by a caret $\hat{}$). The evolution in time is described by the operator

$$\hat{U}(t_1, t_2) = \exp[-i\hat{H}(t_1 - t_2)/\hbar], \tag{2.2}$$

with $\hat{H}$ the Hamilton operator, $\hat{H} = H(\hat{p}, \hat{q})$. Instead of working with q-numbers (operators) $\hat{p}$ and $\hat{q}$ we can also work with time dependent c-numbers (commuting numbers) $q(t)$, in the path-integral formalism. (Later we shall use anti-commuting numbers to incorporate Fermi–Dirac statistics.) In the coordinate basis $|q\rangle$ characterized by

$$\hat{q}|q\rangle = q|q\rangle, \tag{2.3}$$

$$\langle q'|q\rangle = \delta(q' - q), \quad \int dq\, |q\rangle\langle q| = 1, \tag{2.4}$$

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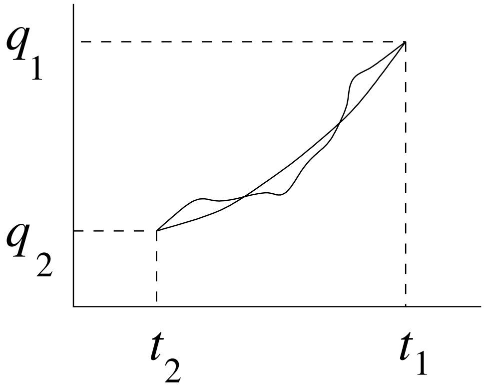

Fig. 2.1. Illustration of two functions $q(t)$ contributing to the path integral.

we can represent the matrix element of $\hat{U}(t_1, t_2)$ by a path integral

$$\langle q_1|\hat{U}(t_1,t_2)|q_2\rangle = \int Dq\, \exp[iS(q)/\hbar]. \tag{2.5}$$

Here S is the action functional of the system,

$$S(q) = \int_{t_2}^{t_1} dt\, L(q(t), \dot{q}(t)), \tag{2.6}$$

and $\int Dq$ symbolizes an integration over all functions $q(t)$ such that

$$q(t_1) = q_1, \quad q(t_2) = q_2, \tag{2.7}$$

as illustrated in figure 2.1. The path integral is a summation over all 'paths' ('trajectories', 'histories') $q(t)$ with given end points. The classical path, which satisfies the equation of motion $\delta S(q) = 0$, or

$$\frac{\partial L}{\partial q} - \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{q}} = 0, \tag{2.8}$$

is only one out of infinitely many possible paths. Each path has a 'weight' $\exp(iS/\hbar)$. If $\hbar$ is relatively small such that the phase $\exp(iS/\hbar)$ varies rapidly over the paths, then a stationary-phase approximation will be good, in which the classical path and its small neighborhood give the dominant contributions. The other extreme is when the variation of $S/\hbar$ is of order one. In the following we shall use again units in which $\hbar = 1$.

A formal definition of $\int Dq$ is given by

$$\int Dq = \prod_{t_2<t<t_1} \int dq(t), \tag{2.9}$$

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i.e. for every $t \in (t_2, t_1)$ we integrate over the domain of q, e.g. $-\infty < q < \infty$. The definition is formal because the continuous product $\prod_t$ still has to be defined. We shall give such a definition with the help of a discretization procedure.

2.2 Regularization by discretization

To define the path integral properly we discretize time in small units a, writing $t = na$, $q(t) = q_n$, with n integer. For a smooth function $q(t)$ the time derivative $\dot{q}(t)$ can be approximated by $\dot{q}(t) = (q_{n+1} - q_n)/a$, such that the discretized Lagrange function may be written as†

$$L(t) = \frac{m}{2a^2}(q_{n+1} - q_n)^2 - \frac{1}{2}V(q_{n+1}) - \frac{1}{2}V(q_n), \tag{2.10}$$

where we have divided the potential term equally between q_n and q_{n+1}. We define a discretized evolution operator $\hat{T}$ by its matrix elements as follows:

$$\langle q_1|\hat{T}|q_2\rangle = c \exp\left\{ia\left[\frac{m}{2a^2}(q_1 - q_2)^2 - \frac{1}{2}V(q_1) - \frac{1}{2}V(q_2)\right]\right\}, \tag{2.11}$$

where c is a constant to be specified below. Note that the exponent is similar to the Lagrange function. The operator $\hat{T}$ is called the transfer operator, its matrix elements the transfer matrix. In terms of the transfer matrix we now give a precise definition of the discretized path integral:

$$\begin{aligned}
\langle q'|\hat{U}(t', t'')|q''\rangle = &\int dq_1 \cdots dq_{N-1} \langle q'|\hat{T}|q_{N-1}\rangle \\
&\times \langle q_{N-1}|\hat{T}|q_{N-2}\rangle \cdots \langle q_1|\hat{T}|q''\rangle \\
= &\, c\int \left(\prod c\, dq\right) \exp\left[\frac{im}{2a}(q' - q_{N-1})^2\right. \\
&- \frac{ia}{2}V(q') - iaV(q_{N-1}) + \frac{im}{2a}(q_{N-1} - q_{N-2})^2 \\
&\left. - iaV(q_{N-2}) + \cdots + \frac{im}{2a}(q_1 - q'')^2 - \frac{ia}{2}V(q'')\right] \\
\equiv &\int Dq\, e^{iS}.
\end{aligned} \tag{2.12}$$

Here the discretized action is defined by

$$S = a\sum_{n=0}^{N-1} L(na), \tag{2.13}$$

† For notational simplicity we shall denote the discretized forms of L, S, ..., by the same symbols as their continuum counterparts.

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where $q_N \equiv q'$ and $q_0 \equiv q''$. In the limit $N \to \infty$ this becomes equal to the continuum action, when we substitute smooth functions $q(t)$. Since the q_n are integrated over on every 'time slice' n, such smoothness is not typically present in the integrand of the path integral (typical paths q_n will look like having a very discontinuous derivative) and a continuum limit at this stage is formal.

It will now be shown that, with a suitable choice of the constant c, the transfer operator can be written in the form

$$\hat{T} = e^{-iaV(\hat{q})/2}\, e^{-ia\hat{p}^2/2m}\, e^{-iaV(\hat{q})/2}. \tag{2.14}$$

Taking matrix elements between $\langle q_1|$ and $|q_2\rangle$ we see that this formula is correct if

$$\langle q_1|e^{-ia\hat{p}^2/2m}|q_2\rangle = c e^{im(q_1-q_2)^2/2a}. \tag{2.15}$$

Inserting eigenstates $|p\rangle$ of the momentum operator $\hat{p}$ using

$$\langle q|p\rangle = e^{ipq}, \quad \int \frac{dp}{2\pi}\, |p\rangle\langle p| = 1, \tag{2.16}$$

we find that (2.15) is true provided that we choose

$$c = \sqrt{\frac{m}{2\pi i a}} = \sqrt{\frac{m}{2\pi a}} e^{-i\pi/4}. \tag{2.17}$$

The transfer operator $\hat{T}$ is the product of three unitary operators, so we may write

$$\hat{T} = e^{-ia\hat{H}}. \tag{2.18}$$

This equation defines a Hermitian Hamiltonian operator $\hat{H}$ modulo $2\pi/a$. For matrix elements between eigenstates with energy $E \ll 2\pi/a$ the expansion

$$\hat{T} = 1 - ia\hat{H} + O(a^2) \tag{2.19}$$

leads to the identification

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) + O(a^2), \tag{2.20}$$

in which we recognize the usual Hamilton operator. It should be kept in mind though that, as an operator equation, the expansion (2.19) is formal: because $\hat{p}^2$ is an unbounded operator there may be matrix elements for which the expansion does not converge.

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2.3 Analytic continuation to imaginary time

It is very useful in practice to make an analytic continuation to imaginary time according to the substitution $t \to -it$. This can be justified if the potential $V(q)$ is bounded from below, as is the case, for example, for the anharmonic oscillator

$$V(q) = \tfrac{1}{2}m\omega^2 q^2 + \tfrac{1}{4}\lambda q^4. \tag{2.21}$$

Consider the discretized path integral (2.12). The integration over the variables q_n continues to converge if we rotate a in the complex plane according to

$$a = |a|e^{-i\varphi}, \quad \varphi\colon 0 \to \frac{\pi}{2}. \tag{2.22}$$

The reason is that, for all $\varphi \in (0, \pi/2]$, the real part of the exponent in (2.12) is negative:

$$\frac{i}{|a|e^{-i\varphi}} = \frac{1}{|a|}(-\sin\varphi + i\cos\varphi), \quad -i|a|e^{-i\varphi} = |a|(-\sin\varphi - i\cos\varphi). \tag{2.23}$$

The result of this analytic continuation in a is that the discretized path integral takes the form

$$\langle q'|\hat{U}_{\Im}(t', t'')|q''\rangle = |c| \int \left(\prod_n |c| dq_n\right) e^{S_{\Im}},$$
$$S_{\Im} = -|a| \sum_{n=0}^{N-1} \left[\frac{m}{2|a|^2}(q_{n+1} - q_n)^2 + \frac{1}{2}V(q_{n+1}) + \frac{1}{2}V(q_n)\right]. \tag{2.24}$$

Here the subscript $\Im$ denotes the imaginary-time versions of U and S.

The integrand in the imaginary-time path integral is real and bounded from above. This makes numerical calculations and theoretical analysis very much easier. Furthermore, in the generalization to field theory there is a direct connection to statistical physics, which has led to many fruitful developments. For most purposes the imaginary-time formulation is sufficient to extract the relevant physical information such as the energy spectrum of a theory. If necessary, one may analytically continue back to real time, by implementing the inverse of the rotation (2.22). (This can be done only in analytic calculations, since statistical errors in e.g. Monte Carlo computations have the tendency to blow up upon continuation.) In the following the subscript $\Im$ will be dropped and we will redefine $|a| \to a$, with a positive.

After transformation to imaginary time the transfer operator takes the Hermitian form

$$\hat{T} = e^{-aV(\hat{q})/2}\, e^{-a\hat{p}^2/2m}\, e^{-aV(\hat{q})/2}. \tag{2.25}$$

This is a positive operator, i.e. all its expectation values and hence all its eigenvalues are positive. We may therefore redefine the Hamiltonian operator $\hat{H}$ according to

$$\hat{T} = e^{-a\hat{H}}. \tag{2.26}$$

A natural object in the imaginary-time formalism is the partition function

$$Z = \mathrm{Tr}\, e^{-\hat{H}(t_+ - t_-)} = \int dq\, \langle q|e^{-\hat{H}(t_+ - t_-)}|q\rangle = \mathrm{Tr}\, \hat{T}^N, \tag{2.27}$$

where we think of t_+ (t_-) as the largest (smallest) time under consideration, with $t_+ - t_- = Na$. From quantum statistical mechanics we recognize that Z is the canonical partition function corresponding to the temperature

$$T = (t_+ - t_-)^{-1} \tag{2.28}$$

in units such that Boltzmann's constant $k_{\mathrm{B}} = 1$. The path-integral representation of Z is obtained by setting in (2.24) $q_N = q_0 \equiv q$ ($q' = q'' \equiv q$) and integrating over q:

$$Z = \int_{\mathrm{pbc}} Dq\, e^S. \tag{2.29}$$

Here 'pbc' indicates the fact that the integration is now over all discretized functions $q(t)$, $t_- < t < t_+$, with 'periodic boundary conditions' $q(t_+) = q(t_-)$.

2.4 Spectrum of the transfer operator

Creation and annihilation operators are familiar from the theory of the harmonic oscillator. Here we shall use them to derive the eigenvalue spectrum of the transfer operator of the harmonic oscillator, for which

$$V(q) = \tfrac{1}{2} m\omega^2 q^2. \tag{2.30}$$

For simplicity we shall use units in which $a = 1$ and $m = 1$, which may be obtained by transforming to variables $q' = q/a$, $p' = ap$, $m' = am$,

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and $\omega' = a\omega$, then to $q'' = q'\sqrt{m'}$ and $p'' = p'/\sqrt{m'}$, such that (omitting the primes) $[\hat{p}, \hat{q}] = -i$ and

$$\hat{T} = e^{-\omega^2 \hat{q}^2/4} e^{-\hat{p}^2/2} e^{-\omega^2 \hat{q}^2/4}. \tag{2.31}$$

Using the representation $\hat{q} \to q$, $\hat{p} \to -i\,\partial/\partial q$ or vice-versa one obtains the relation

$$\hat{T}\begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix} = M \begin{pmatrix} \hat{p} \\ \hat{q} \end{pmatrix} \hat{T}, \tag{2.32}$$

where the matrix M is given by

$$M = \begin{pmatrix} 1 + \frac{1}{2}\omega^2 & i \\ -i(2 + \frac{1}{2}\omega^2)\frac{1}{2}\omega^2 & 1 + \frac{1}{2}\omega^2 \end{pmatrix}. \tag{2.33}$$

We want to find linear combinations $\kappa\hat{q} + \lambda\hat{p}$ such that

$$\hat{T}(\kappa\hat{q} + \lambda\hat{p}) = \mu(\kappa\hat{q} + \lambda\hat{p})\hat{T}, \tag{2.34}$$

from which it follows that (κ, λ) have to form an eigenvector of M^{T} (the transpose of M) with eigenvalue μ. The eigenvalues $\mu_\pm$ of M can be expressed as

$$\mu_\pm = e^{\pm\tilde{\omega}}, \;\; \cosh\tilde{\omega} = 1 + \tfrac{1}{2}\omega^2, \tag{2.35}$$

and the linear combinations sought are given by

$$\begin{aligned} \hat{a} &= \nu[\sinh(\tilde{\omega}\hat{q}) + i\hat{p}], \\ \hat{a}^\dagger &= \nu[\sinh(\tilde{\omega}\hat{q}) - i\hat{p}], \end{aligned} \tag{2.36}$$

where ν is a normalization constant. The $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation operators for the discretized harmonic oscillator. They satisfy the usual commutation relations

$$[\hat{a}, \hat{a}^\dagger] = 1, \;\; [\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0, \tag{2.37}$$

provided that

$$\nu = \frac{1}{\sqrt{2\sinh\tilde{\omega}}}, \tag{2.38}$$

and furthermore

$$\hat{T}\hat{a} = e^{\tilde{\omega}}\,\hat{a}\hat{T}, \;\; \hat{T}\hat{a}^\dagger = e^{-\tilde{\omega}}\,\hat{a}^\dagger\hat{T}. \tag{2.39}$$

The ground state $|0\rangle$ with the highest eigenvalue of $\hat{T}$ satisfies $\hat{a}|0\rangle = 0$, from which one finds (using for example the coordinate representation)

$$\begin{aligned}\langle q|0\rangle &= e^{-\frac{1}{2}\sinh\tilde{\omega}\, q^2},\\ \hat{T}|0\rangle &= e^{-E_0}|0\rangle,\\ E_0 &= \tfrac{1}{2}\tilde{\omega}.\end{aligned} \tag{2.40}$$

The ground-state energy is $E_0 = \frac{1}{2}\tilde{\omega}$ and using (2.39) one finds that the excitation energies occur in units of $\tilde{\omega}$, for example

$$\hat{T}\hat{a}^\dagger|0\rangle = e^{-\tilde{\omega}}\,\hat{a}^\dagger\hat{T}|0\rangle = e^{-(3/2)\,\tilde{\omega}}\hat{a}^\dagger|0\rangle. \tag{2.41}$$

Hence, the energy spectrum is given by

$$E_n = \left(n + \tfrac{1}{2}\right)\tilde{\omega}, \tag{2.42}$$

which looks familiar, except that $\tilde{\omega} \neq \omega$.

We now can take the continuum limit $a \to 0$ in the physical quantities E_n. Recalling that ω is really $a\omega$, and similarly for $\tilde{\omega}$, we see by expanding (2.35) in powers of a, i.e. $\cosh(a\tilde{\omega}) = 1 + a^2\tilde{\omega}^2/2 + a^4\tilde{\omega}^4/24 + \cdots = 1 + a^2\omega^2/2$, that

$$\tilde{\omega} = \omega + O(a^2). \tag{2.43}$$

Note that the corrections are $O(a^2)$, which is much better than $O(a)$ as might be expected naively. This is the reason for the symmetric division of the potential in (2.11).

2.5 Latticization of the scalar field

We now transcribe these ideas to field theory, taking the scalar field as the first example. The dynamical variables generalize as

$$q(t) \to \varphi(\mathbf{x}, t) \tag{2.44}$$

(i.e. there is a q for every $\mathbf{x}$). The coordinate representation is formally characterized by

$$\hat{\varphi}(\mathbf{x})|\varphi\rangle = \varphi(\mathbf{x})|\varphi\rangle, \tag{2.45}$$

$$|\varphi\rangle = \prod_{\mathbf{x}} |\varphi_{\mathbf{x}}\rangle, \tag{2.46}$$

$$\langle\varphi'|\varphi\rangle = \prod_{\mathbf{x}} \delta(\varphi'(\mathbf{x}) - \varphi(\mathbf{x})), \tag{2.47}$$

$$\prod_{\mathbf{x}} \int_{-\infty}^{\infty} d\varphi(\mathbf{x})\, |\varphi\rangle\langle\varphi| = 1. \tag{2.48}$$

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The evolution operator is given by

$$\langle\varphi_1|\hat{U}(t_1,t_2)|\varphi_2\rangle = \int D\varphi\, e^{S(\varphi)}, \tag{2.49}$$

where the integral is over all functions $\varphi(\mathbf{x},t)$ with $\varphi(\mathbf{x},t_{1,2}) = \varphi_{1,2}(\mathbf{x})$. The theory is specified furthermore by the choice of action S. For the standard φ^4 model

$$S(\varphi) = -\int_{t_2}^{t_1} dx_4 \int d^3x \left[\frac{1}{2}\partial_\mu\varphi(x)\partial_\mu\varphi(x) + \frac{\mu^2}{2}\varphi^2(x) + \frac{\lambda}{4}\varphi^4(x)\right], \tag{2.50}$$

where $x = (\mathbf{x}, x_4)$ and $x_4 = t$. Note that in the imaginary-time formalism the symmetry between space and time is manifest, since the metric tensor is simply equal to the Kronecker $\delta_{\mu\nu}$. Consequently, we shall not distinguish between upper and lower indices $\mu, \nu, \ldots$. One often speaks of the *Euclidean formalism*, since the space–time symmetries of the theory consist of Euclidean rotations, reflections and translations.

The partition function is given by

$$Z = \int D\varphi\, e^{S(\varphi)}, \tag{2.51}$$

where the integral is over all functions periodic in the time direction, $\varphi(\mathbf{x}, t+\beta) = \varphi(\mathbf{x}, t)$, with $\beta = T^{-1}$ the inverse temperature.

The path integral Z will be given a precise definition with the lattice regularization, by a straightforward generalization of the example of quantum mechanics with one degree of freedom. Let x_μ be restricted to a four-dimensional hypercubic lattice,

$$x_\mu = m_\mu a, \quad m_\mu = 0, 1, \ldots, N-1, \tag{2.52}$$

where a is the lattice distance. The size of the hypercubic box is $L = Na$ and its space–time volume is L^4. The notation

$$\sum_x \equiv a^4 \sum_{m_1=0}^{N-1} \cdots \sum_{m_4=0}^{N-1} \equiv a^4 \sum_m \tag{2.53}$$

will be used in this book. For smooth functions $f(x)$ we have in the continuum limit

$$\sum_x f(x) \to \int_0^L d^4x\, f(x), \quad N \to \infty, \;\; a = L/N \to 0, \;\; L \text{ fixed}. \tag{2.54}$$

We have put $x = 0$ at the edge of the box. If we want it in the middle of the box we can choose $m_\mu = -N/2+1, -N/2+2, \ldots, N/2$. Below we

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shall choose such a labeling for Fourier modes and we shall assume N to be even in the following.

The scalar field on the lattice is assigned to the sites x, we write φ_x. The part of the action without derivatives is transcribed to the lattice as $\sum_x(\mu^2\varphi_x^2/2 + \lambda\varphi_x^4/4)$.

Derivatives can be replaced by differences. We shall use the notation

$$\partial_\mu\varphi_x = \frac{1}{a}(\varphi_{x+a\hat{\mu}} - \varphi_x), \tag{2.55}$$

$$\partial'_\mu\varphi_x = \frac{1}{a}(\varphi_x - \varphi_{x-a\hat{\mu}}), \tag{2.56}$$

where $\hat{\mu}$ is a unit vector in the μ direction. For smooth functions $f(x)$,

$$\partial_\mu f(x),\ \partial'_\mu f(x) \to \frac{\partial}{\partial x_\mu} f(x), \quad a \to 0. \tag{2.57}$$

It is convenient to use periodic boundary conditions (such that the lattice has no boundary), which are specified by

$$\varphi_{x+Na\hat{\mu}} = \varphi_x, \tag{2.58}$$

and, for example,

$$\partial_4\varphi_{\mathbf{x},(N-1)a} = \frac{1}{a}(\varphi_{\mathbf{x},0} - \varphi_{\mathbf{x},(N-1)a}). \tag{2.59}$$

With periodic boundary conditions the derivative operators ∂_μ and ∂'_μ are related by 'partial summation' (the analog of partial integration)

$$\sum_x \varphi_{1x}\,\partial_\mu\varphi_{2x} = -\sum_x \partial'_\mu\varphi_{1x}\,\varphi_{2x}. \tag{2.60}$$

In matrix notation,

$$\partial_\mu\varphi_x = (\partial_\mu)_{xy}\,\varphi_y, \tag{2.61}$$

∂'_μ is minus the transpose of ∂_μ, $\partial'_\mu = -\partial_\mu^{\mathrm{T}}$:

$$(\partial_\mu)_{xy} = \frac{1}{a}(\delta_{x+a\hat{\mu},y} - \delta_{x,y}), \tag{2.62}$$

$$(\partial'_\mu)_{xy} = \frac{1}{a}(\delta_{x,y} - \delta_{x-a\hat{\mu},y}) = -(\partial_\mu)_{yx} = -(\partial_\mu^{\mathrm{T}})_{xy}. \tag{2.63}$$

After these preliminaries, the path integral will now be defined by

$$Z = \int D\varphi\, e^{S(\varphi)}, \tag{2.64}$$

$$\int D\varphi = \prod_x \left(c\int_{-\infty}^{\infty}\right) d\varphi_x, \quad \prod_x \equiv \prod_m, \tag{2.65}$$

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$$S(\varphi) = -\sum_x \left(\frac{1}{2}\partial_\mu\varphi_x\partial_\mu\varphi_x + \frac{\mu^2}{2}\varphi_x^2 + \frac{\lambda}{4}\varphi_x^4\right), \tag{2.66}$$

$$c = a/\sqrt{2\pi}. \tag{2.67}$$

Note that $c\varphi$ is dimensionless. The dimension of φ follows from the requirement that the action S is dimensionless. In d space–time dimensions,

$$[\varphi] = a^{-(d-2)/2}, \quad c = a^{(d-2)/2}. \tag{2.68}$$

The factor $1/\sqrt{2\pi}$ is an inessential convention, chosen such that there is no additional factor in the expression for the transfer operator (2.74) below, which would lead to an additional constant in the Hamiltonian (2.80).

The lattice action was chosen such that for smooth functions $f(x)$, $S(f) \to S_{\rm cont}(f)$ in the *classical* continuum limit $a \to 0$. However, it is useful to keep in mind that typical field configurations φ_x contributing to the path integral are not smooth at all on the lattice scale. The previous sentence is meant in the following sense. The factor $Z^{-1}\exp S(\varphi)$ can be interpreted as a normalized probability distribution for an ensemble of field configurations φ_x. Drawing a typical field configuration φ from this ensemble, e.g. one generated by a computer with some Monte Carlo algorithm, one finds that it varies rather wildly from site to site on the lattice. This has the consequence that different discretizations (e.g. different discrete differentiation schemes) may lead to different answers for certain properties, although this should not be the case for physically observable properties. The discussion of continuum behavior in the *quantum* theory is a delicate matter, which involves concepts like renormalization, scaling and universality.

2.6 Transfer operator for the scalar field

The derivation of the transfer operator for the scalar field on the lattice follows the steps made earlier in the example with one degree of freedom. For later use we generalize to different lattice spacings for time and space, a_t and a, respectively. We use the notation $x_4 = t = na_t$, $\varphi_x = \varphi_{n,\mathbf{x}}$, with $n = 0, 1, \ldots, N-1$ and $\varphi_{N,\mathbf{x}} = \varphi_{0,\mathbf{x}}$. Then the action can be written as

$$S(\varphi) = -a_t \sum_n \sum_{\mathbf{x}} \frac{1}{2a_t^2}(\varphi_{n+1,\mathbf{x}} - \varphi_{n,\mathbf{x}})^2 - a_t \sum_n V(\varphi_n), \tag{2.69}$$

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$$V(\varphi_n) = \sum_{\mathbf{x}} \left[\frac{1}{2} \sum_{j=1}^{3} \partial_j \varphi_{n,\mathbf{x}} \partial_j \varphi_{n,\mathbf{x}} + \frac{\mu^2}{2} \varphi_{n,\mathbf{x}}^2 + \frac{\lambda}{4} \varphi_{n,\mathbf{x}}^4 \right]. \tag{2.70}$$

The transfer operator $\hat{T}$ is defined by its matrix elements

$$\begin{aligned} \langle \varphi_{n+1} | \hat{T} | \varphi_n \rangle = c^{N^3} \exp \left[-a_t \sum_{\mathbf{x}} \frac{1}{2a_t^2} (\varphi_{n+1,\mathbf{x}} - \varphi_{n,\mathbf{x}})^2 \right] \\ \times \exp \left[-a_t \frac{1}{2} (V(\varphi_{n+1}) + V(\varphi_n)) \right], \end{aligned} \tag{2.71}$$

such that

$$\begin{aligned} Z &= \left(\prod_x \int d\varphi_x \right) \langle \varphi_N | \hat{T} | \varphi_{N-1} \rangle \cdots \langle \varphi_1 | \hat{T} | \varphi_0 \rangle & (2.72) \\ &= \mathrm{Tr}\, \hat{T}^N. & (2.73) \end{aligned}$$

The transfer operator $\hat{T}$ can be written in the form

$$\hat{T} = \exp \left[-a_t \frac{1}{2} V(\hat{\varphi}) \right] \exp \left[-a_t \frac{1}{2} \sum_{\mathbf{x}} \hat{\pi}_{\mathbf{x}}^2 \right] \exp \left[-a_t \frac{1}{2} V(\hat{\varphi}) \right], \tag{2.74}$$

where $\hat{\pi}_{\mathbf{x}}$ is the canonical conjugate operator of $\hat{\varphi}_{\mathbf{x}}$, with the property

$$[\hat{\varphi}_{\mathbf{x}}, \hat{\pi}_{\mathbf{y}}] = i a^{-3} \delta_{\mathbf{x},\mathbf{y}}. \tag{2.75}$$

To check (2.74) we take matrix elements between $|\varphi_n\rangle$ and $\langle \varphi_{n+1}|$ and compare with (2.71). Using

$$e^{-a_t \frac{1}{2} V(\hat{\varphi})} |\varphi_n\rangle = e^{-a_t \frac{1}{2} V(\varphi_n)} |\varphi_n\rangle, \tag{2.76}$$

we see that (2.74) is correct provided that

$$\langle \varphi_{n+1} | e^{-a_t \frac{1}{2} \sum_{\mathbf{x}} \hat{\pi}_{\mathbf{x}}^2} | \varphi_n \rangle = c^{N^3} \exp \left[-a_t \sum_{\mathbf{x}} (\varphi_{n+1,\mathbf{x}} - \varphi_{n,\mathbf{x}})^2 / 2a_t^2 \right]. \tag{2.77}$$

This relation is just a product over $\mathbf{x}$ of relations of the one-degree-of-freedom type

$$\langle q_1 | e^{-\hat{p}^2/2\xi} | q_2 \rangle = \sqrt{\frac{\xi}{2\pi}}\, e^{-\xi (q_1 - q_2)^2/2}, \tag{2.78}$$

with the identification, for given $\mathbf{x}$, $q = a\varphi$, $\hat{p} = a^2 \hat{\pi} \to -i\, \partial/\partial q$, and $|\varphi\rangle = \sqrt{a} |q\rangle$ (such that $\langle \varphi' | \varphi \rangle = a \langle q' | q \rangle = a\delta(q' - q) = \delta(\varphi' - \varphi)$). It follows that

$$c = a\sqrt{\frac{\xi}{2\pi}}, \quad \xi = \frac{a}{a_t}. \tag{2.79}$$

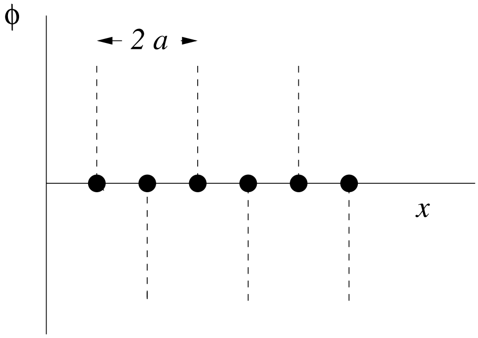

Fig. 2.2. Shortest wave length of a lattice field.

Making the formal continuous-time limit by letting $a_t \to 0$ and expanding $\hat{T} = 1 - a_t\hat{H} + \cdots$, we find a conventional-looking Hamiltonian[1] on a spatial lattice,

$$\hat{H} = \sum_x \left(\tfrac{1}{2}\hat{\pi}_{\mathbf{x}}^2 + \tfrac{1}{2}\partial_j\hat{\varphi}_{\mathbf{x}}\partial_j\hat{\varphi}_{\mathbf{x}} + \tfrac{1}{2}\mu^2\hat{\varphi}_{\mathbf{x}}^2 + \tfrac{1}{4}\lambda\hat{\varphi}_{\mathbf{x}}^4\right) + O(a^2). \tag{2.80}$$

2.7 Fourier transformation on the lattice

We record now some frequently used formulas involving the Fourier transform. The usual plane waves in a finite volume with periodic boundary conditions are given by

$$e^{ipx}, \quad p_\mu = n_\mu \frac{2\pi}{L}, \tag{2.81}$$

where the n_μ are integers. We want to use these functions for (Fourier) transformations of variables. On the lattice the x_μ are restricted to $x_\mu = m_\mu a$, $m_\mu = 0, \ldots, N-1$, $L = Na$. There should not be more p_μ than x_μ; we take

$$n_\mu = -N/2+1, -N/2+2, \ldots, N/2. \tag{2.82}$$

Indeed, the shortest wave length and largest wave vector are given by (cf. figure 2.2)

$$\lambda_{\min} = 2a, \quad p_{\max} = \frac{\pi}{a} = \frac{N}{2}\frac{2\pi}{L}. \tag{2.83}$$

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Apart from these intuitive arguments, the reason for (2.82) is the fact that (in d dimensions, $mn = m_\mu n_\mu$)

$$U_{mn} \equiv N^{-d/2} e^{i2\pi mn/N} \equiv N^{-d/2} \big(e^{ipx}\big)_{mn} \tag{2.84}$$

is a unitary matrix,

$$U_{mn} U^*_{mn'} = \delta_{n,n'}. \tag{2.85}$$

We check this for the one-dimensional case, $d = 1$:

$$U_{mn} U^*_{mn'} = \frac{1}{N} \sum_{m=0}^{N-1} r^m = \frac{1}{N} \frac{1 - r^N}{1 - r} = \bar{\delta}_{n,n'}, \tag{2.86}$$

$$r \equiv e^{i2\pi(n-n')/N}, \tag{2.87}$$

where

$$\bar{\delta}_{n,n'} \equiv 0, \quad n \neq n' \mod N \tag{2.88}$$

$$= 1, \quad n = n' \mod N. \tag{2.89}$$

We shall use this result in the form

$$\sum_x e^{-i(p-p')x} = \bar{\delta}_{p,p'} \equiv \prod_\mu \Big(N|a_\mu| \bar{\delta}_{m_\mu, m'_\mu}\Big), \tag{2.90}$$

$$\sum_p e^{ip(x-x')} = \bar{\delta}_{x,x'} \equiv \prod_\mu \Big(|a_\mu|^{-1} \bar{\delta}_{n_\mu, n'_\mu}\Big), \tag{2.91}$$

$$\sum_x \equiv \prod_\mu \left(|a_\mu| \sum_{m_\mu}\right), \tag{2.92}$$

$$\sum_p \equiv \prod_\mu \left(\frac{1}{N|a_\mu|} \sum_{n_\mu}\right), \tag{2.93}$$

where $|a_\mu|$ is the lattice spacing in the μ direction (unless stated otherwise, $|a_\mu| = a$). With this notation we can write the Fourier transformation of variables ('from position space to momentum space') and its inverse as

$$\tilde{\varphi}_p = \sum_x e^{-ipx} \varphi_x, \tag{2.94}$$

$$\varphi_x = \sum_p e^{ipx} \tilde{\varphi}_p. \tag{2.95}$$

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For smooth functions $f(p)$ we have, in the infinite-volume limit $L = Na \to \infty$,

$$\sum_p f(p) = \frac{(\Delta p)^4}{(2\pi)^4} \sum_n f\left(\frac{2\pi n}{Na}\right) \tag{2.96}$$

$$\to \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4}\, f(p), \quad N \to \infty, \quad a \text{ fixed}, \tag{2.97}$$

where $\Delta p = 2\pi/Na$.

2.8 Free scalar field

For $\lambda = 0$ we get the free scalar field action. For this case the path integral can be done easily. Assuming $\mu^2 \equiv m^2 > 0$, we write

$$S = -\sum_x \left(\tfrac{1}{2}\partial_\mu \varphi_x \partial_\mu \varphi_x + \tfrac{1}{2} m^2 \varphi_x^2\right) \tag{2.98}$$

$$= \tfrac{1}{2} \sum_{xy} S_{xy}\, \varphi_x \varphi_y, \tag{2.99}$$

where

$$S_{xy} = -\sum_z \left[\sum_\mu (\bar{\delta}_{z+a\hat{\mu},x} - \bar{\delta}_{z,x})(\bar{\delta}_{z+a\hat{\mu},y} - \bar{\delta}_{z,y}) + m^2 \bar{\delta}_{z,x}\bar{\delta}_{z,y}\right]. \tag{2.100}$$

It is useful to introduce an external source J_x, which can be chosen as we wish. The partition function with an external source is defined as

$$Z(J) = \int D\varphi\, \exp\left(S + \sum_x J_x \varphi_x\right). \tag{2.101}$$

The transformation of variables

$$\varphi_x \to \varphi_x + \sum_y G_{xy} J_y, \tag{2.102}$$

with G_{xy} minus the inverse of S_{xy},

$$S_{xy} G_{yz} = -\bar{\delta}_{x,z}, \tag{2.103}$$

brings $Z(J)$ into the form

$$Z(J) = Z(0)\, \exp\left(\tfrac{1}{2} G_{xy} J_x J_y\right). \tag{2.104}$$

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The integral $Z(0)$ is just a multiple Gaussian integral,

$$Z(0) = \int D\varphi \, \exp\left(-\tfrac{1}{2} G_{xy}^{-1} \varphi_x \varphi_y\right)$$
$$= \frac{1}{\sqrt{\det G^{-1}}} = \exp\left(\tfrac{1}{2} \ln \det G\right). \tag{2.105}$$

There is finite-temperature physics that can be extracted from the partition function $Z(0)$, but here we shall not pay attention to it.

The propagator G can be easily found in 'momentum space'. First we determine the Fourier transform of S_{xy}, using lattice units $a = 1$,

$$S_{p,-q} \equiv \sum_{xy} e^{-ipx+iqy} S_{xy} \tag{2.106}$$
$$= -\sum_z \left[\sum_\mu (e^{-ip\hat{\mu}} - 1)(e^{iq\hat{\mu}} - 1) + m^2\right] e^{-ipz+iqz}$$
$$= S_p \, \bar{\delta}_{p,q}, \tag{2.107}$$
$$-S_p = m^2 + \sum_\mu (2 - 2\cos p_\mu) \tag{2.108}$$
$$= m^2 + \sum_\mu 4\sin^2\left(\frac{p_\mu}{2}\right). \tag{2.109}$$

Since $S_{p,-q}$ is diagonal in momentum space, its inverse is given by

$$G_{p,-q} = G_p \, \bar{\delta}_{p,q}, \quad G_p = \frac{1}{m^2 + \sum_\mu (2 - 2\cos p_\mu)}. \tag{2.110}$$

From this we can restore the lattice distance by using dimensional analysis: $p \to ap$, $m \to am$ and $G_p \to a^2 G(p)$. This gives

$$G(p) = \frac{1}{m^2 + a^{-2} \sum_\mu (2 - 2\cos ap_\mu)}, \tag{2.111}$$

and in the continuum limit $a \to 0$,

$$G(p) = \frac{1}{m^2 + p^2 + O(a^2)}, \tag{2.112}$$

which is the usual covariant expression for the scalar field propagator. It is instructive to check that the corrections to the continuum form are already quite small for $ap_\mu < \frac{1}{2}$.

From the form (2.104) we calculate the correlation function of the free theory,

$$\langle\varphi_x\rangle = \left[\frac{\partial \ln Z}{\partial J_x}\right]_{J=0} = 0, \tag{2.113}$$

$$\langle\varphi_x\varphi_y\rangle = \left[\frac{\partial \ln Z}{\partial J_x\,\partial J_y}\right]_{J=0} = G_{xy}. \tag{2.114}$$

Hence, the propagator G is the correlation function of the system (cf. problem (v)).

We now calculate the time dependence of G_{xy}, assuming that the temporal extent of the lattice is infinite (zero temperature),

$$G(x-y) \equiv G_{xy} = \int_{-\pi}^{\pi}\frac{dp_4}{2\pi}\sum_{\mathbf{p}} e^{ip(x-y)}G(p), \tag{2.115}$$

$$G(\mathbf{x},t) = \sum_{\mathbf{p}} e^{i\mathbf{px}}\int_{-\pi}^{\pi}\frac{dp_4}{2\pi}\,\frac{e^{ip_4 t}}{2b-2\cos p_4}, \tag{2.116}$$

$$b = 1+\frac{1}{2}\left(m^2+\sum_{j=1}^{3}4\sin^2\frac{p_j}{2}\right), \tag{2.117}$$

where we reverted to lattice units. The integral over p_4 can be done by contour integration. We shall take $t>0$. Note that, in lattice units, t is an integer and $b>1$. With $z=\exp(ip_4)$ we have

$$I \equiv \int_{-\pi}^{\pi}\frac{dp_4}{2\pi}\,\frac{e^{ip_4 t}}{2b-2\cos p_4} \tag{2.118}$$

$$= -\int\frac{dz}{2\pi i}\,\frac{z^t}{z^2-2bz+1}, \tag{2.119}$$

where the integration is counter clockwise over the contour $|z|=1$, see figure 2.3. The denominator has a pole at $z=z_-$ within the unit circle,

$$\begin{aligned} z^2-2bz+1 &= (z-z_+)(z-z_-),\\ &\quad z_\pm = b\pm\sqrt{b^2-1},\quad z_+z_-=1,\quad z_+>1,\quad z_-<1,\\ &\quad z_- = e^{-\omega},\quad \cosh\omega=b,\quad \omega=\ln\left(b+\sqrt{b^2-1}\right). \end{aligned} \tag{2.120}$$

The residue at $z=z_-$ gives

$$I = \frac{e^{-\omega t}}{2\sinh\omega}, \tag{2.121}$$

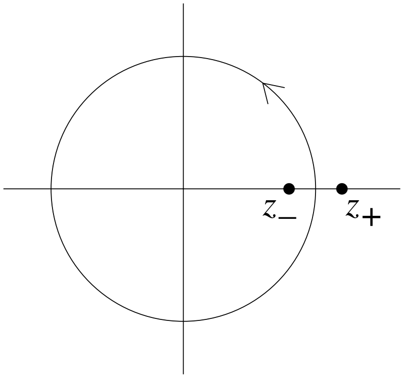

Fig. 2.3. Integration contour in the complex $z = e^{ip_4}$ plane. The crosses indicate the positions of the poles at $z = z_\pm$.

and it follows that (ω depends on $\mathbf{p}$)

$$G(\mathbf{x}, t) = \sum_{\mathbf{p}} \frac{e^{i\mathbf{px}-\omega t}}{2\sinh\omega}. \tag{2.122}$$

Notice that the pole $z = z_-$ corresponds to a pole in the variable p_4 at $p_4 = i\omega$.

In the continuum limit ($m \to am$, $p_j \to ap_j$, $\omega \to a\omega$, $a \to 0$) we get the familiar Lorentz covariant expression,

$$\omega \to \sqrt{m^2 + \mathbf{p}^2}. \tag{2.123}$$

The form (2.122) is a sum of exponentials $\exp(-\omega t)$. For large t the exponential with the smallest ω, $\omega = m$, dominates,

$$G \propto e^{-mt}, \quad t \to \infty, \tag{2.124}$$

and we see that the correlation length of the system is $1/m$.

2.9 Particle interpretation

The free scalar field is just a collection of harmonic oscillators, which are coupled by the gradient term $\partial_j\varphi\partial_j\varphi$ in the action or Hamiltonian (2.80). We can diagonalize the transfer operator explicitly by taking similar steps to those for the harmonic oscillator. One then finds (cf. problem (iii)) creation and annihilation operators $\hat{a}^\dagger_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}$, which are indexed by the Fourier label $\mathbf{p}$. The ground state $|0\rangle$ has the property $\hat{a}_{\mathbf{p}}|0\rangle = 0$ with energy $E_0 = \sum_{\mathbf{p}} \omega_{\mathbf{p}}/2$. The elementary excitations $|\mathbf{p}\rangle =$

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$\hat{a}^\dagger_{\mathbf{p}}|0\rangle$ are interpreted as particles with momentum $\mathbf{p}$ and energy $\omega_{\mathbf{p}}$. This interpretation is guided by the fact that these states are eigenstates of the translation operators in space and time, namely, $\exp(\hat{H}t)$ (eigenvalue $\exp[(\omega_{\mathbf{p}} + E_0)t]$), and the spatial translation operator $\hat{U}_{\mathbf{x}}$ (eigenvalue $\exp(-i\mathbf{px})$, see problem (vii) for its definition).

In the continuum limit we recover the relativistic energy–momentum relation $\omega(\mathbf{p}) = \sqrt{m^2 + \mathbf{p}^2}$. The mass (rest energy) of the particles is evidently m. They have spin zero because they correspond to a scalar field under rotations (there are no further quantum numbers to characterize their state). They are *bosons* because the (basis) states are symmetric in interchange of labels: $|\mathbf{p}_1\mathbf{p}_2\rangle \equiv \hat{a}^\dagger_{\mathbf{p}_1}\hat{a}^\dagger_{\mathbf{p}_2}||0\rangle = \hat{a}^\dagger_{\mathbf{p}_2}\hat{a}^\dagger_{\mathbf{p}_1}||0\rangle = |\mathbf{p}_2\mathbf{p}_1\rangle$. The ground state is usually called 'the vacuum'.

For interacting fields the above creation and annihilation operators no longer commute with the Hamiltonian – they are said to create 'bare' particles. The 'dressed' particle states are the eigenstates of the Hamiltonian, but only the single-particle states have the simple free energy–momentum relation $\omega(\mathbf{p}) = \sqrt{m^2 + \mathbf{p}^2}$. Multi-particle states have in general interaction energy, unless the particles (i.e. their wavepackets) are far apart.

Using the spectral representation (cf. problem (viii))

$$\langle\varphi_x\varphi_y\rangle - \langle\varphi\rangle^2 = \sum_{\mathbf{p},\gamma\neq 0} |\langle 0|\hat{\varphi}_0|\mathbf{p},\gamma\rangle|^2 \exp[-\omega_{\mathbf{p},\gamma}|x_4 - y_4| + i\mathbf{p}(\mathbf{x}-\mathbf{y})],$$
$$\omega_{\mathbf{p},\gamma} = E_{\mathbf{p},\gamma} - E_0, \tag{2.125}$$

the particle properties can still be deduced from the correlation functions, e.g. by studying their behavior at large time differences, for which the states with lowest excitation energies (i.e. the particles) $\omega_{\mathbf{p}}$ dominate. Alternatively, one can diagonalize the transfer operator by variational methods.

These methods are very general and also apply to confining theories such as QCD. The quantum numbers of the particles excited by the fields out of the vacuum match those of the fields chosen in the correlation functions.

2.10 Back to real time

In (2.22) we analytically continued the lattice distance in the time direction a_t to imaginary values. If we want to go back to real time we have to keep track of a_t. For instance, the action (2.70) may be rewritten in lattice units as

$$S = -\xi \sum_x \tfrac{1}{2}\partial_4\varphi_x\partial_4\varphi_x \\ - \frac{1}{\xi}\sum_x \left[\frac{1}{2}\partial_j\varphi_x\partial_j\varphi_x + \frac{m^2}{2}\varphi_x^2 + \frac{\lambda}{4}\varphi^4\right], \quad \xi = \frac{a}{a_t}, \tag{2.126}$$

which leads to the correlation function in momentum space

$$G_p = \frac{\xi}{m^2 + \sum_j (2 - 2\cos p_j) + \xi^2(2 - 2\cos p_4)}. \tag{2.127}$$

We have to realize that the symbol a_t in the Euclidean notation was really $|a_t|$ (cf. below (2.24)) and that $|a_t| = ia_t = i|a_t|\exp(-i\varphi)$, $\varphi = \pi/2$, according to (2.22). Hence, restoring the φ dependence of ξ means

$$\xi \to |\xi|(-ie^{i\varphi}). \tag{2.128}$$

Rotating back to real time, we keep φ infinitesimally positive in order to avoid singularities in G_p, φ: $\pi/2 \to \epsilon$, $\epsilon > 0$ infinitesimal. This gives

$$G \to \frac{-i|\xi|}{m^2 + \sum_j (2 - 2\cos p_j) - |\xi|^2(2 - 2\cos p_4) - i\epsilon}, \tag{2.129}$$

where we freely rescaled the infinitesimal ϵ by positive values, $[-i\exp(i\epsilon)]^2 = (-i+\epsilon)^2 = -1 - i\epsilon$; $(2 - 2\cos p_4)$ is also positive.

In the continuum limit $m \to am$, $p_j \to ap_j$, $p_4 \to |\xi|^{-1}ap_4$, $G_p \to a^{-2}\xi G(p)$, $a \to 0$ we obtain the Feynman propagator

$$G(p) \to \frac{-i}{m^2 + \mathbf{p}^2 - p_4^2 - i\epsilon} \equiv -iG_{\mathrm{M}}(p). \tag{2.130}$$

In continuum language the rotation to imaginary time is usually called a Wick rotation:

$$x^0 \to -ix_4, \quad p^0 \to -ip_4, \quad p_0 \to ip_4, \tag{2.131}$$

where $-i$ is meant to represent the rotation $\exp(-i\varphi)$, φ: $0 \to \pi/2$ in the complex plane. For instance, one continues the Minkowski space propagator to the Euclidean-space correlation function

$$G_{\mathrm{M}}(x) = \int \frac{dp_0\, d^3p}{(2\pi)^4} \frac{e^{ipx}}{m^2 + \mathbf{p}^2 - p_0^2 - i\epsilon} \tag{2.132}$$

$$\to i\int \frac{dp_4\, d^3p}{(2\pi)^4} \frac{e^{ipx}}{m^2 + \mathbf{p}^2 + p_4^2} \tag{2.133}$$

$$= iG(x), \tag{2.134}$$

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without encountering the singularities at $p_0 = \pm\sqrt{m^2+\mathbf{p}^2} \mp i\epsilon$. Notice that $\exp(ipx)$ is invariant under the rotation: $\sum_{\mu=0}^{3} p_\mu x^\mu \to \sum_{\mu=1}^{4} p_\mu x_\mu$.

In (2.130) the timelike momentum is still denoted by p_4 instead of p_0, because the p_μ (and x_μ) in lattice units are just dummy indices denoting lattice points. The actual values of G in the scaling region $|x| \gg a$ are the same as in the continuum.

2.11 Problems

We use lattice units $a = 1$ unless indicated otherwise.

(i) *Restoration of rotation invariance*
Consider the free scalar field propagator in two dimensions

$$G_{xy} = \int \frac{d^2p}{(2\pi)^2} \frac{e^{ip(x-y)}}{m^2 + 4 - 2\cos p_1 - 2\cos p_2}. \tag{2.135}$$

Let $x - y \to \infty$ along a lattice direction, or along the diagonal: $x - y = nt$, $t \to \infty$, $n = (1,0)$ or $n = (1,1)/\sqrt{2}$. The correlation length $\xi(n)$ in direction n is identified by $G \propto \exp(-t/\xi(n))$. Use the saddle-point technique to show that, along a lattice direction,

$$\xi^{-1} = \omega, \quad \cosh\omega = 1 + m^2/2, \tag{2.136}$$

whereas along the diagonal

$$\xi'^{-1} = \sqrt{2}\omega', \quad \cosh\omega' = 1 + m^2/4. \tag{2.137}$$

Discuss the cases $m \ll 1$ and $m \gg 1$. In particular show that in the first case

$$\xi'/\xi = 1 - m^2/48 + O(m^4). \tag{2.138}$$

In non-lattice units $m \to am$, and we see restoration of rotation invariance, $\xi'/\xi \to 1$ as $a \to 0$. Corrections are of order a^2m^2.

(ii) *Real form of the Fourier transform*
Consider for simplicity one spatial dimension. Since φ_x is real, $\tilde\varphi_p^* = \tilde\varphi_{-p}$. Let $\tilde\varphi_p = \tilde\varphi_p^{'} + i\tilde\varphi_p^{''}$. The real and imaginary parts $\tilde\varphi_p^{'}$ and $\tilde\varphi_p^{''}$ satisfy $\tilde\varphi_p^{'} = \tilde\varphi_{-p}^{'}$ and $\tilde\varphi_p^{''} = -\tilde\varphi_{-p}^{''}$. The $\tilde\varphi_p^{'}$, $p \geq 0$, and $\tilde\varphi_{-p}^{''}$, $p < 0$, may be considered independent variables equivalent to φ_x. Expressing φ_x in these variables gives the real form of the

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Fourier transform, and the matrix O given by

$$\begin{aligned} O_{mn} &= \frac{1}{\sqrt{N}}, && n = 0, \\ &= \sqrt{\frac{2}{N}} \cos\left(\frac{2\pi mn}{N}\right), && n = 1, \ldots, \frac{N}{2} - 1, \\ &= \frac{1}{\sqrt{N}}, && n = \frac{N}{2}, \\ &= -\sqrt{\frac{2}{N}} \sin\left(\frac{2\pi mn}{N}\right), && n = -\frac{N}{2} + 1, \ldots, -1, \end{aligned} \tag{2.139}$$

where $m = 0, \ldots, N-1$, is orthogonal: $O\,O^{\mathrm{T}} = \mathbb{1}$.

Similar considerations apply to canonical conjugate π_x and $\tilde{\pi}_p$. Verify that the operators $\hat{\tilde{\varphi}}_p$ and $\hat{\tilde{\pi}}_p$ satisfy the commutation relations

$$[\hat{\tilde{\varphi}}_p, \hat{\tilde{\pi}}_q^\dagger] = i\bar{\delta}_{p,q}, \quad [\hat{\tilde{\varphi}}_p, \hat{\tilde{\pi}}_q] = 0, \quad [\hat{\tilde{\varphi}}_p^\dagger, \hat{\tilde{\pi}}_q^\dagger] = 0, \quad [\hat{\tilde{\varphi}}_p^\dagger, \hat{\tilde{\pi}}_q] = i\bar{\delta}_{p,q}, \tag{2.140}$$

in addition to $[\hat{\tilde{\varphi}}_p, \hat{\tilde{\varphi}}_q] = [\hat{\tilde{\varphi}}_p, \hat{\tilde{\varphi}}_q^\dagger] = [\hat{\tilde{\pi}}_p, \hat{\tilde{\pi}}_q] = [\hat{\tilde{\pi}}_p, \hat{\tilde{\pi}}_q^\dagger] = 0$.

(iii) *Creation and annihilation operators*

For a free scalar field show that

$$\begin{aligned} \hat{T} &= e^{-\sum_p m_p^2 |\hat{\tilde{\varphi}}_p|^2/4}\, e^{-\sum_p |\hat{\tilde{\pi}}_p|^2/2}\, e^{-\sum_p m_p^2 |\hat{\tilde{\varphi}}_p|^2/4}, \\ m_p^2 &= m^2 + 2(1 - \cos p), \end{aligned} \tag{2.141}$$

where $|\hat{\tilde{\varphi}}_p|^2 = \hat{\tilde{\varphi}}_p^\dagger \hat{\tilde{\varphi}}_p$, etc. Hence, the transfer operator has the form $\hat{T} = \prod_p \hat{T}_p$.

Obtain the commutation relations of the creation ($\hat{a}_p^\dagger$) and annihilation ($\hat{a}_p$) operators defined by

$$\hat{a}_p = \sqrt{\frac{1}{2\sinh\omega_p}}\,[\sinh(\omega_p)\,\hat{\tilde{\varphi}}_p + i\hat{\tilde{\pi}}_p^\dagger]. \tag{2.142}$$

Using the results derived for the harmonic oscillator, show that the energy spectrum is given by

$$E = L\sum_p \left(N_p + \tfrac{1}{2}\right)\omega_p, \quad \cosh\omega_p = 1 + \tfrac{1}{2}m_p^2. \tag{2.143}$$

where N_p is the occupation number of the mode p (recall that in our notation $L\sum_p = \sum_n$, $p = 2\pi n/L$).

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Verify that

$$\hat{\varphi}_x = \sum_p \sqrt{\frac{1}{2\sinh\omega_p}}\big(e^{ipx}\hat{a}_p + e^{-ipx}\hat{a}_p^\dagger\big). \tag{2.144}$$

(iv) *Ground-state wave functional*
For the free scalar field, write down the wave function for the ground state in the coordinate representation, $\Psi_0(\varphi) = \langle\varphi|0\rangle$.

(v) *Correlation functions*
We define expectation values

$$\langle\varphi_{x_1}\cdots\varphi_{x_n}\rangle = \frac{1}{Z(J)}\int D\varphi\, e^{S(\varphi)+J_x\varphi_x}\,\varphi_{x_1}\cdots\varphi_{x_n}, \tag{2.145}$$

and correlation functions (connected expectation values)

$$G_{x_1\cdots x_n} = \langle\varphi_{x_1}\cdots\varphi_{x_n}\rangle_{\rm conn} = \frac{\partial}{\partial J_{x_1}}\cdots\frac{\partial}{\partial J_{x_1}}\ln Z(J). \tag{2.146}$$

Verify that

$$G_x = \langle\varphi_x\rangle, \tag{2.147}$$

$$G_{x_1x_2} = \langle\varphi_{x_1}\varphi_{x_2}\rangle - \langle\varphi_{x_1}\rangle\langle\varphi_{x_2}\rangle. \tag{2.148}$$

Give similar expressions for the three- and four-point functions $G_{x_1x_2x_3}$ and $G_{x_1x_2x_3x_4}$. Note that $\langle\varphi_x\rangle$ may be non-zero in cases of spontaneous symmetry breaking even when $J_x = 0$.

(vi) *Ground-state expectation values of Heisenberg operators*
On an $L^3\times\beta$ space–time lattice, verify that

$$\langle\varphi_x\varphi_y\rangle = \frac{{\rm Tr}\, e^{-(\beta-x_4+y_4)\hat{H}}\,\hat{\varphi}_{\mathbf{x}}\, e^{-(x_4-y_4)\hat{H}}\,\hat{\varphi}_{\mathbf{y}}}{{\rm Tr}\, e^{-\beta\hat{H}}}, \tag{2.149}$$

where $x_4 > y_4$ and $J = 0$.

Let $|n\rangle$ be a complete set of energy eigenstates of the Hamiltonian,

$$\hat{H}|n\rangle = E_n|n\rangle. \tag{2.150}$$

The ground state $|0\rangle$ has lowest energy, E_0. Show that for $\beta\to\infty$ (zero temperature)

$$\langle\varphi_x\varphi_y\rangle = \langle 0|T\hat{\varphi}_x\hat{\varphi}_y|0\rangle, \tag{2.151}$$

where T is the time ordering 'operator' and $\hat{\varphi}_x$ is the Heisenberg operator

$$\hat{\varphi}_{\mathbf{x},x_4} = e^{x_4\hat{H}}\hat{\varphi}_{\mathbf{x},0}e^{-x_4\hat{H}}. \tag{2.152}$$

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(vii) *Translation operator*
The translation operator $\hat{U}_{\mathbf{x}}$ may be defined by

$$\hat{U}_{\mathbf{x}}|\varphi_{\mathbf{y}}\rangle = |\varphi_{\mathbf{x}-\mathbf{y}}\rangle, \tag{2.153}$$

with $|\varphi_{\mathbf{y}}\rangle$ the factor in the tensor product $|\varphi\rangle = \prod_{\mathbf{y}} |\varphi_{\mathbf{y}}\rangle$. This operator has the properties

$$\hat{U}_{\mathbf{x}}^{\dagger}\,\hat{\varphi}_{\mathbf{y}}\hat{U}_{\mathbf{x}} = \hat{\varphi}_{\mathbf{x}-\mathbf{y}}, \tag{2.154}$$

$$\hat{U}_{\mathbf{x}}^{\dagger}\,\hat{\pi}_{\mathbf{y}}\hat{U}_{\mathbf{x}} = \hat{\pi}_{\mathbf{x}-\mathbf{y}}, \tag{2.155}$$

such that the expectation value of e.g. $\hat{\varphi}_{\mathbf{x}}$ in an actively translated state $|\psi'\rangle \equiv \hat{U}_{\mathbf{z}}|\psi\rangle$ behaves in a way to be expected intuitively: $\langle\psi'|\hat{\varphi}_{\mathbf{x}}|\psi'\rangle = \langle\psi|\hat{\varphi}_{\mathbf{x}-\mathbf{z}}|\psi\rangle$.

Verify that for periodic boundary conditions the Hamiltonian is translation invariant,

$$\hat{U}_{\mathbf{x}}^{\dagger}\hat{H}\hat{U}_{\mathbf{x}} = \hat{H}. \tag{2.156}$$

(viii) *Spectral representation*
Let $|\mathbf{p},\gamma\rangle$ be simultaneous eigenvectors of $\hat{H}$ and $\hat{U}_{\mathbf{x}}$ (γ is some label needed to specify the state in addition to $\mathbf{p}$),

$$\hat{H}|\mathbf{p},\gamma\rangle = E_{\mathbf{p},\gamma}|\mathbf{p},\gamma\rangle, \quad \hat{U}_{\mathbf{x}}|\mathbf{p},\gamma\rangle = e^{-i\mathbf{p}\mathbf{x}}|\mathbf{p},\gamma\rangle \tag{2.157}$$

Derive the spectral representation for zero temperature:

$$\begin{aligned}\langle\varphi_x\varphi_y\rangle - \langle\varphi\rangle^2 &= \sum_{\mathbf{p},\gamma\neq 0} |\langle 0|\hat{\varphi}_0|\mathbf{p},\gamma\rangle|^2 \\ &\qquad \times \exp[-\omega_{\mathbf{p},\gamma}|x_4 - y_4| + i\mathbf{p}(\mathbf{x}-\mathbf{y})], \\ \omega_{\mathbf{p},\gamma} &= E_{\mathbf{p},\gamma} - E_0,\end{aligned} \tag{2.158}$$

where $\gamma \neq 0$ indicates that the ground state is not included.

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