Introduction to Quantum Fields on a Lattice

'a robust mate'

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Introduction

We introduce here quarks and gluons. The analogy with electrodynamics at short distances disappears at larger distances with the emergence of the string tension, the force that confines the quarks and gluons permanently into bound states called hadrons.

Subsequently we introduce the simplest relativistic field theory, the classical scalar field.

1.1 QED, QCD, and confinement

Quantum electrodynamics (QED) is the quantum theory of photons (γ) and charged particles such as electrons ($e^{\pm}$), muons ($\mu^{\pm}$), protons (p), pions ($\pi^{\pm}$), etc. Typical phenomena that can be described by perturbation theory are Compton scattering ($\gamma + e^- \to \gamma + e^-$), and pair annihilation/production such as $e^+ + e^- \to \mu^+ + \mu^-$. Examples of non-perturbative phenomena are the formation of atoms and molecules. The expansion parameter of perturbation theory is the fine-structure constant[1] $\alpha = e^2/4\pi$.

Quantum chromodynamics (QCD) is the quantum theory of quarks (q) and gluons (g). The quarks u, d, c, s, t and b ('up', 'down', 'charm', 'strange', 'top' and 'bottom') are analogous to the charged leptons ν_e, e, ν_μ, μ, ν_τ, and τ. In addition to electric charge they also carry 'color charges', which are the sources of the gluon fields. The gluons are analogous to photons, except that they are self-interacting because they also carry color charges. The strength of these interactions is measured by $\alpha_{\rm s} = g^2/4\pi$ (alpha strong), with g analogous to the electromagnetic charge e. The 'atoms' of QCD are $q\bar{q}$ ($\bar{q}$ denotes the antiparticle of q)

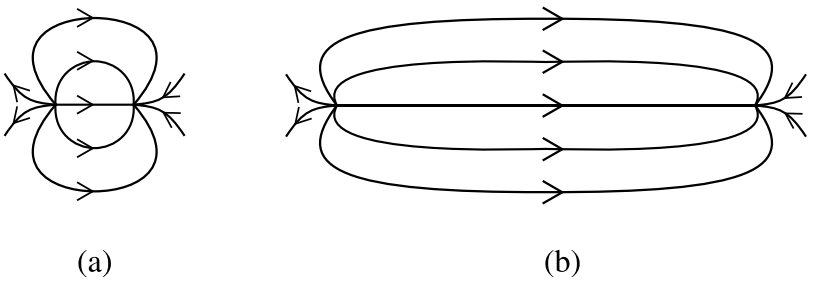

Fig. 1.1. Intuitive representation of chromoelectric field lines between a static quark–antiquark source pair in QCD: (a) Coulomb-like at short distances; (b) string-like at large distances, at which the energy content per unit length becomes constant.

bound states called mesons† (π, K, η, η', ρ, K^*, ω, ϕ, ...) and $3q$ bound states called baryons (the nucleon N, and furthermore Σ, Λ, Ξ, Δ, Σ^*, Λ^*, ...). The mesons are bosons and the baryons are fermions. There may be also multi-quark states analogous to molecules. Furthermore, there are expected to be glueballs consisting mainly of gluons. These bound states are called 'hadrons' and their properties as determined by experiment are recorded in the tables of the Particle Data Group [2].

The way that the gluons interact among themselves has dramatic effects. At distances of the order of the hadron size, the interactions are strong and α_s effectively becomes arbitrarily large as the distance scale increases. Because of the increasing potential energy between quarks at large distances, it is not possible to have single quarks in the theory: they are permanently confined in bound states.

For a precise characterization of confinement one considers the theory with gluons only (no dynamical quarks) in which static external sources are inserted with quark quantum numbers, a distance r apart. The energy of this configuration is the quark–antiquark potential $V(r)$. In QCD confinement is realized such that $V(r)$ increases linearly with r as $r \to \infty$,

$$V(r) \approx \sigma r, \quad r \to \infty. \tag{1.1}$$

The coefficient σ is called the string tension, because there are effective string models for $V(r)$. Such models are very useful for grasping some of the physics involved (figure 1.1).

Because of confinement, quarks and gluons cannot exist as free parti-

† The quark content of these particles is given in table 7.1 in section 7.5.

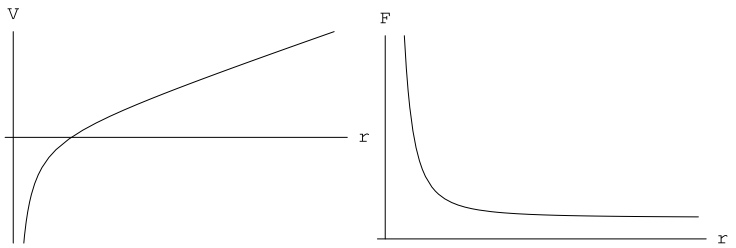

Fig. 1.2. Shape of the static $q\bar{q}$ potential and the force $F = \partial V/\partial r$.

cles. No such free particles have been found. However, scattering experiments at high momentum transfers (corresponding to short distances) have led to the conclusion that there are quarks and gluons inside the hadrons. The effective interaction strength $\alpha_{\rm s}$ is *small* at short distances. Because of this, perturbation theory is applicable at short distances or large momentum transfers. This can also be seen from the force derived from the $q\bar{q}$ potential, $F = \partial V/\partial r$. See figure 1.2. Writing conventionally

$$F(r) = \frac{4}{3}\frac{\alpha_{\rm s}(r)}{r^2}, \tag{1.2}$$

we know that $\alpha_{\rm s} \to 0$ very slowly as the distance decreases,

$$\alpha_{\rm s}(r) \approx \frac{4\pi}{11\ln(1/\Lambda^2 r^2)}. \tag{1.3}$$

This is called *asymptotic freedom*. The parameter Λ has the dimension of a mass and may be taken to set the dimension scale in quark-less 'QCD'. For the glueball mass m or string tension σ we can then write

$$m = C_m\Lambda, \qquad \sqrt{\sigma} = C_\sigma\Lambda. \tag{1.4}$$

Constants like C_m and C_σ, which relate short-distance to long-distance properties, are non-perturbative quantities. They are pure numbers whose computation is a challenge to be met by the theory developed in the following chapters.

The value of the string tension σ is known to be approximately $(400\ \text{MeV})^2$. This information comes from a remarkable property of the hadronic mass spectrum, the fact that, for the leading spin states, the spin J is approximately linear in the squared mass m^2,

$$J = \alpha_0 + \alpha' m^2. \tag{1.5}$$

See figure 1.3. Such approximately straight 'Regge trajectories' can be

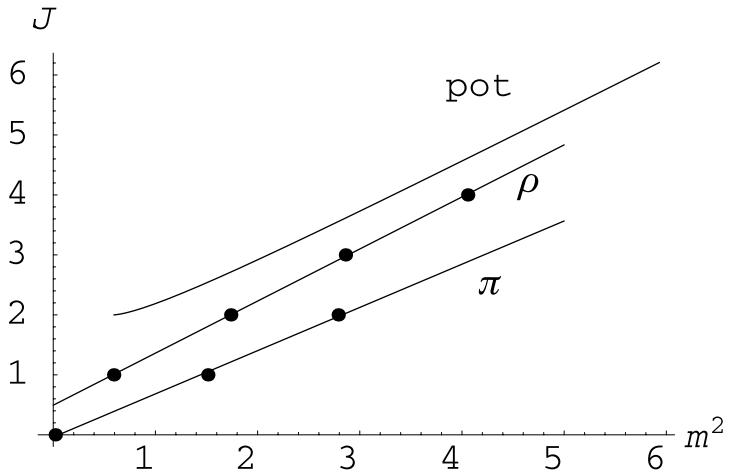

Fig. 1.3. Plot of spin J versus m^2 (GeV^2) for ρ- and π-like particles. The dots give the positions of particles, the straight lines are fits to the data, labeled by their particles with lowest spin. The line labeled 'pot' is L versus H^2 for the solution (1.10), for clarity shifted upward by two units, for $m_q = m_\rho/2$, $\sigma = 1/8\alpha'_\rho$.

understood from the following simple effective Hamiltonian for binding of a $q\bar{q}$ pair,

$$H = 2\sqrt{m_q^2 + p^2} + \sigma r. \tag{1.6}$$

Here m_q is the mass of the constituent quarks, taken to be equal for simplicity, $p = |\mathbf{p}|$ is the relative momentum, $r = |\mathbf{r}|$ is the relative separation, and the spin of the quarks is ignored. The potential is taken to be purely linear, because we are interested in the large-mass bound states with large relative angular momentum L, for which one expects that only the long-distance part of $V(r)$ is important.

For such states with large quantum number L the classical approximation should be reasonable. Hence, consider the classical Hamilton equations,

$$\frac{dr_k}{dt} = \frac{\partial H}{\partial p_k}, \quad \frac{dp_k}{dt} = -\frac{\partial H}{\partial r_k}. \tag{1.7}$$

and the following Ansatz for a circular solution:

$$\begin{aligned} r_1 = a\cos(\omega t), \quad r_2 = a\sin(\omega t), \quad r_3 = 0, \\ p_1 = -b\sin(\omega t), \quad p_2 = b\cos(\omega t), \quad p_3 = 0. \end{aligned} \tag{1.8}$$

Substituting (1.8) into (1.7) we get relations among ω, a, and b, and expressions for p and r, which can be written in the form

$$p = b = \sigma\omega^{-1}, \quad r = a = 2s^{-1}\sigma^{-1}p, \quad s \equiv \sqrt{1 + m_q^2/p^2}, \tag{1.9}$$

such that L and H can be written as

$$L = rp = 2s^{-1}\sigma^{-1}p^2, \quad H = 2(s + s^{-1})p. \tag{1.10}$$

For $p^2 \gg m_q^2$, $s \approx 1$, $L \propto p^2$ and $H \propto p$. Then $L \propto H^2$ and, because $H = m$ is the mass (rest energy) of the bound state, we see that

$$\alpha' \equiv \left[LH^{-2}\right]_{p/m_q \to \infty} = (8\sigma)^{-1}. \tag{1.11}$$

It turns out that L is approximately linear in H^2 even for quite small p^2, such that $L < 1$, as shown in figure 1.3. Of course, the classical approximation is suspect for L *not* much larger than unity, but the same phenomenon appears to take place quantum mechanically in nature, where the lower spin states are also near the straight line fitting the higher spin states.[2]

With $\alpha' = 1/8\sigma$, the experimental value $\alpha' \approx 0.90$ GeV^{-2} gives $\sqrt{\sigma} \approx$ 370 MeV. The effective string model (see e.g. [3] section 10.5) leads approximately to the same answer: $\alpha' = 1/2\pi\sigma$, giving $\sqrt{\sigma} \approx 420$ MeV. The string model is perhaps closer to reality if most of the bound-state energy is in the string-like chromoelectric field, but it should be kept in mind that both the string model and the effective Hamiltonian give only an approximate representation of QCD.

1.2 Scalar field

We start our exploration of field theory with the scalar field. Scalar fields $\varphi(x)$ ($x = (\mathbf{x}, t)$, $t \equiv x^0$) are used to describe spinless particles. Particles appearing elementary on one distance scale may turn out to be be composite bound states on a smaller distance scale. For example, protons, pions, etc. appear elementary on the scale of centimeters, but composed of quarks and gluons on much shorter distance scales. Similarly, fields may also be elementary or composite. For example, for the description of pions we may use elementary scalar fields $\varphi(x)$, or composite scalar fields of the schematic form $\bar{\psi}(x)\gamma_5\psi(x)$, where $\psi(x)$ and $\bar{\psi}(x)$ are quark fields and γ_5 is a Dirac matrix. Such composite fields can still be approximately represented by elementary $\varphi(x)$, which are then called effective fields. This is useful for the description of effective

interactions, which are the result of more fundamental interactions on a shorter distance scale.

A basic tool in the description is the action $S = \int dt\, L$, with L the Lagrangian. For a nonrelativistic particle described by coordinates q_k, $k = 1, 2, 3$, the Lagrangian has the form kinetic energy minus potential energy, $L = \dot{q}_k \dot{q}_k/2m - V(q)$.† For the anharmonic oscillator in three dimensions the potential has the form $V(q) = \omega^2 q^2/2 + \lambda (q^2)^2/4$, $q^2 \equiv q_k q_k$. In field theory a simple example is the action for the φ^4 theory,

$$S = \int\limits_M d^4x\, \mathcal{L}(x), \quad d^4x = dx^0\, dx^1\, dx^2\, dx^3, \tag{1.12}$$

$$\mathcal{L}(x) = \tfrac{1}{2}\partial_t \varphi(x) \partial_t \varphi(x) - \tfrac{1}{2} \nabla \varphi(x) \cdot \nabla \varphi(x) - \tfrac{1}{2}\mu^2 \varphi(x)^2 - \tfrac{1}{4}\lambda \varphi(x)^4, \tag{1.13}$$

Here M is a domain in space–time, $\varphi(x)$ is a scalar field, $\mathcal{L}(x)$ is the action density or Lagrange function, and λ and μ^2 are constants (λ is dimensionless and μ^2 has dimension $(\text{mass})^2 = (\text{length})^{-2}$). Note that the index $\mathbf{x}$ is a continuous analog of the discrete index k: $\varphi(\mathbf{x}, t) \leftrightarrow q_k(t)$.

Requiring the action to be stationary under variations $\delta\varphi(x)$ of $\varphi(x)$, such that $\delta\varphi(x) = 0$ for x on the boundary of M, leads to the equation of motion:

$$\begin{aligned} \delta S &= \int d^4x \big[-\partial_t^2 \varphi(x) + \nabla^2 \varphi(x) - \mu^2 \varphi(x) - \lambda \varphi(x)^3 \big]\, \delta\varphi(x) \\ &= 0 \quad \Rightarrow \quad (\partial_t^2 - \nabla^2 + \mu^2)\varphi + \lambda \varphi^3 = 0. \end{aligned} \tag{1.14}$$

In the first step we made a partial integration. In classical field theory the equations of motion are very important (e.g. Maxwell theory). In quantum field theory their importance depends very much on the problem and method of solution. The action itself comes more to the foreground, especially in the path-integral description of quantum theory.

Various states of the system can be characterized by the energy $H = \int d^3x\, \mathcal{H}$. The energy density has the form kinetic energy plus potential energy, and is given by

$$\mathcal{H} = \tfrac{1}{2}\dot{\varphi}^2 + \tfrac{1}{2}(\nabla \varphi)^2 + U, \tag{1.15}$$

$$U = \tfrac{1}{2}\mu^2 \varphi^2 + \tfrac{1}{4}\lambda \varphi^4. \tag{1.16}$$

The field configuration with lowest energy is called the ground state. It has $\dot{\varphi} = \nabla \varphi = 0$ and minimal U. We shall assume $\lambda > 0$, such that $\mathcal{H}$ is

† Unless indicated otherwise, summation over repeated indices is implied, $\dot{q}_k \dot{q}_k \equiv \sum_k \dot{q}_k \dot{q}_k$.

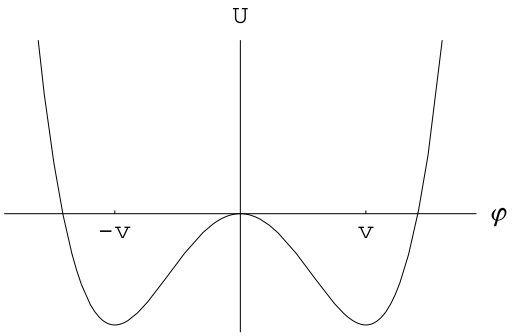

Fig. 1.4. The energy density for constant fields for $\mu^2 < 0$.

bounded from below for all φ. From a graph of $U(\varphi)$ (figure 1.4) we see that the cases $\mu^2 > 0$ and $\mu^2 < 0$ are qualitatively different:

$$\begin{aligned} &\mu^2 > 0: \quad \varphi_{\mathrm{g}} = 0, \quad U_{\mathrm{g}} = 0; \\ &\mu^2 < 0: \quad \varphi_{\mathrm{g}} = \pm v, \quad v^2 = -\frac{\mu^2}{\lambda}, \quad U_{\mathrm{g}} = -\frac{1}{4}\frac{\mu^2}{\lambda}. \end{aligned} \tag{1.17}$$

So the case $\mu^2 < 0$ leads to a doubly degenerate ground state. In this case the symmetry of S or $\mathcal{H}$ under $\varphi(x) \to -\varphi(x)$ is broken, because a non-zero φ_{g} is not invariant, and one speaks of spontaneous (or dynamical) symmetry-breaking.

Small disturbances away from the ground state propagate and disperse in space and time in a characteristic way, which can be found by linearizing the equation of motion (1.14) around $\varphi = \varphi_{\mathrm{g}}$. Writing $\varphi = \varphi_{\mathrm{g}} + \varphi'$ and neglecting $O(\varphi'^2)$ gives

$$(\partial_t^2 - \nabla^2 + m^2)\varphi' = 0, \tag{1.18}$$

$$m^2 = U''(\varphi_{\mathrm{g}}) = \begin{cases} \mu^2, & \mu^2 > 0; \\ \mu^2 + 3\lambda v^2 = -2\mu^2, & \mu^2 < 0. \end{cases} \tag{1.19}$$

Wavepacket solutions of (1.18) propagate with a group velocity $\mathbf{v} = \partial\omega/\partial\mathbf{k}$, where $\mathbf{k}$ is the average wave vector and $\omega = \sqrt{m^2 + \mathbf{k}^2}$. In the quantum theory these wavepackets are interpreted as particles with energy–momentum $(\omega, \mathbf{k})$ and mass m. The particles can scatter with an interaction strength characterized by the coupling constant λ. For $\lambda = 0$ there is no scattering and the field is called 'free'.

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 $\hat{\cdot}$). 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

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

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

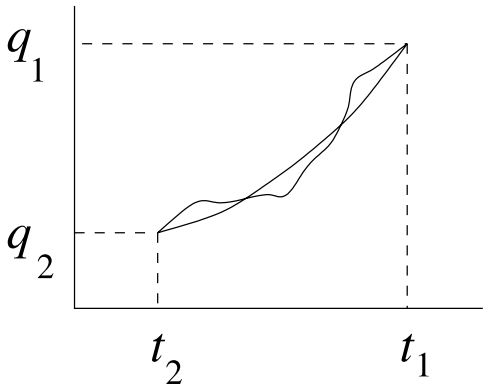

Fig. 2.1. Illustration of two functions $q(t)$ contributing to the path integral.

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

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

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:

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

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.

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

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

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

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

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.

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

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

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

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

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 $q' = q/a$, $p' = ap$, $m' = am$,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$Z = \left(\prod_x \int d\varphi_x \right) \langle \varphi_N | \hat{T} | \varphi_{N-1} \rangle \cdots \langle \varphi_1 | \hat{T} | \varphi_0 \rangle \tag{2.72}$$

$$= \operatorname{Tr} \hat{T}^N. \tag{2.73}$$

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

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

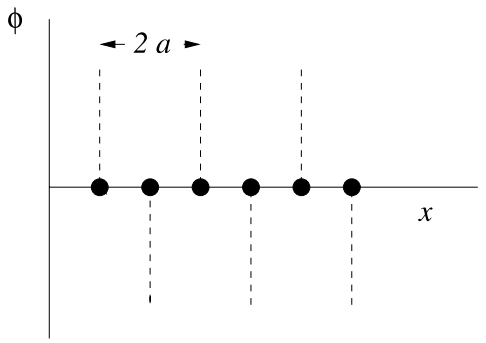

Fig. 2.2. Shortest wave length of a lattice field.

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)

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