Chapter 1
Lattice QCD: A Brief Introduction

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Abstract A general introduction to lattice QCD is given. The reader is assumed to have some basic familiarity with the path integral representation of quantum field theory. Emphasis is placed on showing that the lattice regularization provides a robust conceptual and computational framework within quantum field theory. The goal is to provide a useful overview, with many references pointing to the following chapters and to freely available lecture series for more in-depth treatments of specifics topics.

1.1 Introduction and Scope

Lattice QCD is a framework in which the strong interactions can be studied from first principles, from low to high energy scales. It is a mature subject started in 1974 [1]. Deep inelastic experiments had shown that in reactions involving a very high momentum transfer, weakly coupled quarks appear as the prominent degrees of freedom at the interaction point. The asymptotic states of the theory, however, were clearly bound states of quarks called hadrons. Lattice QCD provided for the first time a framework in which this apparent dichotomy could be addressed. However, due to the complexity of non-perturbative phenomena at low energies, it is only with the advent of supercomputers that the approach acquired the potential of being quantitatively predictive [2]. By now, lattice QCD is an important source of information for tests of the Standard Model, where it provides results for various hadronic matrix elements that are complementary to those obtained using phenomenological approaches. It has also become a viable basis for calculations of nuclear few-body quantities (see chapter "Nuclear Physics from Lattice QCD"), and for the exploration of part of the QCD phase diagram (chapter "High Temperature and Density in Lattice QCD").

The goal of this introduction is to give a concise overview of the theoretical basis on which the lattice QCD calculations described in the following chapters

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H.-W. Lin, H.B. Meyer (eds.), *Lattice QCD for Nuclear Physics*, Lecture Notes
in Physics 889, DOI 10.1007/978-3-319-08022-2_1

rest. Several textbooks are available [3–6] for more detailed introductions. Quantum field theory has many facets, and those that are of central importance in lattice QCD are not necessarily the ones most emphasized in standard QFT textbooks, which are mostly concerned with the perturbative calculation of the scattering amplitudes. The presentation is meant to help the interested reader orient himself in the subject, and also to provide the young practitioner with a minimum background to embark on a lattice calculation. A number of excellent lecture series on more specific topics are freely available on the arXiv preprint server, and often I refer the reader to them. The reader is assumed to have had some exposure to the path integral formulation of quantum field theory, and to have some familiarity with the basics of strong interaction physics.

1.2 The Lattice Formulation of Quantum Field Theory

In this section we introduce lattice field theory as a way to 'discretize' continuum field theories. The Euclidean path integral is introduced, but the discussion remains largely at the classical level; quantum effects are treated in the next sections. We treat the cases of the scalar, Dirac spinor and (non-Abelian) gauge fields.

1.2.1 Scalar Field Theory

In this chapter we will be working entirely in d-dimensional Euclidean space; the scalar product of two vectors reads $a \cdot b = a_\mu \delta_{\mu\nu} b_\nu = a_\mu b_\mu$ and there is no distinction between covariant and contravariant indices.

The Euclidean partition function for a real scalar field ϕ reads

$$Z = \int D\phi \ \exp(-S[\phi]) \tag{1.1}$$

with the measure formally defined as $D\phi = \prod_x d\phi(x)$. In continuum field theory, the action in d spacetime dimensions is defined as

$$S[\phi] = \int d^d x \ \left(\frac{1}{2}(\partial_\mu \phi(x))^2 + \frac{1}{2} m^2 \phi^2 + \frac{1}{4!} \lambda \phi^4 \right). \tag{1.2}$$

The parameter m corresponds to the mass of the scalar particle and λ to the strength of its self-interaction. The path integral measure needs to be given a precise meaning, since the partition function (1.1) involves an integral over an accountable number of degrees of freedom. If a perturbative treatment of the theory is desired, propagators and Feynman rules can nonetheless be derived and the corresponding momentum integrals can be regulated using dimensional regularization.

The lattice regularization provides an intuitive way of rendering the number of degrees of freedom countable and all correlation functions finite. The limit of the lattice spacing going to zero can be taken once the (renormalized) correlation functions have been calculated; it is referred to as the 'continuum limit'. Here the interactions do not have to be treated perturbatively.

We will restrict ourselves to four-dimensional cubic lattices,

$$\Lambda = \left\{ x \in \mathbb{R}^d \;\middle|\; x = a\,n,\; n \in \mathbb{Z}^d \right\}. \tag{1.3}$$

The length a is referred to as the lattice spacing. A lattice field $\phi(x)$ is the assignment of a real number to every point on the lattice.

We write unit vectors in the four directions as $\hat{\mu}$, $\mu = 0, 1, \ldots d$. In order to formulate an action for the lattice field theory, it is natural to introduce the discretized forward and backward derivatives

$$\partial_\mu \phi(x) = \frac{1}{a}(\phi(x + a\hat{\mu}) - \phi(x)), \qquad \partial^\star_\mu \phi(x) = \frac{1}{a}(\phi(x) - \phi(x - a\hat{\mu})), \tag{1.4}$$

as well as the symmetric derivative $\tilde{\partial}_\mu = \frac{1}{2}(\partial_\mu + \partial^\star_\mu)$. Discretizing the continuum action in the same way one would discretize differential equations, (making the simplest choices) we arrive at

$$S[\phi] = a^d \sum_x \left(\frac{1}{2}(\partial_\mu \phi(x))^2 + \frac{1}{2} m^2 \phi(x)^2 + \frac{1}{4!} \lambda \phi(x)^4 \right). \tag{1.5}$$

Exercises

1. Show that the finite-difference operators ∂_μ, ∂^*_ν all commute.
2. Show the following properties of the forward and backward derivatives:

$$\partial_\mu(\chi(x)\psi(x)) = \partial_\mu \chi(x)\, \psi(x) + \chi(x)\partial_\mu \psi(x) + a\partial_\mu \chi(x)\partial_\mu \psi(x), \tag{1.6}$$

$$a^d \sum_x \chi(x)\partial_\mu \phi(x) = -a^d \sum_x \partial^*_\mu \chi(x)\, \phi(x). \tag{1.7}$$

3. Show that in the $\lambda \to \infty$ limit, the scalar lattice action reduces to the Ising model

$$S_{\text{Ising}} = -\kappa \sum_x \sigma(x)\sigma(x + a\hat{\mu}) \tag{1.8}$$

with the rescaled field $\sigma(x)$ taking values in $\mathbb{Z}_2 = \{+1, -1\}$. Remember that additive constants in the action do not influence correlation functions and can be dropped.

4. Generalize the lattice treatment of the scalar field theory to a complex scalar field, and to a two-component complex scalar field. The latter case is the relevant model for the Standard Model Higgs.

1.2.1.1 Analysis in Momentum Space

It is worth recalling the representation of lattice fields in momentum space, perhaps familiar to the reader from condensed matter physics. If we set

$$\tilde{\phi}(p) = a^d \sum_x e^{-ipx}\phi(x), \tag{1.9}$$

then clearly $\tilde{\phi}(p + \frac{2\pi}{a}n) = \tilde{\phi}(p)$ for $n \in \mathbb{Z}^d$. The independent momenta are therefore restricted to the Brillouin zone,

$$\mathcal{B} = \left\{ p \in \mathbb{R}^d \;\middle|\; |p_\mu| \leq \frac{\pi}{a} \right\} \tag{1.10}$$

and the position-space field can be written as

$$\phi(x) = \int_{\mathcal{B}} \frac{d^d p}{(2\pi)^d}\, e^{ipx}\, \tilde{\phi}(p). \tag{1.11}$$

This representation shows very clearly that the lattice thus introduces a momentum cutoff of order $\frac{1}{a}$, since higher-momentum modes do not appear in Eq. (1.11).

Exercises

1. Show that in momentum space the forward and backward derivatives operators act multiplicatively with the factors

$$\partial_\mu \longrightarrow \tfrac{1}{a}(e^{iap_\mu} - 1), \tag{1.12}$$

$$\partial^*_\mu \longrightarrow \tfrac{1}{a}(1 - e^{-iap_\mu}), \tag{1.13}$$

$$\tilde{\partial}_\mu \longrightarrow i\,\mathring{p}_\mu, \tag{1.14}$$

$$\triangle \equiv \sum_\mu \partial^*_\mu \partial_\mu \longrightarrow -\hat{p}^2, \tag{1.15}$$

where

$$\mathring{p}_\mu \equiv \tfrac{1}{a}\sin(ap_\mu), \qquad \hat{p}_\mu \equiv \tfrac{2}{a}\sin(\tfrac{1}{2}ap_\mu). \tag{1.16}$$

2. Show that the propagator is given by

$$\langle\phi(x)\phi(y)\rangle = \int_{\mathcal{B}} \frac{d^d p}{(2\pi)^d} \frac{e^{ip(x-y)}}{\hat{p}^2 + m^2} \tag{1.17}$$

$$= \int_{-\pi/a}^{\pi/a} \frac{d^{d-1}\boldsymbol{p}}{(2\pi)^{d-1}} \frac{e^{-\Omega_{\boldsymbol{p}}|x_0-y_0|+i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})}}{\frac{2}{a}\sinh(a\Omega_{\boldsymbol{p}})} \tag{1.18}$$

with $\Omega_{\boldsymbol{p}} = \frac{2}{a}\,\mathrm{asinh}(\frac{a}{2}\sqrt{\hat{\boldsymbol{p}}^2 + m^2})$. The second equality is best established using contour integration (see Sect. 1.2.2.2).

1.2.1.2 Symmetries

A very important aspect of any regularization is, how much symmetry of the original action (1.2) it preserves. More precisely, the question is which of the discrete symmetries and which of the continuous symmetry generators are preserved. It is clear that translations, rotations and boosts are no longer continuous symmetries of the lattice action. This is a general downside of the lattice regularization: it breaks space-time symmetries, i.e. the Poincaré group, and only a discrete subgroup remain as a symmetry. Recalling that Noether's theorem applies to continuous symmetries, this implies that on the lattice we cannot expect to find four conserved currents associated with space-time symmetries (the energy-momentum tensor). Fortunately this does not represent an obstacle to most calculations, for reasons explained below.

Exercise Give the list of symmetries of the complex scalar field theory on the lattice. Apart from Poincaré symmetry, have any other symmetries of the continuum theory been broken by the regularization? Give the expression of the conserved current associated with the U(1) symmetry transformation

$$\phi'(x) = e^{i\alpha}\phi(x), \qquad (\phi^*)'(x) = \phi^*(x)e^{-i\alpha}. \tag{1.19}$$

1.2.2 Fermions

From here on, we consider field theories in four spacetime dimensions. In the continuum Euclidean theory, the action for a Dirac fermion of mass m reads

$$S_{\mathrm{f}}[\psi,\bar{\psi}] = \int d^4x\ \bar{\psi}(x)(\gamma_\mu\partial_\mu + m)\psi(x) \tag{1.20}$$

where all four 4×4 matrices γ_μ are hermitian and satisfy $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$. Correspondingly, the propagator, which coincides with the Green's function of $(\gamma_\mu \partial_\mu + m)$, reads

$$\langle \psi(x)\bar{\psi}(y)\rangle = \int \frac{d^4 p}{(2\pi)^4} \frac{e^{ip(x-y)}}{i\not{p} + m} \tag{1.21}$$

with $\not{p} \equiv p_\mu \gamma_\mu$. Via Wick's theorem, n-point functions can be expressed as a sum of products of propagators with appropriate minus signs.

The original Wilson formulation of fermions on the lattice assigns a Dirac spinor $\psi(x)$ to every lattice site $x \in \Lambda$. The corresponding action [1] reads

$$S_{\rm f}[\psi, \bar{\psi}] = a^4 \sum_x \bar{\psi}(x)(D_{\rm w} + m)\psi(x), \tag{1.22}$$

$$D_{\rm w} = \sum_\mu \left(\gamma_\mu \tilde{\partial}_\mu - a\partial^*_\mu \partial_\mu\right). \tag{1.23}$$

The first-order derivatives are discretized symmetrically in the first term, but an additional term proportional to the lattice Laplacian operator has been added. It is clear that the first-order derivatives alone would not couple neighbouring points, thereby not attributing a large action to certain high-momentum modes; this feature would lead to unwanted additional long-range degrees of freedom called ‘doublers’. The doubling problem is fixed by the addition of the Laplacian term. A more precise analysis will be given below in momentum space.

Exercises

1. Verify that the following transformations are symmetries of the Wilson action: Parity:

$$\psi(x) \to \gamma_0 \psi(x_0, -\boldsymbol{x}), \qquad \bar{\psi}(x) \to \bar{\psi}(x_0, -\boldsymbol{x})\gamma_0\,; \tag{1.24}$$

Euclidean time reversal: with $\gamma_5 \equiv \gamma_0\gamma_1\gamma_2\gamma_3$,

$$\psi(x) \to \gamma_0\gamma_5 \psi(-x_0, \boldsymbol{x}), \qquad \bar{\psi}(x) \to \bar{\psi}(-x_0, \boldsymbol{x})\gamma_5\gamma_0\,; \tag{1.25}$$

Charge conjugation[1]:

$$\psi(x) \to (\bar{\psi}(x)\gamma_0\gamma_2)^\top, \qquad \bar{\psi}(x) \to (\gamma_0\gamma_2\psi(x))^\top. \tag{1.26}$$

[1] This transformation law applies for certain representations of the Dirac matrices, e.g.

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \gamma_i = \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix}$$

with σ^i the Pauli matrices.

2. Give the expression of the conserved current associated with the U(1) symmetry transformation

$$\psi'(x) = e^{i\alpha}\psi(x), \qquad \bar{\psi}'(x) = \bar{\psi}(x)e^{-i\alpha}. \tag{1.27}$$

3. With respect to the obvious scalar product of lattice fermion fields, show that the Wilson-Dirac operator satisfies the γ_5-hermiticity relation

$$D_{\mathrm{w}}^{\dagger} = \gamma_5 D_{\mathrm{w}} \gamma_5. \tag{1.28}$$

1.2.2.1 Path-Integral Representation of Correlation Functions

Wick's theorem for fermionic n-point functions (see for instance [7], Sec. 4.2.2) has a representation in terms of a path integral over Grassmann variables. Let us recall how this works. Let $\eta_1, \dots, \eta_n$ and $\bar{\eta}_1, \dots, \bar{\eta}_n$ be anticommuting generators of a Grassmann algebra. Let also ζ and $\bar{\zeta}$ be n-component vectors of anticommuting variables and A an $n \times n$ c-number matrix. If the 'integration' rules are defined as

$$\int d\eta_i = \int d\bar{\eta}_i = 0, \tag{1.29}$$

$$\int d\eta_i \, \eta_j = \int d\bar{\eta}_i \, \bar{\eta}_j = \delta_{ij}, \tag{1.30}$$

$$\int d\eta_i \, \bar{\eta}_j = \int d\bar{\eta}_i \, \eta_j = 0, \tag{1.31}$$

then the Gaussian integral for the generating functional

$$Z[\zeta, \bar{\zeta}] \equiv \int d\eta_1 \dots d\eta_n \, d\bar{\eta}_1 \dots d\bar{\eta}_n \tag{1.32}$$
$$\exp\Big(-\sum_{i,j} (\bar{\eta}_i A_{ij} \eta_j) + \sum_i (\bar{\eta}_i \zeta_i + \bar{\zeta}_i \eta_i) \Big)$$

is given by

$$Z[\zeta, \bar{\zeta}] = c \cdot \det(A) \ \exp\Big(\sum_{i,j} \bar{\zeta}_i (A^{-1})_{ij} \zeta_j \Big). \tag{1.33}$$

Note that the determinant appears in the numerator rather than in the denominator. Applying this machinery to a lattice fermion field ($\eta_i := \psi_\alpha(x)$, $A := D_{\mathrm{w}} + m$), one obtains the following 'path-integral' representation of the lattice n-point functions,

$$\langle \psi(x_1) \dots \psi(x_n) \, \bar{\psi}(y_1) \dots \bar{\psi}(y_n) \rangle \tag{1.34}$$
$$= \frac{1}{Z[0,0]} \int D[\psi] D[\bar{\psi}] \, \psi(x_1) \dots \psi(x_n) \, \bar{\psi}(y_1) \dots \bar{\psi}(y_n) \ \exp(-S_{\mathrm{f}}[\psi, \bar{\psi}])$$

with

$$D[\psi] = \prod_{\alpha,x} d\psi_\alpha(x), \qquad D[\bar{\psi}] = \prod_{\alpha,x} d\bar{\psi}_\alpha(x). \tag{1.35}$$

Since Wick's theorem gives all correlation functions in terms of the propagator, only the latter remains to be specified. Using Eq. (1.14, 1.15), the expression for the propagator is easily found,

$$\langle\psi(x)\bar{\psi}(y)\rangle = \int_{\mathcal{B}} \frac{d^4p}{(2\pi)^4} \frac{e^{ip(x-y)}}{i\sum_\mu(\mathring{p}_\mu\gamma_\mu) + \frac{1}{2}a\hat{p}^2 + m}. \tag{1.36}$$

The spectrum of a theory is given by the location of the poles in its two-point functions. To find the poles, we first rewrite the momentum-space propagator as

$$\frac{1}{i\sum_\mu(\gamma_\mu\mathring{p}_\mu) + \frac{1}{2}a\hat{p}^2 + m} = \frac{-i\sum_\mu(\gamma_\mu\mathring{p}_\mu) + \frac{1}{2}a\hat{p}^2 + m}{\mathring{p}^2 + (\frac{1}{2}a\hat{p}^2 + m)^2}\,. \tag{1.37}$$

Exercises

1. Show that

$$\mathring{p}_\mu^2 = \hat{p}_\mu^2 - \frac{1}{4}a^2\hat{p}_\mu^4. \tag{1.38}$$

2. Use this identity to write the denominator of Eq. (1.37) as

$$\mathring{p}^2 + (\tfrac{1}{2}a\hat{p}^2 + m)^2 = \alpha(\boldsymbol{p})\hat{p}_0^2 + \sigma(\boldsymbol{p}), \tag{1.39}$$

$$\alpha(\boldsymbol{p}) \equiv 1 + am + \frac{1}{2}a^2\hat{\boldsymbol{p}}^2, \tag{1.40}$$

$$\sigma(\boldsymbol{p}) \equiv m^2 + (1+am)\hat{\boldsymbol{p}}^2 + \frac{1}{2}a^2\sum_{k<l}\hat{p}_k^2\hat{p}_l^2. \tag{1.41}$$

3. Conclude that the poles of the propagator are located at $p_0 = \pm i\omega_{\boldsymbol{p}}$ with

$$\omega_{\boldsymbol{p}} \equiv \frac{2}{a}\,\mathrm{asinh}\left(\frac{a}{2}\sqrt{\sigma(\boldsymbol{p})/\alpha(\boldsymbol{p})}\right) = \sqrt{m^2 + \boldsymbol{p}^2} + \mathrm{O}(a). \tag{1.42}$$

1.2.2.2 The Propagator in the Time-Momentum Representation

A representation of correlation functions that is particularly useful in lattice QCD is the mixed time-momentum representation $(x_0, \boldsymbol{p})$. The reason is that it allows for a spectral interpretation in terms of energy eigenstates of definite overall momentum $\boldsymbol{p}$. Having located the poles of the propagator, its time-momentum representation can be obtained by a contour integration using the residue theorem. We choose a rectangular contour with one side coinciding with the segment $[-\pi/a, \pi/a]$ on the real axis, and long vertical sides going up for $x_0 - y_0 > 0$. The contributions from the vertical sides of the rectangle cancel each other, and the contribution from the horizontal side at large Im p_0 is exponentially small; therefore, the $\int_{-\pi/a}^{\pi/a}$ integral is entirely given by the residue of the integrand at the pole $p_0 = +i\omega_{\boldsymbol{p}}$,

$$\langle\psi(x)\bar{\psi}(y)\rangle \overset{x_0>y_0}{=} \int_{-\pi/a}^{\pi/a} \frac{d^3\boldsymbol{p}}{(2\pi)^3} e^{-\omega_{\boldsymbol{p}}(x_0-y_0)} e^{i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} \rho(\boldsymbol{p}), \tag{1.43}$$

$$\rho(\boldsymbol{p}) = \left\{ \frac{-i\gamma_\mu \mathring{p}_\mu + \frac{1}{2}a\hat{p}^2 + m}{\alpha(\boldsymbol{p})(-i)\frac{\partial \hat{p}_0^2}{\partial p_0}} \right\}_{p_0 = i\omega_{\boldsymbol{p}}}. \tag{1.44}$$

Explicitly, the result is

$$\langle\psi(x)\bar{\psi}(y)\rangle \overset{x_0\neq y_0}{=} \int_{-\pi/a}^{\pi/a} \frac{d^3\boldsymbol{p}}{(2\pi)^3} \frac{e^{-\omega_{\boldsymbol{p}}|x_0-y_0|+i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{2\mathcal{E}_{\boldsymbol{p}}} \cdot \left(\text{sign}(x_0-y_0)\frac{1}{a}\sinh(a\omega_{\boldsymbol{p}})\gamma_0 - i\boldsymbol{\gamma}\cdot\mathring{\boldsymbol{p}} + \frac{1}{2}a\hat{\boldsymbol{p}}^2 + m - \frac{a\sigma(\boldsymbol{p})}{2\alpha(\boldsymbol{p})}\right). \tag{1.45}$$

with $\mathcal{E}_{\boldsymbol{p}}$ defined in Eq. (1.47). The case $x_0 < y_0$ is treated analogously and can be checked by using relation (1.28).

Exercises

1. Show that

$$\rho(\boldsymbol{p}) = \frac{1}{2\mathcal{E}_{\boldsymbol{p}}}\left(\frac{1}{a}\sinh(a\omega_{\boldsymbol{p}})\gamma_0 - i\boldsymbol{\gamma}\cdot\mathring{\boldsymbol{p}} + \frac{1}{2}a\hat{\boldsymbol{p}}^2 + m - \frac{a\sigma(\boldsymbol{p})}{2\alpha(\boldsymbol{p})}\right), \tag{1.46}$$

$$\mathcal{E}_{\boldsymbol{p}} \equiv \frac{\alpha(\boldsymbol{p})}{a}\sinh(a\omega_{\boldsymbol{p}}). \tag{1.47}$$

2. For the case $x_0 = y_0$, show by direct calculation of the p_0 integral that

$$\langle\psi(x)\bar{\psi}(y)\rangle \overset{x_0=y_0}{=} \int_{-\pi/a}^{\pi/a} \frac{d^3\boldsymbol{p}}{(2\pi)^3} \frac{e^{i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{2\mathcal{E}_{\boldsymbol{p}}} \cdot \left(-i\boldsymbol{\gamma}\cdot\mathring{\boldsymbol{p}} + \frac{1}{2}a\hat{\boldsymbol{p}}^2 + m + \frac{2\mathcal{E}_{\boldsymbol{p}} - a\sigma(\boldsymbol{p})}{2\alpha(\boldsymbol{p})}\right). \tag{1.48}$$

3. Verify, using Eqs. (1.48) and (1.45), that the propagator satisfies

$$(D_{\text{w}} + m)\langle\psi(x)\bar{\psi}(y)\rangle = \frac{1}{a^4}\delta_{x,y}. \tag{1.49}$$

1.2.3 Gauge Fields

We start by recalling a few properties of gauge fields in the continuum. The fermion theory (1.20) has a global U(1) symmetry. If the single fermion field is replaced by an N-tuplet (corresponding to N 'colors'), the global symmetry becomes $U(N)$. Here we will focus on the SU(N) subgroup. Promoting the latter symmetry to a local one requires introducing gauge fields $A_\mu(x) = A_\mu^a(x)T^a \in \mathrm{su}(N)$ belonging to the Lie algebra. We will use traceless hermitian generators T^a, normalized according to $\mathrm{Tr}\{T^aT^b\} = \frac{1}{2}\delta^{ab}$ and satisfying the commutation relations $[T^a, T^b] = if^{abc}T^c$. The structure constants f^{abc} are real and totally antisymmetric. With $\Lambda(x) \in SU(N)$, the gauge-transformed fields are defined as

$$\psi^\Lambda(x) = \Lambda(x)\psi(x), \qquad \bar{\psi}^\Lambda(x) = \bar{\psi}(x)\Lambda(x)^{-1}, \tag{1.50}$$

$$A_\mu^\Lambda(x) = \Lambda(x)A_\mu(x)\Lambda(x)^{-1} + i\Lambda(x)\partial_\mu\Lambda(x)^{-1}. \tag{1.51}$$

The covariant derivative of the fermion field

$$D_\mu\psi(x) = (\partial_\mu - iA_\mu(x))\psi(x) \tag{1.52}$$

then transforms like $\psi(x)$ and the fermion action

$$S_\mathrm{f}[\psi,\bar{\psi}] = \int d^4x\ \bar{\psi}(x)(\gamma_\mu D_\mu + m)\psi(x) \tag{1.53}$$

is gauge invariant. The field strength tensor

$$G_{\mu\nu} = G_{\mu\nu}^a T^a \equiv \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu] \tag{1.54}$$

(or equivalently $G_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + f^{abc}A_\mu^b A_\nu^c$) transforms covariantly,

$$G_{\mu\nu}^\Lambda(x) = \Lambda(x)G_{\mu\nu}(x)\Lambda(x)^{-1}. \tag{1.55}$$

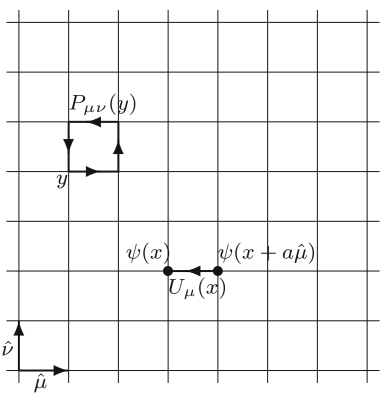

Fig. 1.1 Geometric interpretation of the dynamical variables $\psi(x)$ and $U_\mu(x)$ on a cubic spacetime lattice. The product $U_\mu(x)\psi(x+a\hat{\mu})$ transforms in the same way as $\psi(x)$ under the gauge transformation (1.50). The plaquette defined in Eq. (1.64) is also displayed

In particular, the gauge action

$$S_{\rm g}[A] = \frac{1}{2g_0^2} \int d^4x \; {\rm Tr}\{G_{\mu\nu}(x)G_{\mu\nu}(x)\} \tag{1.56}$$

is gauge invariant.

The logic to be followed is similar on the lattice. We consider a gauge transformation acting on a lattice fermion field as in Eq. (1.50). The *raison d'être* of the gauge field is to make finite-difference operators gauge covariant. Specifically, if $U_\mu(x) \in SU(N)$ is a variable which transforms as

$$U_\mu^\Lambda(x) = \Lambda(x)U_\mu(x)\Lambda(x+a\hat{\mu})^{-1}, \tag{1.57}$$

then

$$\nabla_\mu\psi(x) \equiv \frac{1}{a}\left(U_\mu(x)\psi(x+a\hat{\mu}) - \psi(x)\right). \tag{1.58}$$

transforms like $\psi(x)$ itself (see Fig. 1.1). Because of its role in the finite-difference operator, $U_\mu(x)$ is naturally associated with the 'link' joining the points x and $x + a\hat{\mu}$. It is therefore referred to as a 'link variable'. Similarly,

$$\nabla_\mu^*\psi(x) \equiv \frac{1}{a}\left(\psi(x) - U_\mu(x-a\hat{\mu})^{-1}\psi(x-a\hat{\mu})\right). \tag{1.59}$$

also transforms like $\psi(x)$.

From the classical point of view that the lattice action ought to be a discretization of the continuum action, the question of the relation between the link variable $U_\mu(x)$ and the continuum gauge field $A_\mu(x)$ poses itself. To answer this question we recall the definition of a Wilson line. If $x(s)$ is a path from $x(0) = y$ to $x(1) = z$, the Wilson line for a given gauge field is defined by a path-ordered exponential,

$$U([A]; z, y) = \mathcal{P}\exp\left(i\int_0^1 ds \, \frac{{\rm d}x_\mu}{{\rm d}s} \, A_\mu(x(s))\right) \tag{1.60}$$

$$\equiv 1 + \sum_{n=1}^{\infty} i^n \int_0^1 ds_1 \int_0^{s_1} ds_2 \ldots \int_0^{s_{n-1}} ds_n \, \frac{{\rm d}x_{\mu_1}}{{\rm d}s_1} \ldots \frac{{\rm d}x_{\mu_n}}{{\rm d}s_n} \cdot \cdot A_{\mu_1}(x(s_1)) \ldots A_{\mu_n}(x(s_n)). \tag{1.61}$$

A crucial property of the Wilson is its transformation under a gauge transformation (1.51) of the field $A_\mu(x)$,

$$U([A^\Lambda]; z, y) = \Lambda(z)U([A]; z, y)\Lambda(y)^{-1}. \tag{1.62}$$

Comparing this transformation law to Eq. (1.57), we conclude that the link variable can (at the classical level) be thought of as the straight Wilson line going from $x + a\hat{\mu}$ to x, defined on the continuum gauge field.

Exercises

1. Show that $U_t \equiv U([A]; x(t), y)$ satisfies $(\partial_t + \dot{x}_\mu(t) A_\mu(x(t)))U_t = 0$ with $U_0 = 1$.
2. Prove that $U([A]; z, y) \in \mathrm{SU}(N)$. Hint: show that $\partial_t (U_t^\dagger U_t) = 0$.
3. Prove relation (1.62). Hint: show that $\Lambda(z(t))U([A]; z(t), y)\Lambda(y)^{-1}$ satisfies the differential equation in Exercise (1) for the gauge transformed field A^Λ.

1.2.4 Lattice QCD

Given the transformation property (1.58) of the covariant derivative, the following fermion action is gauge invariant,

$$S_{\mathrm{f}}[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x)(D_{\mathrm{w}} + m_0)\psi(x), \tag{1.63}$$

$$D_{\mathrm{w}} = \sum_\mu (\gamma_\mu \tilde{\nabla}_\mu - a \nabla_\mu \nabla_\mu^*)$$

with ∇_μ, ∇_μ^* and $\tilde{\nabla}_\mu$ respectively the forward, backward and symmetrized covariant derivatives, $\tilde{\nabla}_\mu = \frac{1}{2}(\nabla_\mu + \nabla_\mu^*)$. More generally, operators such as

$$\bar{\psi}(x)\gamma_\mu\psi(x), \qquad \bar{\psi}(x)\gamma_\mu\nabla_\nu\psi(x), \quad \text{and} \quad \bar{\psi}(z)U_{\mu_1}(z)\dots U_{\mu_n}(y - a\hat{\mu}_n)\psi(y),$$

where a quark and an antiquark field are joined by a product of link variables along a given path, are gauge invariant.

Gauge invariant operators made solely of the link variables are easily constructed. The gauge transformation of a Wilson line returning to its starting point, $U([A]; y, y)$ is a similarity transformation (see Eq. (1.57)), and therefore the trace of the loop is gauge invariant. The simplest non-trivial Wilson loop on the lattice is the *plaquette*

$$P_{\mu\nu}(x) = U_\mu(x)U_\nu(x + a\hat{\mu})U_\mu(x + a\hat{\nu})^{-1}U_\nu(x)^{-1}. \tag{1.64}$$

The trace $\mathrm{Tr}\,\{P_{\mu\nu}(x)\}$ is gauge invariant. For a long-wavelength classical continuum field $A_\mu(x)$, it must therefore be possible to represent it as a linear combination of local gauge invariant operators with appropriate powers of the lattice spacing

a to get the dimensions right. The lowest-dimensional non-trivial gauge invariant operator is $\mathrm{Tr}\,\{G_{\mu\nu}(x)G_{\rho\sigma}(x)\}$. A straightforward calculation then shows that

$$P_{\mu\nu}(x) = N - \frac{1}{2}a^4\mathrm{Tr}\,\{G_{\mu\nu}(x)G_{\mu\nu}(x)\} + \ldots \qquad (1.65)$$

The simplest lattice action for the gauge fields is thus

$$S_{\mathrm{g}}[U] = \frac{2}{g_0^2}\sum_x\sum_{\mu<\nu}\mathrm{Re}\,\mathrm{Tr}\,\{1 - P_{\mu\nu}(x)\}. \qquad (1.66)$$

The total action

$$S[U,\psi,\bar{\psi}] = S_{\mathrm{f}}[U,\psi,\bar{\psi}] + S_{\mathrm{g}}[U] \qquad (1.67)$$

can thus be regarded (for $N = 3$) as a discretization of the continuum QCD action. For every quark flavor $u, d, s, c \ldots$, a term (1.63) is added to the action with the appropriate (bare) quark mass.

The details of the action (1.67) appear quite arbitrary, however, the precise form of the action should not matter—in a sense specified in Sect. 1.3—in the regime where the correlation lengths are much longer than the lattice spacing. For instance, another widely used type of fermion action is the Kogut-Susskind or 'staggered' action [8,9]. See [10] for a description of staggered fermions as they are used today.

Exercise How do the discrete symmetries C, P and T act on the lattice gauge fields for the action (1.67)?

1.2.4.1 The Path Integral

So far we have presented a lattice action for the fermion and gauge fields. In order to fully formulate the quantum theory, we need to specify the integration measure in the path integral. While this was done in Sect. 1.2.2.1 for the fermions, the definition of the measure

$$D[U] = \prod_{x,\mu} dU_\mu(x) \qquad (1.68)$$

still needs to be given. With an integration measure in hand, expectation values are defined as[2]

$$\langle \mathcal{O}_1 \ldots \mathcal{O}_n \rangle = \frac{1}{Z}\int D[U]\int D[\psi]D[\bar{\psi}]\ \mathcal{O}_1 \ldots \mathcal{O}_n\ \exp(-S[U,\psi,\bar{\psi}]). \qquad (1.69)$$

[2]The partition function Z is chosen such that $\langle 1 \rangle = 1$.

The measure is required to be '$SU(N)$ invariant'; that is

$$\int dU\ f(UV) = \int dU\ f(VU) = \int dU\ f(U) \qquad \forall\, V \in SU(N). \tag{1.70}$$

An immediate consequence of this property is the following. Suppose we calculate the expectation value of $\mathcal{O}[\psi, \bar{\psi}, U]$. The latter operator can be decomposed into irreducible representations of the SU(N) symmetry group associated with any given point x. It then follows from Eq. (1.70) and the gauge invariance of the action that all the non-singlet contributions vanish. A further crucial observation is that gauge-fixing is not required for the path integral to make sense, because the volume of the gauge group is finite,

$$\int \prod_x d\Lambda(x) = 1. \tag{1.71}$$

An explicit form for the measure is given in the exercise below.

Exercises If $U \in$ SU(N) is parametrized by $t_1, \ldots t_n$, $n \equiv N^2 - 1$, let

$$g_{ij} \equiv -2\,\mathrm{Tr}\left\{(U^{-1}\tfrac{\partial}{\partial t_i}U)\ (U^{-1}\tfrac{\partial}{\partial t_j}U)\right\} \tag{1.72}$$

1. Verify that g_{ij} is a positive-definite metric on SU(N).
2. Let

$$dU = c\ dt_1 \ldots dt_n\ \sqrt{\det(g)} \tag{1.73}$$

   with c chosen such that $\int dU = 1$. Show that the measure is independent of the parametrization.
3. Show that property (1.70) is satisfied.

1.3 The Approach to the Continuum and Renormalization

We give an overview of how the weak-coupling expansion is set up in the lattice regularization. A systematic and rigorous derivation of the expansion can be found in [11]; many explicit formulae are given in [12]; and a general strategy for numerical perturbative computations was first given in [13]. We then discuss the renormalization group, the approach to the continuum and the 'improvement' of the lattice theory.

1.3.1 The Weak-Coupling Expansion

The perturbative expansion is based on the idea that for g_0 very small, the path integral should be dominated by the fields that minimize the action. Perturbation theory is then a saddle point expansion around such field configurations. The gauge fields minimizing $S_\mathrm{g}[U]$ are of the form $U_\mu(x) = \Lambda(x)\Lambda(x + a\hat{\mu})^{-1}$ and are thus gauge-equivalent to the 'unit-configuration' $U_\mu(x) = 1 \;\forall \mu, x$. The small fluctuations of the link variables are then parametrized by a gauge potential,

$$U_\mu(x) = \exp(ig_0 a A_\mu(x)), \qquad A_\mu(x) = A_\mu^a(x) T^a. \tag{1.74}$$

If the plaquette entering the action is expanded in the $A_\mu(x)$,

$$P_{\mu\nu}(x) \equiv \exp(ig_0 a^2 G_{\mu\nu}(x)), \qquad G_{\mu\nu}(x) = G_{\mu\nu}^a(x) T^a, \tag{1.75}$$

then one finds

$$S_\mathrm{g}[U] = \frac{a^4}{4} \sum_x G_{\mu\nu}^a(x) G_{\mu\nu}^a(x) + \mathrm{O}(g_0^2), \tag{1.76}$$

$$G_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + \mathrm{O}(g_0). \tag{1.77}$$

The relations familiar from continuum field theory are thus recovered, with the derivatives replaced by finite differences. One can also show that the Jacobian of the change of integration variables is of the form

$$dU_\mu(x) = \Big(\prod_{a=1}^{N^2-1} dA_\mu^a(x) \Big) \Big(1 + \frac{g_0^2 N}{12} a^2 A_\nu^b(x) A_\nu^b(x) + \ldots \Big). \tag{1.78}$$

Although the lattice QCD path integral exists even prior to gauge fixing, an important aspect of perturbation theory is to factor out the integration over the gauge group. One can show that the condition $\partial_\mu^* A_\mu = 0$ is equivalent to the condition that the variation $\epsilon \partial_\omega A_\mu(x)$ of the field $A_\mu(x)$ under any infinitesimal gauge transformation $\Lambda(x) = 1 + i\epsilon\omega(x)$ is orthogonal to $A_\mu(x)$ itself[3]; it is thus a natural gauge-fixing condition. The result of the procedure is that the perturbative expansion of an observable $\mathcal{O}$ is given by the functional integral

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D[U] D[c] D[\bar{c}]\, \mathcal{O}[U]\, \exp(-S_\mathrm{tot}[A, c, \bar{c}]), \tag{1.79}$$

[3] With respect to the scalar product $(A, B) = a^4 \sum_{x,\mu,a} A_\mu^a(x) B_\mu^a(x)$.

where c and $\bar{c}$ are Fadeev-Popov ghosts, and

$$S_{\text{tot}}[A, c, \bar{c}] = S_{\text{g}}[U] + S_{\text{gf}}[A] + S_{\text{FP}}[A, c, \bar{c}], \tag{1.80}$$

$$S_{\text{FP}}[A, c, \bar{c}] = a^4 \sum_x \bar{c}^a(x) \triangle_{\text{FP}}^{ab} c^b(x), \tag{1.81}$$

$$S_{\text{gf}}[A] = \frac{\lambda_0 a^4}{2} \sum_x \partial_\mu^* A_\mu^a(x) \partial_\nu^* A_\nu^a(x). \tag{1.82}$$

It is understood that $U_\mu(x) = \exp(ig_0 a A_\mu(x))$ and that the integration measure is given by Eq. (1.78), and the Fadeev-Popov operator is given by $\triangle_{\text{FP}}\omega(x) \equiv g_0 \partial_\mu^* \, \partial_\omega A_\mu(x)$.

The gauge-fixed action leads to Feynman rules in the usual way. The gauge-field and ghost propagators read

$$\langle A_\mu^a(x) A_\nu^b(y) \rangle = \delta^{ab} \int_{\mathcal{B}} \frac{d^4 p}{(2\pi)^4} \frac{e^{i(p(x-y) + \frac{1}{2}ap_\mu - \frac{1}{2}ap_\nu)}}{\hat{p}^2} \cdot \left(\delta_{\mu\nu} - (1 - \lambda_0^{-1}) \frac{\hat{p}_\mu \hat{p}_\nu}{\hat{p}^2} \right), \tag{1.83}$$

$$\langle c^a(x) c^b(y) \rangle = \delta^{ab} \int_{\mathcal{B}} \frac{d^4 p}{(2\pi)^4} \frac{e^{ip(x-y)}}{\hat{p}^2}. \tag{1.84}$$

In the continuum formulation, a momentum cutoff can be problematic in gauge theories since the modes that are cut off depend on the gauge. The way the lattice regularization preserves the consequences of gauge invariance (BRS symmetry [14]) while introducing a momentum cutoff is that more and more vertices appear at higher orders.

The fermions also lead to Feynman rules as in the continuum; the propagator was given in Eq. (1.36), and the quark-quark-gluon vertex is given by

$$ig_0 (T^a)_{ij} \left(\gamma_\mu \cos(\tfrac{1}{2}a(p + p')_\mu) - i \sin(\tfrac{1}{2}a(p + p')_\mu) \right), \tag{1.85}$$

with p the incoming momentum of a quark with color index j and p' the outgoing momentum of the other quark line.

The vertices rapidly become algebraically complex to write down. It soon becomes essential to employ an automated way of generating the Feynman rules [13], see [15] for an overview of recent results obtained in this way. High-order lattice perturbation theory has been used to determine the strong coupling constant [16].

1.3.2 The Renormalization Group

Lattice QCD (see Eqs. (1.63), (1.66), (1.67)) can formally be viewed as a four-dimensional classical statistical mechanics system. Thus removing the cutoff from the quantum field theory, i.e. taking the continuum limit, can be viewed as the approach to a second order phase transition where all correlation lengths in lattice units[4] diverge. First the values of the parameters for which this happens must be found. We consider initially the case of the pure-gauge theory.

For illustration, we consider one particular observable that may be computed in perturbation theory, the rectangular Wilson loop

$$\mathcal{L}_\mu(x,d) \equiv U_\mu(x)U_\mu(x+a\hat{\mu})\dots U_\mu(x+(d-a)\hat{\mu}), \tag{1.86}$$

$$W_{\mu\nu}(x,d,d') \equiv \mathcal{L}_\mu(x,d)\mathcal{L}_\nu(x+d\hat{\mu},d')\mathcal{L}_\mu(x+d'\hat{\nu},d)^{-1}\mathcal{L}_\nu(x,d')^{-1} \tag{1.87}$$

As we shall see in Sect. 1.4.1, if we define a *static potential* $V(R)$ via

$$\langle W_{0k}(x,R,T)\rangle \overset{T\to\infty}{=} c(R)\exp(-TV(R)) + \dots, \tag{1.88}$$

it has the interpretation of the potential energy between two quarks in the limit where the latter become infinitely massive. To remove an ultraviolet-divergent additive constant, we consider the 'static force' $F(R) \equiv -\frac{\partial V}{\partial R}$. Computationally, the force also depends on the bare coupling and the lattice spacing.[5] A one-loop calculation in the pure SU(N) gauge theory yields the result

$$F(R,g_0,a) \overset{R\gg a}{=} \frac{C_F}{4\pi R^2}\left(g_0^2 + \frac{11N}{24\pi^2}g_0^4(\log(R/a)+c) + \mathrm{O}(g_0^6)\right) \tag{1.89}$$

with $C_F = (N^2-1)/(2N)$ and c a numerical constant. Now, we expect the force at a fixed separation R to reach a finite limit when $a \to 0$. The form (1.89) clearly shows that this is only possible if g_0 is adjusted as a function of a. How exactly it must be adjusted can be worked out by requiring that F actually be independent of a,

$$0 = a\frac{d}{da}F(R,g_0(a),a) = \left(a\frac{\partial}{\partial a} - \beta(g_0)\frac{\partial}{\partial g_0}\right)F(R,g_0,a)\Big|_{g_0=g_0(a)}, \tag{1.90}$$

with

$$\beta(g_0) \equiv -a\frac{\partial g_0}{\partial a}. \tag{1.91}$$

[4]The correlation lengths λ are defined by the fall-off of correlation functions, $C(x) \sim \exp(-|x|/\lambda)$.

[5]Dimensional analysis implies $F(R,g_0,a) = \frac{1}{a^2}\hat{F}(R/a,g_0)$.

Inserting the one-loop expression (1.89) into Eq. (1.90), one finds

$$\beta(g_0) = -b_0 g_0^3, \qquad b_0 = \frac{11N}{48\pi^2}. \tag{1.92}$$

The definition (1.91) of $\beta(g_0)$ can now be read as a differential equation for g_0. The negative value of the beta function means that g_0 must be made smaller in order to reduce the lattice spacing. The asymptotic solution of the differential equation is

$$g_0^2 = -\frac{1}{b_0 \log(a\mu)} + \dots \tag{1.93}$$

This is the expression of the 'asymptotic freedom' property of QCD at the level of the bare regularized theory. Note that an arbitrary mass scale μ had to be introduced. Its appearance is sometimes referred to as dimensional transmutation.

More generally, consider first the pure SU(N) gauge theory in perturbation theory. The bare parameters of the theory, g_0 and λ_0, as well as the momentum-space bare n-point correlation functions $G_0(p_1, \dots, p_n)$ of the gauge potential A_μ^a, can be traded for renormalized parameters g, λ and renormalized correlation functions $G(p_1, \dots, p_n)$. The latter have a finite continuum limit; they are well-defined functions of the external momenta, g, λ and a renormalization scale μ that is introduced when defining the finite-part of correlation functions. One could say that the divergences have been absorbed into the bare parameters. The latter can be adjusted as a function of the lattice spacing in such a way that g, μ and λ stay constant as $a \to 0$. The bare coupling g_0 can then be expressed as a function of $a\mu$ and a renormalized coupling g. For instance, a renormalized coupling based on the static force may be introduced by setting

$$F(R) = \frac{C_F g^2(R)}{4\pi R^2} \qquad \text{(defines } g(R)\text{)}. \tag{1.94}$$

The perturbative result (1.89) then shows that

$$g^2(r) = g_0^2 + \frac{11N}{24\pi^2} g_0^4 \log(\bar{r}/a) + \mathrm{O}(g_0^6), \qquad \bar{r} \equiv r\ \exp(c). \tag{1.95}$$

In the presence of fermions, the coefficient of the beta function is modified,

$$b_0 = \frac{11N - 2N_\mathrm{f}}{48\pi^2}. \tag{1.96}$$

Thus asymptotic freedom remains a property of the theory as long as $N_\mathrm{f} < \frac{11}{2}N$. In addition to g_0 and λ_0, the fermion masses need to be renormalized. While in the continuum theory, chiral symmetry prevents the appearance of an additive correction to the masses, the explicit breaking of chiral symmetry by the Wilson action (see Sect. 1.5.2) means that a tuning of the bare mass m_0 to a 'critical' value m_c is necessary in order to reach the point where the renormalized quark mass $\overline{m}$ vanishes. One writes

$$\overline{m} = Z_m(m_0 - m_c). \tag{1.97}$$

In the statistical-mechanics language, $g_0 = 0$ corresponds to a free-field theory and the critical point is thus a Gaussian one. However, the quantities that are of interest from the quantum field theory point of view are typically ratios of correlation lengths corresponding (at the non-perturbative level) to ratios of hadron masses.

1.3.3 The Continuum Limit and Universality

We have so far looked at a specific discretization of the continuum action, the Wilson action. There is a degree of arbitrariness in the choice of the discretization. However, the continuum limit is *universal*, as implied by the theory of critical phenomena. Ratios of correlation lengths associated with source fields of different quantum numbers do not depend on the details of the action. Only the list of long-wavelength modes, the dimensionality of space and the symmetries of the action matter.

As far as the quantum field theory is concerned, the property of universality implies in particular that if physical renormalization conditions are imposed (e.g. a momentum-subtraction scheme, or the renormalized coupling defined from the static $\bar{Q}Q$ force), the results will be exactly the same as if dimensional regularization had been used. If a renormalization scheme is used which is tied up with the regularization (such as minimal subtraction), the results differ by a finite renormalization of the parameters $(g, \bar{m}, \lambda)$ and the fields. We refer the reader to [17] for an in-depth discussion of renormalization.

In practical calculations it is important to know at what rate the continuum limit is approached. An important framework to analyze this question was developed by Symanzik [18]. The idea is to write down an effective (continuum) theory for the long-wavelength[6] degrees of freedom of the lattice fields. The effective theory is non-renormalizable, but comes with a clear power-counting scheme. The lowest-order Lagrangian, if all goes according to plan, is the continuum QCD Lagrangian. All higher-dimensional operators consistent with the symmetries of the lattice action contribute, however their coefficients are suppressed by powers of the lattice spacing. The discussion is thus analogous to the low-energy description of beyond the Standard Model physics if one identifies a^{-1} with the scale of 'new physics'. One unusual aspect is that here not only Lorentz-scalar operators can appear, due to the breaking of Lorentz symmetry by the lattice regulator.

[6] Compared to the lattice spacing.

In the language of the Symanzik effective field theory, the dimension-three operator $\bar{\psi}\psi$ must be included with a coefficient of order $1/a$ for the case of the Wilson action. This statement is equivalent to the additive renormalization of the quark mass in Eq. (1.97). However, direct inspection of the symmetries shows that no other operators of dimension $d < 5$ appear that are not already included in the naive continuum limit of the Wilson action. This is the real reason why Wilson lattice QCD is a valid regularization of QCD. The discretization of the continuum QCD action in a classical way was, in retrospect, only a useful guide. However, this procedure did allow for the setup of the perturbative expansion in a relatively standard way.[7]

From a practical point of view, the most important prediction of Symanzik's analysis applied to the Wilson action is that the continuum limit is approached asymptotically with a correction term of $O(a)$ multiplying a power series in $\log(a)$. In the pure gauge theory, the corrections are of order a^2. It should be emphasized that the approach to the continuum is predictable because of asymptotic freedom. Since the continuum limit is at $g_0 = 0$, the scaling dimension of operators is in first approximation equal to their naive engineering dimension.

1.3.4 Improvement

In practice, the approach to the continuum with $O(a)$ corrections can lead to large systematic uncertainties on the final results, since it is computationally very costly to reduce the lattice spacing. Therefore, a strategy has been developed to accelerate the approach to the continuum [20, 21].

One way to formulate the problem is the following. One wants to tune the coefficients of certain operators in the lattice theory such that in the action of the Symanzik effective theory, the coefficients of the dimension-five operators vanish. This condition guarantees for instance that the spectrum (masses and dispersion relations of hadrons) approaches its continuum limit with $O(a^2)$ corrections (up to logarithms).

The symmetries of continuum QCD and the equations of motion can be used to reduce the list of dimension-five operators in the Symanzik effective theory. Then these operators are carried over in 'discretized' form to the lattice theory. It turns out that, apart from a rescaling of the gauge action and the quark mass term, the only new term appearing is the 'Pauli' or 'clover' term,

$$S \to S + \frac{i}{4} c_{\rm sw} a^5 \sum_x \bar{\psi}(x) \sigma_{\mu\nu} \hat{G}_{\mu\nu} \psi(x). \tag{1.98}$$

[7] Recently, the use of a gauge action with no obvious classical continuum limit, but respecting the same symmetries as the Wilson gauge action has been studied [19].

Here $\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu]$ and $\hat{G}_{\mu\nu}$ is a lattice-site centered discretization [20] of the field strength tensor $G_{\mu\nu}$. A condition to determine the value of the coefficient $c_{\rm sw}$ that will eliminate the $\mathrm{O}(a)$ effects is provided by requiring that the PCAC relation (see Sect. 1.5.1.1) be satisfied under different kinematic conditions [22]. In imposing the condition, one must take into account that also composite operators such as the axial current receive improvement terms.

1.4 Observables

In order to illustrate the way lattice QCD is used, we describe three types of observables: the Wilson loop, the hadron spectrum and the chiral condensate.

1.4.1 The Wilson Loop and Its Interpretation

Apart from local operators, extended gauge-invariant operators such as

$$\mathcal{O}_r(x) = \bar{Q}(x)\mathcal{L}_1(x,r)Q'(x + r\boldsymbol{e}_1), \tag{1.99}$$

$$\tilde{\mathcal{O}}_r(x) = \bar{Q}'(x + r\boldsymbol{e}_1)\mathcal{L}_1(x,r)^{-1}Q(x), \tag{1.100}$$

can be used to probe mesons with different quantum numbers. Here Q and Q' are meant to represent different quark flavors. It is interesting to consider the two-point function $\langle \tilde{\mathcal{O}}_r(x + t\boldsymbol{e}_0)\, \mathcal{O}_r(x)\rangle$ in the limit where the quark mass goes to infinity.

For a large quark mass, the quark propagator in a given background gauge field can be expanded in a geometric series,

$$(D_{\rm w} + m)^{-1} = \frac{1}{m}\sum_{n=0}^{\infty}\left(\frac{-D_{\rm w}}{m}\right)^n. \tag{1.101}$$

Since $D_{\rm w}$ only couples nearest neighbours, $(D_{\rm w}^n\psi)(x)$ vanishes for $\frac{1}{a}\sum_{\mu=0}^{3}|x_\mu| > n$ if $\psi(x) = u\delta_{0,x}$ is a source field located at the origin, u being a 12-component colored spinor. For $x = (x_0, \mathbf{0})$ with $x_0 > 0$, the leading contribution

$$((D_{\rm w} + m)^{-1}\psi)(x) = \frac{\exp(-x_0 \log(am))}{2m}\,\mathcal{L}_0(0, x_0)\,(1 + \gamma_0)\,u \cdot (1 + \mathrm{O}((am)^{-2})) \tag{1.102}$$

is determined by the Wilson line joining the origin to x.

Thus, if we perform the Wick contractions for the correlator $\langle \mathcal{O}_r(x)\, \tilde{\mathcal{O}}_r(0)\rangle$, we obtain a Wilson loop,

$$\langle \tilde{\mathcal{O}}_r(x + t\boldsymbol{e}_0)\, \mathcal{O}_r(x)\rangle = c\, \exp(-2x_0 \log(am))\, \mathrm{Tr}\,\{W_{01}(x, r, t)\} \\ \sim \exp(-tV(r)), \tag{1.103}$$

with c a constant. Writing the expectation value of the Wilson loop as the two-point function of $\bar{Q}Q$ operators with static quarks separated by a distance r suggests the interpretation anticipated in Eq. (1.88), namely, that it falls off exponentially in Euclidean time, with an exponent given by the meson energy. The latter consists of the (divergent) quark self-energies and the r-dependent interaction energy, or 'static potential'. The quark self-energies drop out in the force $F(r) = -\frac{\partial V}{\partial r}$. The latter is often used in practice as a way of 'setting the scale', most commonly by defining the reference length r_0 through the condition $r_0^2 F(r_0) = 1.65$ [23]. The physical value of r_0 is about 0.50 fm [24].

1.4.1.1 The Strong-Coupling Expansion

The Wilson loop was originally proposed as an order parameter for the confinement of quarks [1]. If all quarks are made very massive, the potential energy between any two quarks has either an area law, $\langle W_{0k}(0, r, t)\rangle \sim \exp(-\sigma r t)\rangle$, or a perimeter law, $\langle W_{0k}(0, r, t)\rangle \sim \exp(-m(r + t))\rangle$. According to the interpretation derived in Sect. 1.4.1, the two cases distinguish respectively between the static force $F(r)$ going to a non-vanishing or vanishing value at long distances.

The strong-coupling expansion is, in a sense, particularly natural on the lattice, and simpler than the weak-coupling expansion. In this context it is customary to introduce the parameter

$$u \equiv \frac{1}{g_0^2} \tag{1.104}$$

and to expand the partition functions and observables in powers of β. The Haar measure plays a central role. Consider a single link variable U. The only non-vanishing integrals of a monomial in components of U and U^* up to order 2 included are

$$\int dU = 1, \qquad \int dU\, U_{ij} U^*_{lk} = \frac{1}{N}\delta_{il}\delta_{jk}. \tag{1.105}$$

In addition, there is the 'baryon-like' contribution

$$\int dU\, U_{i_1 j_1} \dots U_{i_N j_N} = \frac{1}{N} \epsilon_{i_1 \dots i_N}\, \epsilon_{j_1 \dots j_N}. \tag{1.106}$$

To compute the partition function

$$Z_u = \int DU \ \ \exp\Big(u \sum_{x,\mu,\nu} \mathrm{Tr}\{P_{\mu\nu}(x)\}\Big), \tag{1.107}$$

we write

$$\begin{aligned}\exp\Big(u \sum_{x,\mu,\nu} \mathrm{Tr}\{P_{\mu\nu}(x)\}\Big) &= \prod_p \exp(u\mathrm{Tr}\{P_p\}) \\ &= \sum_{\{n_p\}} u^{\sum_p n_p} \prod_p \frac{1}{n_p!} \mathrm{Tr}\{P_p\}^{n_p},\end{aligned} \tag{1.108}$$

where $p \equiv (x, \mu, \nu)$ is the label of an oriented plaquette. Diagrammatically, in order to compute the order u^n we must lay down n tiles on the cubic faces of the lattice.

Consider then the expectation of a Wilson loop,

$$\langle W_{0k}(0,r,t)\rangle = \frac{1}{Z_u}\int DU \ W_{0k}(0,r,t) \ \exp\Big(u \sum_{x,\mu,\nu} \mathrm{Tr}\{P_{\mu\nu}(x)\}\Big). \tag{1.109}$$

The Wilson loop contains at most a single power of any link variable. In view of Eq. (1.105), each link variable must be 'saturated' by a corresponding factor of the link variable coming from the expansion of the exponential. Let $A = rt/a^2$. The first non-trivial contribution appears at order u^A and comes when the entire surface of the Wilson loop is 'tiled' with plaquettes from the action. The integral then gives

$$\langle W_{0k}(0,r,t)\rangle \sim u^A. \tag{1.110}$$

Thus we have obtained an area law with

$$a^2\sigma = -\log u, \qquad\qquad u \to 0. \tag{1.111}$$

Similarly, the mass gap m_G of the pure gauge theory (corresponding to a 'glueball') can be computed by considering the plaquette-plaquette correlator, $\sum_{i,j=1}^{3}\langle P_{ii}(t,\mathbf{0})P_{jj}(0)\rangle \sim \exp(-m_G t)$. The result is in leading order

$$am_G = -4\log u, \qquad\qquad u \to 0. \tag{1.112}$$

The reader is invited to consult [3] for a systematic discussion of the strong-coupling expansion.

1.4.1.2 Quark Confinement

That the theory exhibits linear confinement in the strong coupling regime $g_0^2 \gg 1$ does not mean that this feature is present near the continuum limit ($g_0^2 \ll 1$). As a case in point, the 'compact' formulation of U(1) gauge theory admits a phase transition at a bare coupling of order unity, beyond which the static potential is of the Coulomb type. All numerical evidence points to a finite string tension σ in the continuum limit of SU($N \geq 2$) gauge theory; see for instance [25, 26]. Quite a bit can be inferred, however, by assuming that the linear potential survives the continuum limit, and that the relevant effective degrees of freedom of a large Wilson loop are the two transverse fluctuations of a two-dimensional sheet in four dimensions [27, 28]. An effective bosonic string theory has been developed based on this picture, yielding an expansion of the static potential in powers of $1/r$,

$$V(r) = \mu + \sigma r - \frac{\pi}{12r} + \dots \tag{1.113}$$

The effective string theory makes even stronger predictions for the corrections to the linear potential at large r; see [29] and references therein. These sharp predictions still remain to be fully tested by numerical simulations, but there is good numerical evidence that the static potential follows the prediction (1.113). Moreover, the spectrum predicted by the Nambu-Goto string action provides an excellent description of the low-lying (closed-string) states [30].

1.4.2 Hadron Spectroscopy

Here we will adopt a continuum notation and consider that we are in the infinite-volume, continuum Euclidean theory. The main purpose of this section is to show that the spectrum of stable hadrons can be extracted from the long-distance behavior of Euclidean correlation functions. An explicit analytic continuation of the correlation functions to Minkowski space is not required.

For concreteness we will consider the simplest case of the pion. From Eq. (1.18), we saw that the energy of a scalar particle could be read off from the large Euclidean time of the propagator in the time-momentum representation. The form of the free-field propagator, however, generalizes to (even non-perturbatively) interacting field theories via the Källen-Lehmann spectral representation. The Heisenberg representation, continued to Euclidean time, reads

$$\hat{\phi}(x) = e^{H|x_0| - i\boldsymbol{P}\cdot\boldsymbol{x}}\, \hat{\phi}(0)\, e^{-H|x_0| + i\boldsymbol{P}\cdot\boldsymbol{x}} \tag{1.114}$$

Suppose we use as an interpolating operator $\hat{\phi}(x) = \bar{d}\gamma_5 u$ and write

$$\langle 0|\hat{\phi}(x)|\boldsymbol{p}\rangle = \sqrt{\phi_\pi}\, e^{-E_{\boldsymbol{p}}|x_0| + i\boldsymbol{p}\cdot\boldsymbol{x}}. \tag{1.115}$$

Then define

$$G(x_0, \boldsymbol{p}) \equiv \int d^3x\ e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \langle 0|\hat{\phi}(x)\hat{\phi}(0)^\dagger|0\rangle = \int d^3x\ e^{-i\boldsymbol{p}\cdot\boldsymbol{x}}\ \langle \phi(x)\phi(0)^\dagger\rangle. \tag{1.116}$$

Inserting a complete set of states of total momentum $\boldsymbol{p}$, and taking into account the fact that the next states above the pion form a continuum of three-pion states,[8]

$$1 = \int \frac{d^3\boldsymbol{p}}{(2\pi)^3 2E_{\boldsymbol{p}}} |\boldsymbol{p}\rangle\langle\boldsymbol{p}| + (\text{projector onto states of energy} > 3m_\pi). \tag{1.117}$$

we have

$$G(x_0, \boldsymbol{p}) \overset{|x_0|\to\infty}{=} \phi_\pi \frac{e^{E_{\boldsymbol{p}}|x_0|}}{2E_{\boldsymbol{p}}} + \mathrm{O}(e^{-3m_\pi|x_0|}). \tag{1.118}$$

A typical operator that couples to the nucleon is (here $C = \gamma_0\gamma_2$)

$$\chi_\alpha(x) = \epsilon_{abc}(u^{a\top} C\gamma_5 d^b)u^a_\alpha(x). \tag{1.119}$$

However, often operators are used that do not transform as a Dirac spinor under boosts. In that case the other symmetries can still be used to constrain the possible form of the two-point function. One can decompose

$$C_2(x_0, \boldsymbol{p})_{\alpha\beta} \equiv \int d^3x\ e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \langle\chi_\alpha(x)\bar{\chi}_\beta(0)\rangle \tag{1.120}$$

$$= (C_2^+(x_0, \boldsymbol{p}) + C_2^-(x_0, \boldsymbol{p}))_{\alpha\beta}, \tag{1.121}$$

with

$$C_2^+(x_0, \boldsymbol{p}) \equiv \tfrac{1}{2}(1+\gamma_0)C_2(x_0, \boldsymbol{p}) \tag{1.122}$$

$$= \tfrac{1}{2}(1+\gamma_0)\Big(\mathcal{F}(x_0, \boldsymbol{p}^2) - i\,\mathcal{G}(x_0, \boldsymbol{p}^2)\ \boldsymbol{p}\cdot\boldsymbol{\gamma}\Big),$$

$$C_2^-(x_0, \boldsymbol{p}) \equiv \tfrac{1}{2}(1-\gamma_0)C_2(x_0, \boldsymbol{p}) \tag{1.123}$$

$$= \tfrac{1}{2}(1-\gamma_0)\Big(\mathcal{F}(-x_0, \boldsymbol{p}^2) - i\,\mathcal{G}(x_0, \boldsymbol{p}^2)\ \boldsymbol{p}\cdot\boldsymbol{\gamma}\Big).$$

Charge conjugation implies that $\mathcal{G}$ is even in x_0. Spectral positivity implies that $\gamma_0 C_2$ is a Hermitian, positive-definite matrix. Thus, the functions $\mathcal{F}$ and $\mathcal{G}$ are real and must satisfy

$$-\mathcal{F}(x_0, \boldsymbol{p}^2)\ \mathcal{F}(-x_0, \boldsymbol{p}^2) \geq \boldsymbol{p}^2\mathcal{G}(x_0, \boldsymbol{p}^2)^2, \tag{1.124}$$

$$\mathrm{sign}(x_0)\ (\mathcal{F}(x_0, \boldsymbol{p}^2) - \mathcal{F}(-x_0, \boldsymbol{p}^2)) \geq 0. \tag{1.125}$$

[8] One-particle states are normalized according to $\langle\boldsymbol{p}'|\boldsymbol{p}\rangle = (2\pi)^3 2E_{\boldsymbol{p}}\delta(\boldsymbol{p}-\boldsymbol{p}')$.

At zero momentum, $C_2^+(x_0, \mathbf{0})$ receives contributions only from positive-parity baryons, while $C_2^-(x_0, \mathbf{0})$ only couples to negative-parity baryons (see the transformation of spinors under parity, Eq. (1.24)). Thus, one may extract the proton mass m_p from the long-distance part of the projected correlator

$$\mathrm{Tr}\,\{C_2^+(x_0, \mathbf{0})\} \sim |\chi_\mathrm{p}|^2 \exp(-m_\mathrm{p} x_0), \qquad x_0 \to +\infty, \tag{1.126}$$

where the trace acts on the spin indices. Many more aspects of spectroscopy calculations are covered in chapter “Lattice Methods for Hadron Spectroscopy”.

1.4.3 *Spontaneous Chiral Symmetry Breaking and Low-Energy Constants*

In view of the special role of the pions in QCD as pseudo-Goldstone bosons associated with the spontaneous breaking of chiral symmetry, both their masses and couplings to the axial current are of interest. Consider the case where two degenerate quark flavors, up and down, are very light and let $\psi = (u, d)^\top$. Current-algebra relations imply the Gell-Mann–Oakes–Renner (GMOR) relation

$$F_\pi^2 m_\pi^2 \overset{m\to 0}{=} 2m\,\Sigma, \qquad \Sigma = -\frac{1}{2} \lim_{m\to 0} \lim_{V\to 0} \langle \bar{\psi}\psi \rangle, \tag{1.127}$$

giving the leading-order dependence of the pion mass in terms of the quark mass. The pion decay constant F_π is defined by (the axial current A_μ^a is defined in Eq. (1.143) below)

$$\langle 0|A_\mu^a(0)|\pi^b\rangle = ip_\mu\,\delta^{ab} F_\pi, \tag{1.128}$$

and its value (92.2 MeV) is extracted from the weak decay $\pi^- \to \mu^-\bar{\nu}_\mu$. In lattice QCD it can be extracted for instance from the two-point function

$$\int d^3x\ \langle A_0^a(x) A_0^b(0)\rangle \overset{|x_0|\to\infty}{=} \frac{\delta^{ab}}{2} F_\pi^2 m_\pi \exp(-m_\pi |x_0|). \tag{1.129}$$

The GMOR relation (1.127) can be used to estimate the chiral condensate Σ, knowing m_π and F_π for a range of small quark masses. However, the condensate can also be extracted in an independent way. Consider the average spectral density of the Dirac operator,

$$\rho(\lambda, m) = \frac{1}{V}\sum_{k=1}^{\infty} \langle \delta(\lambda - \lambda_k)\rangle. \tag{1.130}$$

The Banks-Casher relation [31] gives the condensate as the density of modes of the Dirac operator around the origin in the chiral limit,

$$\lim_{\lambda\to 0}\lim_{m\to 0}\lim_{V\to\infty}\rho(\lambda,m)=\frac{\Sigma}{\pi}. \tag{1.131}$$

This relation has been used as a way to compute the chiral condensate in the chiral limit [32]. Other methods exist as well,[9] and a recent average given by the FLAG2 report [34] is

$$\Sigma^{1/3}=270(7)\,\mathrm{MeV} \tag{1.132}$$

in QCD with two flavors. The GMOR relation is found to be a good approximation well beyond the physical values of the light-quark masses. The level of accuracy reached in lattice calculations is however such that low-energy constants that appear at higher orders in chiral perturbation theory are being determined with competitive accuracy [34].

1.5 Theory Topics for the Lattice Practitioner

We give an introduction to a few theory topics which are, on one hand, of general interest for aspiring quantum field theorists, and which on the other hand have proved important in practical lattice calculations.

1.5.1 Ward Identities

Suppose that the Euclidean action $S[\psi,\bar\psi,U]$ is invariant under a global transformation of the fields. Promoting the transformation to a local one generates interesting relations among correlation functions. As an example in lattice QCD with the Wilson action, consider then the local transformation

$$\psi'(x)=e^{i\alpha(x)}\psi(x), \qquad \bar\psi'(x)=\bar\psi(x)e^{-i\alpha(x)}. \tag{1.133}$$

One finds, for an infinitesimal transformation,

$$S[\psi',\bar\psi',U]=S[\psi,\bar\psi,U]+\delta S[\psi,\bar\psi,U], \tag{1.134}$$

[9] At the time of writing, the Yang-Mills gradient flow provides probably the most efficient way to compute the chiral condensate with precision [33].

$$\delta S[\psi, \bar{\psi}, U] = i\ a^4 \sum_x \partial_\mu \alpha(x) J_\mu(x) + \mathrm{O}(\alpha^2), \tag{1.135}$$

with

$$J_\mu(x) = \tfrac{1}{2}\big(\bar{\psi}(x + a\hat{\mu})(1 + \gamma_\mu)U_\mu^\dagger(x)\psi(x) \tag{1.136}$$
$$- \bar{\psi}(x)(1 - \gamma_\mu)U_\mu(x)\psi(x + a\hat{\mu})\big),$$

while the integration measure is left invariant. If $\mathcal{O}$ is an observable which transforms according to

$$\mathcal{O}[\psi', \bar{\psi}', U] = \mathcal{O}[\psi, \bar{\psi}, U] + \delta\mathcal{O}[\psi, \bar{\psi}, U] + \mathrm{O}(\alpha^2), \tag{1.137}$$

then

$$\langle \mathcal{O} \rangle = \int DU\, D\psi' D\bar{\psi}'\ \mathcal{O}[\psi', \bar{\psi}', U]\ \exp(-S[\psi', \bar{\psi}', U]) \tag{1.138}$$

$$= \int DU\ \underbrace{D\psi' D\bar{\psi}'}_{=D\psi D\bar{\psi}}\ (\mathcal{O}[\psi, \bar{\psi}, U] + \delta\mathcal{O}[\psi, \bar{\psi}, U]) \tag{1.139}$$
$$\exp(-S[\psi, \bar{\psi}, U] - \delta S[\psi, \bar{\psi}, U])$$
$$= \langle \mathcal{O} \rangle + \langle \delta\mathcal{O} - \mathcal{O}\delta S \rangle + \mathrm{O}(\alpha^2).$$

We conclude

$$\langle \delta\mathcal{O} \rangle = \langle \mathcal{O}\delta S \rangle. \tag{1.140}$$

For instance, for $\mathcal{O} = J_\nu(y)$, we have $\delta\mathcal{O} = -ia\partial_\nu \alpha(y) S^{(\nu)}(y)$,

$$S^{(\nu)}(y) = \tfrac{1}{2}\big(\bar{\psi}(y + a\hat{\nu})(1 + \gamma_\nu)U_\nu(y)^{-1}\psi(y) \tag{1.141}$$
$$+ \bar{\psi}(y)(1 - \gamma_\nu)U_\nu(y)\psi(y + a\nu)\big).$$

It can be thought of as a point-split discretization of the continuum scalar operator $\bar{\psi}\psi$. Now choosing $\alpha(x) = \epsilon\, e^{ikx}$, we finally obtain the relation [35]

$$a^4 \sum_{x,\mu} \hat{k}_\mu \Big\langle J_\nu(y) J_\mu(x) \Big\rangle e^{ik(x - y + \frac{a}{2}\hat{\mu} - \frac{a}{2}\hat{\nu})} = -a\hat{k}_\nu\ \langle S^{(\nu)}(y) \rangle. \tag{1.142}$$

This relation tells us that the longitudinal part of the polarization tensor is a pure contact term, and specifies the latter for the present regularization of QCD.

1.5.1.1 Chiral Ward Identities

The consequences of the global continuous symmetries of QCD can be elegantly worked out as Ward identities in the continuum Euclidean path integral (cf. [21], Sec. 4); the results are equivalent to those derived in the algebra of currents acting on the Hilbert space of the quantum states.

Perhaps the most important use of Ward identities in lattice QCD is to impose renormalization and/or improvement conditions on composite operators. The Ward identities can be derived in the continuum theory, and as long as on-shell correlation functions[10] are considered, they can be imposed in the lattice theory, thus providing renormalization conditions for certain local operators.

As an important example, consider QCD with a doublet of degenerate quark flavors, represented by a field $\psi(x) = (u(x), d(x))^\top$ (there may be more flavors in addition). The isovector axial current and pseudoscalar density read

$$A^a_\mu(x) = \bar\psi \gamma_\mu \gamma_5 \frac{\tau^a}{2} \psi(x), \qquad P^a(x) = \bar\psi(x)\gamma_5 \frac{\tau^a}{2}\psi(x), \tag{1.143}$$

where τ^a are the Pauli matrices acting in flavor space. For instance, the identity of the partially conserved axial current (PCAC) for QCD with a doublet of degenerate quark flavors

$$\partial_\mu A^a_\mu(x) = 2mP^a(x), \tag{1.144}$$

valid in all on-shell correlation functions, is used to define the quark mass m in Wilson lattice QCD, as well as to determine the finite renormalization of the axial current [21, 36, 37]. Equation (1.144) also shows that the renormalization of the quark mass m is known once the axial current and the pseudoscalar density are renormalized, see [38].

Similar to the axial current, the energy-momentum tensor requires a finite renormalization in order to satisfy the Ward identities of translation invariance. See e.g. [39] for the use of continuum Ward identities to renormalize the energy-momentum tensor in lattice field theory.

1.5.2 Chiral Symmetry on the Lattice

One drawback of the Wilson-Dirac operator (1.63) is that it does not preserve chiral symmetry: in the massless continuum theory, the action is invariant under the variation

$$\delta\psi(x) = \gamma_5\psi(x), \qquad \delta\bar\psi(x) = \bar\psi(x)\gamma_5 \tag{1.145}$$

[10] By 'on-shell correlation function', we mean that all operators involved are located at a physical distance from each other. By focusing on these, we avoid the discussion of contact terms, which in general are regularization-dependent.

of the fields. This property follows from the fact that, at vanishing quark mass, the Dirac operator anticommutes with γ_5. The Laplacian term in the Wilson-Dirac operator clearly spoils this property.

This is no coincidence, as the Nielsen-Ninomiya theorem [40–42] implies that chiral symmetry cannot be realized in this form on the lattice. We give here a particularly simple version of the theorem quoted in [43]. If $S = a^4 \sum_x \bar{\psi}(x) D \psi(x)$ is the free-fermion action, and $D e^{ipx} u = \tilde{D}(p) e^{ipx} u$ for u a constant spinor and $\tilde{D}(p)$ a 4×4 matrix, then the following four properties cannot be realized simultaneously:

i. $\tilde{D}(p)$ is analytic and periodic in p_μ with a period $2\pi/a$;
ii. $\tilde{D}(p) = i\gamma_\mu p_\mu + \mathrm{O}(ap^2)$ at small momenta;
iii. $\tilde{D}(p)$ is invertible at all momenta that are non-vanishing mod $2\pi/a$;
iv. D anticommutes with γ_5.

As an example in one dimension, consider the case $\tilde{D}(p) = \frac{1}{a}\gamma_1 \sin(p_1 a)$. It satisfies the one-dimensional analogue of the conditions (i), (ii) and (iv) above, but violates (iii). The presence of a second zero of $\tilde{D}(p)$ within the Brillouin zone at $p_1 = \pi/a$ is a consequence of the existence of a zero at the origin, and that by periodicity it must cross zero again with the same slope at $p_1 = 2\pi/a$ [44].

However one can show that a modified 'chiral' transformation [43],

$$\delta\psi(x) = \gamma_5(1 - \tfrac{1}{2}aD)\psi(x), \qquad \delta\bar{\psi}(x) = \bar{\psi}(x)(1 - \tfrac{1}{2}aD)\gamma_5, \tag{1.146}$$

is indeed a symmetry of the action if the following 'Ginsparg-Wilson' relation [45] is satisfied by the Dirac operator,

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D. \tag{1.147}$$

In term of the propagator, this relation reads

$$\langle \psi(x)\bar{\psi}(y)\rangle \,\gamma_5 + \gamma_5 \,\langle \psi(x)\bar{\psi}(y)\rangle = a^{-3}\gamma_5 \delta_{x,y}, \tag{1.148}$$

which shows that the ordinary chiral symmetry is realized on the mass shell. An explicit lattice Dirac operator that satisfies Eq. (1.147) is the 'overlap' operator [46]

$$D = \frac{1}{a}(1 - A(A^\dagger A)^{-1/2}), \qquad A = 1 - aD_{\mathrm{w}}. \tag{1.149}$$

It also satisfies the conditions (i), (ii) and (iii) above. The analyticity of $\tilde{D}(p)$ for real momenta implies the locality of D on a range of the order a.

The realization of a form of chiral symmetry on the lattice has important consequences. In particular, relation (1.147) implies that the 'topological charge' Q defined as

$$Q = a^4 \sum_x q(x), \qquad q(x) \equiv -\frac{a}{2}\mathrm{Tr}\{\gamma_5 D(x,x)\}, \tag{1.150}$$

is equal to the index $\mathrm{Tr}\{\gamma_5 P_0\}$ of the Dirac operator [47], where P_0 is the projector onto the subspace of its zero modes.

We refer the reader to Sec. 5 of [48] and to [49, 50] for accessible and more complete introductions to the subject of chiral symmetry and lattice fermions. In particular, lattice domain wall fermions [51–53] are a widely used formulation of chiral fermions.

1.5.3 Topology of the Gauge Field

Let D be a Dirac operator obeying the Ginsparg-Wilson relation (1.147). Then Q provides a definition of the topological charge obeying the index theorem. Its cumulants can be rewritten in such a way that, by power counting, no short-distance singularities appear. A universal (i.e. regularization-independent) definition of the cumulants of the topological charge can then be given [54]. In particular, the topological susceptibility χ_t can be written

$$\chi_t \equiv \frac{1}{V}\langle Q^2\rangle = m_1 \dots m_5 \int d^4x_1 \dots d^4x_4 \left\langle P_{31}(x_1)S_{12}(x_2)S_{23}(x_3)P_{54}(x_4)S_{45}(0)\right\rangle_{\mathrm{conn}} \tag{1.151}$$

with $P_{rs}(x) = \bar{\psi}_r(x)\gamma_5\psi_s(x)$, $S_{rs}(x) = \bar{\psi}_r(x)\psi_s(x)$ respectively the pseudoscalar and scalar density with respect to quark flavors r and s.

Direct calculations of the topological susceptibility based on the overlap Dirac operator (see Eq. (1.150)) have been performed in SU(3) gauge theory; as an example, we quote [55]

$$r_0^4\chi_t = 0.059 \pm 0.003. \tag{1.152}$$

(the reference length r_0 was defined at the end of Sect. 1.4.1). Other ways of estimating χ_t motivated by semi-classical arguments yield comparable results (see, for instance, [56, 57]).

1.5.4 Recursive Finite-Size Technique: Linking Vastly Different Length Scales

Consider a renormalized coupling $g^2(\mu)$. We saw an example defined via the force between two static quarks, Eq. (1.95), where $\mu = 1/r$. At standard simulation parameters, the smallest lattice spacing for which a linear system size of several fm can be accomodated is about 0.05 fm. However, in order to make contact with perturbation theory in a completely controlled way, it is desirable to compute the renormalized coupling at distances as small as 0.002 fm. It is clear that the large hierarchy between the distances typical of non-perturbative physics and the regime where perturbation theory becomes quantitatively accurate requires a special treatment.

Probably the only strategy that addresses this issue in a completely satisfactory way is the 'recursive finite-size technique' or 'step-scaling'. The general idea is that the inverse size of the system $1/L$ itself plays the role of the renormalization scale μ. This means that the confinement scale ~ 0.5 fm need not be accomodated in a calculation of the renormalized coupling at a large renormalization scale. A second key point is that attention must be paid to avoid zero modes of the quark and the gluon fields in the perturbative regime. The latter can cause serious problems with the stability and ergodicity of simulations. One set of boundary conditions that removes all zero modes is the set implemented in the Schrödinger functional [58]. There may well be other useful choices [59]. The Schrödinger functional has been used extensively to compute the running coupling [60–63] and has also proved very useful in formulating renormalization conditions for various local operators; see, for instance, [38, 64].

The idea of relating a quantity at high energy scales to the same quantity at small energy scales in multiple manageable steps in order to avoid a large hierarchy of scales is also used in other contexts. One of them is the calculation of the QCD equation of state at high temperatures [65, 66].

1.6 Importance Sampling Monte-Carlo Methods: Basic Ideas

In this section we describe the ideas behind the numerical methods that are used in practical calculations. First consider, for concreteness, the case of the pure gauge theory, Eq. (1.66). The first idea is to interpret

$$p[U] = \frac{1}{Z} D[U] \exp(-S_{\rm g}[U]) \tag{1.153}$$

as a normalized probability distribution on the space of all gauge fields. The second idea is to generate a representative sample of field 'configurations' $\{U_1, \ldots, U_{N_c}\}$, meaning that the fraction of the number of configurations belonging to a domain $\mathcal{D}$ of field space is given by

$$\int_{\mathcal{D}} D[U]\, p[U],$$

with an error of order $N_c^{-1/2}$. Third, the path-integral expectation value of observables can be estimated according to

$$\langle \mathcal{O}[U] \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} \mathcal{O}[U_i] + \mathrm{O}(N_c^{-1/2}). \tag{1.154}$$

One thus needs a method of generating the probability distribution (1.153). Usually, a complicated probability distribution must be generated iteratively; a Markov chain is a general method that achieves this. The chain starts from an initial configuration and then visits a sequence of configurations according to a given transition probability. General criteria exist that guarantee that the configurations visited after a sufficient number of iterations are indeed distributed according to the desired probability distribution [67]. For the state-of-the-art update rule, see, for instance, Sec. 2.3 of [67] and Appendix B of [68] and references therein.

The way fermions are treated in virtually all current lattice calculations is by integrating them out, yielding the determinant of the Dirac operator in the numerator of the path integral (see Eqs. (1.32–1.33)). The determinant can be treated as part of the probability distribution $p[U]$, provided it is positive on all gauge-field configurations. The γ_5 hermiticity of the Dirac operator implies that the determinant is real. For a doublet of mass-degenerate quarks, the square of the determinant is thus positive. For the other quark flavors, chiral symmetry, if realized on the lattice, guarantees that the determinant is positive; for non-chiral discretizations, the eigenvalues appear to all be positive with a substantial spectral gap, so that the property holds in practice.

The state-of-the-art algorithm to generate the distribution of gauge fields including the effect of the quarks is the hybrid Monte-Carlo algorithm [69], with its many important refinements of the last decade or so [67, 70, 71]. The generated sample of gauge-field configurations (an 'ensemble') is stored on disk, so that observables can be calculated on the configurations at a later stage. As an example, the two-point function of quark bilinears $\mathcal{O}(x) = \bar{u}(x)\Gamma u(x)$, $\mathcal{O}'(x) = \bar{u}(x)\Gamma' u(x)$ (with Γ, Γ' matrices acting on the spin degrees of freedom) are evaluated as

$$\langle \mathcal{O}(x)\ \mathcal{O}'(y) \rangle = \frac{1}{N} \sum_{i=1}^{N_c} \Big(-\mathrm{Tr}\big\{\Gamma D^{-1}([U_i]; x, y)\Gamma' D^{-1}([U_i]; y, x)\big\} \tag{1.155}$$
$$+\mathrm{Tr}\big\{\Gamma D^{-1}([U_i]; x, x)\}\ \mathrm{Tr}\{\Gamma' D^{-1}([U_i]; y, y)\big\}\Big) + \mathrm{O}(N_c^{-1/2}),$$

where D is the lattice Dirac operator in a given gauge field and the traces are taken with respect to color and spin indices.

1.7 Outlook

I hope that the introduction given here provides a useful overview of the most important concepts and methods in lattice QCD. It is a theoretically sound quantum field theoretic framework, and, with the steady increase in computing power and the improvement of algorithms, it makes predictions that have a high phenomenological impact [34, 72]. It has also had an influence on the way other problems are approached, for instance in the simulation of theories that may represent strongly coupled extensions of the Standard Model [73] and, more distantly, in theories describing a gas of strongly interacting fermions [74–76]. The following chapters give a far more detailed account of nuclear physics applications of lattice QCD.