The low-energy effective theory of QCD at small quark masses in a finite volume

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Abstract

At low energies the theory of quantum chromodynamics (QCD) can be described effectively in terms of the lightest particles of the theory, the pions. This approximation is valid for temperatures well below the mass difference of the pions to the next heavier particles.

We study the low-energy effective theory at very small quark masses in a finite volume V. The corresponding perturbative expansion in $1/\sqrt{V}$ is called ε *expansion*. At each order of this expansion a finite number of *low-energy constants* completely determine the effective theory. These low-energy constants are of great phenomenological importance.

In the leading order of the ε expansion, called ε *regime*, the theory becomes zero-dimensional and is therefore described by random matrix theory (RMT). The dimensionless quantities of RMT are mapped to dimensionful quantities of the low-energy effective theory using the leading-order low-energy constants Σ and F. In this way Σ and F can be obtained from lattice QCD simulations in the ε regime by a fit to RMT predictions.

For typical volumes of state-of-the-art lattice QCD simulations, finite-volume corrections to the RMT prediction cannot be neglected. These corrections can be calculated in higher orders of the ε expansion. We calculate the finite-volume corrections to Σ and F at next-to-next-to-leading order in the ε expansion. We also discuss non-universal modifications of the theory due to the finite volume. These results are then applied to lattice QCD simulations, and we extract Σ and F from eigenvalue correlation functions of the Dirac operator.

As a side result, we provide a proof of equivalence between the parametrization of the partially quenched low-energy effective theory without singlet particle and that of the super-Riemannian manifold used earlier in the literature. Furthermore, we calculate a special version of the massless sunset diagram at finite volume without constant mode which was not known before.

Apart from the universal regime of QCD, random matrix models can be used as schematic models that describe certain features of QCD such as the chiral phase transition. These schematic models are defined at fixed topological charge instead of fixed vacuum angle. Therefore special care has to be taken when different topological sectors are combined. We classify different schematic random matrix models in terms of the *topological domain* of Dirac eigenvalues, i.e., the part of eigenvalues that is affected by topology. If the topological domain extends beyond the microscopic eigenvalues, additional normalization factors need to be included to allow for finite topological fluctuations. This is important since the mass of the pseudoscalar singlet particle eta' is related to topological fluctuations, and the normalization factors thus solve the corresponding $\mathrm{U}(1)_A$ problem.

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Contents

Part I

Introduction

Chapter 1

Construction of QCD

In this first chapter we introduce the theory of quantum chromodynamics (QCD). QCD is a relativistic quantum field theory that describes the strong interactions that act on the constituents of hadrons such as protons or neutrons. These constituents (also called partons) are quarks and gluons. A quark is a massive fermion with spin $1/2$ and a gluon is a massless boson of spin 1 that mediates the force between quarks in the same sense as massless photons of spin 1 mediate the electromagnetic force between, e.g., electrons.

In the following sections we construct the theory based on a discussion of its symmetries. We begin with a review of the Lorentz group, the group that comprises all linear transformations of space and time that leave the speed of light invariant. We then discuss spinor representations of the Lorentz group and show how to construct a Lagrangian of massive spin $1/2$ particles that is invariant under Lorentz transformations. We finally add a local internal symmetry or gauge symmetry and by doing so introduce massless spin 1 particles that mediate an interaction between the spin $1/2$ particles. If we choose this gauge symmetry group to be $\mathrm{SU}(3)$ we recover QCD.

The following discussion is based on the textbooks of Weinberg [1, 2], Ryder [3], and Peskin and Schroeder [4].

1.1 The Lorentz group

Minkowski space

Let us consider a photon moving with the speed of light c. It shall propagate for a distance $d\vec{x}$ in an infinitesimal time dt, i.e.,

$$c^2 dt^2 - d\vec{x}^2 = 0\,. \tag{1.1}$$

If we consider a transformation of space and time coordinates (t, x) to (t', x') the statement that the speed of light c is the same in the new coordinate system is equivalent to the statement that also

$$c^2 dt'^2 - d\vec{x}'^2 = 0\,. \tag{1.2}$$

This property can now be expressed in a convenient mathematical representation by introducing vectors in a four-dimensional pseudo-Euclidean vector space with metric

$$(g_{\mu\nu}) = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}. \tag{1.3}$$

This vector space is called *Minkowski space*. The infinitesimal time dt and the corresponding vector $d\vec{x}$ are combined to a four vector $(dx^\mu) = (c\,dt, d\vec{x})$ and Eq. (1.1) can be written as

$$ds^2 = dx_\mu dx^\mu = g_{\mu\nu} dx^\mu dx^\nu = 0\,. \tag{1.4}$$

In this framework the transformations of coordinates that leave the speed of light invariant are just the isometries that leave the inner products of infinitesimal difference vectors invariant.

For convenience we adopt natural units in the remainder of this thesis and set $c = \hbar = 1$.

Poincaré group

The group of isometries of the Minkowski space is the *Poincaré group* consisting of all transformations of the affine form

$$x'^{\mu} = \Lambda^{\mu}{}_{\nu} x^{\nu} + T^{\mu}\,, \tag{1.5}$$

with

$$dx'^{\mu} dx'_{\mu} = dx^{\mu} dx_{\mu} \tag{1.6}$$

where dx^{μ} is an infinitesimal difference vector in Minkowski spacetime, $\Lambda^{\mu}{}_{\nu}$ is a real four-by-four matrix and T^{μ} is a four vector describing translations. Equation (1.6) implies that

$$dx'^{\mu} dx'_{\mu} = g_{\mu\nu} \Lambda^{\mu}{}_{\alpha} \Lambda^{\nu}{}_{\beta} dx^{\alpha} dx^{\beta} = g_{\alpha\beta} dx^{\alpha} dx^{\beta} \tag{1.7}$$

or

$$g_{\mu\nu} \Lambda^{\mu}{}_{\alpha} \Lambda^{\nu}{}_{\beta} = g_{\alpha\beta}\,. \tag{1.8}$$

This defining condition can be written in matrix form as

$$\Lambda^{T} g \Lambda = g \tag{1.9}$$

and thus

$$\det \Lambda = \pm 1\,. \tag{1.10}$$

The subgroup defined by $T^{\mu} = 0$, i.e., the subgroup of all linear transformations, is the *Lorentz group* and its elements are called *Lorentz transformations*.

Restricted Lorentz group

Let us first consider Lorentz transformations that are continuously connected to the identity transformation $\Lambda = \mathbb{1}$. Lorentz transformations with this property live in a subgroup called the *restricted Lorentz group*. Since a continuous transformation cannot change the sign of Eq. (1.10), restricted Lorentz transformations have $\det \Lambda = 1$.

A well-known subgroup of the restricted Lorentz group is the group of rotations with

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & & & \\ 0 & & R & \\ 0 & & & \end{pmatrix}, \tag{1.11}$$

where $R^{T} R = \mathbb{1}$, $\det R = 1$. Now by first rotating the spatial components appropriately we can restrict the remaining discussion to the two-dimensional subspace of vectors $(dx^{\mu}) = (dt, dx, 0, 0)$. The relevant Lorentz transformations are then of the form

$$\Lambda = \begin{pmatrix} \Lambda^{0}{}_{0} & \Lambda^{0}{}_{1} & 0 & 0 \\ \Lambda^{1}{}_{0} & \Lambda^{1}{}_{1} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{1.12}$$

Thus for infinitesimal transformations $\Lambda = \mathbb{1} + G$ the defining condition of Eq. (1.9) yields $G^T g + gG = 0$, and therefore

$$\begin{aligned} 0 &= \begin{pmatrix} G^0{}_0 & G^1{}_0 \\ G^0{}_1 & G^1{}_1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} G^0{}_0 & G^0{}_1 \\ G^1{}_0 & G^1{}_1 \end{pmatrix} \\ &= \begin{pmatrix} G^0{}_0 & -G^1{}_0 \\ G^0{}_1 & -G^1{}_1 \end{pmatrix} + \begin{pmatrix} G^0{}_0 & G^0{}_1 \\ -G^1{}_0 & -G^1{}_1 \end{pmatrix}, \end{aligned} \tag{1.13}$$

or $G^0{}_0 = G^1{}_1 = 0$ and $G^0{}_1 = G^1{}_0$. A finite transformation is thus given by

$$\Lambda = \exp \begin{pmatrix} 0 & s \\ s & 0 \end{pmatrix} = \begin{pmatrix} \cosh s & \sinh s \\ \sinh s & \cosh s \end{pmatrix} \tag{1.14}$$

with arbitrary $s \in \mathbb{R}$. Let us try to understand what the parameter s means. Consider an infinitesimal vector (dt, dx) that transforms to

$$\begin{pmatrix} dt' \\ dx' \end{pmatrix} = \Lambda \begin{pmatrix} dt \\ dx \end{pmatrix} = \begin{pmatrix} dt \cosh s + dx \sinh s \\ dt \sinh s + dx \cosh s \end{pmatrix}. \tag{1.15}$$

Now we define a transformed velocity

$$v' = \frac{dx'}{dt'} = \frac{v \cosh s + \sinh s}{v \sinh s + \cosh s} \tag{1.16}$$

with $v = dx/dt$. If we have $v = 0$ in the untransformed system we have $v' = \tanh s$ in the transformed system. Therefore transformations of this type describe a change of coordinates to a frame of reference that moves with a constant velocity of $\tanh s$ relative to the original frame of reference. These are the *boosts* in the special theory of relativity with *rapidity* s.

Let us define $\beta = \tanh s$. Since $\cosh^2 s - \sinh^2 s = 1$, we can show that

$$\cosh s = \frac{1}{\sqrt{1 - \tanh^2 s}} = \frac{1}{\sqrt{1 - \beta^2}} = \gamma\,. \tag{1.17}$$

Therefore we can express the transformation also by the matrix

$$\Lambda(\beta) = \begin{pmatrix} \gamma(\beta) & \gamma(\beta)\beta \\ \gamma(\beta)\beta & \gamma(\beta) \end{pmatrix}. \tag{1.18}$$

Discrete Lorentz transformations

Consider the vector $(x^\mu) = (t, 0)$ which is invariant under rotations and transforms to

$$(x'^\mu) = \begin{pmatrix} t \cosh s \\ t \sinh s \end{pmatrix} \tag{1.19}$$

under a boost with rapidity s. Since $\cosh s > 0$, we conclude that the sign of x^0 is invariant under boosts and thus under the complete restricted Lorentz group.

Therefore, in order to obtain all possible Lorentz transformations, the discrete Lorentz transformation

$$T = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \tag{1.20}$$

needs to be included in addition to restricted Lorentz transformations. This is the *time reversal* operator. Furthermore the *space inversion* or *parity* operator

$$P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \tag{1.21}$$

is also not a part of the restricted Lorentz group and needs to be included separately.

The quotient group of the Lorentz group and the restricted Lorentz group is the discrete group with elements

$$\mathbb{1}, P, T, PT\,. \tag{1.22}$$

In other words, the Lorentz group can be partitioned in four disconnected parts defined by

$$\det \Lambda = \pm 1\,, \qquad \mathrm{Sgn}\,\Lambda^0{}_0 = \pm 1\,. \tag{1.23}$$

We call transformations with $\det \Lambda = 1$ *proper* Lorentz transformations and transformations with $\mathrm{Sgn}\,\Lambda^0{}_0 = 1$ *orthochronous* Lorentz transformations.

Generators of the restricted Lorentz group

Recall that infinitesimal restricted Lorentz transformations $\Lambda = \mathbb{1} + G$ satisfy

$$G^T g + gG = 0\,. \tag{1.24}$$

We write G in block form

$$G = \begin{pmatrix} G_{00} & G_{01} \\ G_{10} & G_{11} \end{pmatrix}, \tag{1.25}$$

where G_{00} only acts on the temporal component, G_{11} only acts on the spatial components, and G_{01} and G_{10} mix spatial and temporal components. In this way Eq. (1.24) can be expressed as

$$\begin{aligned} 0 &= \begin{pmatrix} 1 & 0 \\ 0 & -\mathbb{1}_3 \end{pmatrix} \begin{pmatrix} G_{00} & G_{01} \\ G_{10} & G_{11} \end{pmatrix} + \begin{pmatrix} G_{00} & G_{10}^T \\ G_{01}^T & G_{11}^T \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -\mathbb{1}_3 \end{pmatrix} \\ &= \begin{pmatrix} 2G_{00} & G_{01} - G_{10}^T \\ G_{01}^T - G_{10} & -G_{11} - G_{11}^T \end{pmatrix}, \end{aligned} \tag{1.26}$$

where $\mathbb{1}_3$ is the three-dimensional identity matrix. Therefore the defining conditions for generators of the restricted Lorentz group are

$$G_{01} = G_{10}^T\,, \qquad G_{00} = 0\,, \qquad G_{11}^T = -G_{11}\,. \tag{1.27}$$

This implies the following generators of the restricted Lorentz group.

The boosts are generated by

$$K_i = \begin{pmatrix} 0 & e_i^T \\ e_i & 0 \end{pmatrix} \tag{1.28}$$

with $(e_i)_j = \delta_{ij}$ and $i = 1, 2, 3$. They satisfy

$$[K_i, K_j] = \begin{pmatrix} e_i^T e_j - e_j^T e_i & 0 \\ 0 & (e_i e_j^T - e_j e_i^T)_{ab} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & (\delta_{ia}\delta_{jb} - \delta_{ja}\delta_{ib})_{ab} \end{pmatrix}$$
$$= -\varepsilon_{ijk} J_k \tag{1.29}$$

with J_k defined below.

The rotations are generated by

$$J_i = \begin{pmatrix} 0 & 0 \\ 0 & L_i \end{pmatrix} \tag{1.30}$$

with $(L_i)_{jk} = -\varepsilon_{ijk}$ and $i = 1, 2, 3$. They satisfy

$$[J_i, J_j] = \begin{pmatrix} 0 & 0 \\ 0 & ([L_i, L_j])_{ab} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & (\varepsilon_{ial}\varepsilon_{jlb} - \varepsilon_{jal}\varepsilon_{ilb})_{ab} \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 0 \\ 0 & (\delta_{ib}\delta_{aj} - \delta_{jb}\delta_{ia})_{ab} \end{pmatrix} = \varepsilon_{ijk} J_k \,. \tag{1.31}$$

Hence boosts do not form a subgroup of the restricted Lorentz group, but rotations do. Note that

$$[K_i, J_j] = \begin{pmatrix} 0 & e_i^T \\ e_i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & L_j \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & L_j \end{pmatrix} \begin{pmatrix} 0 & e_i^T \\ e_i & 0 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & (e_i^T L_j)_a \\ (-L_j e_i)_a & 0 \end{pmatrix} = \begin{pmatrix} 0 & (\varepsilon_{ija})_a \\ (\varepsilon_{ija})_a & 0 \end{pmatrix} = \varepsilon_{ijk} K_k \,. \tag{1.32}$$

The Lie algebra of the restricted Lorentz group is therefore given by

$$[K_i, K_j] = -\varepsilon_{ijk} J_k \,, \qquad [J_i, J_j] = \varepsilon_{ijk} J_k \,, \qquad [K_i, J_j] = \varepsilon_{ijk} K_k \,. \tag{1.33}$$

A finite transformation is given by

$$\Lambda = \exp[\vec{s} \cdot \vec{K} + \vec{\varphi} \cdot \vec{J}] \,, \tag{1.34}$$

where $\vec{\varphi}$ contains the angles of a rotation and $\vec{s}$ contains the rapidities of a boost.

A convenient representation of the generators is given by

$$S_i^{\pm} = \frac{1}{2}(\pm K_i + i J_i) \tag{1.35}$$

with $(S_i^{\pm})^\dagger = S_i^{\pm}$ and $i = 1, 2, 3$. We find

$$[S_i^a, S_j^b] = (ab[K_i, K_j] + ib[J_i, K_j] + ia[K_i, J_j] - [J_i, J_j])/4$$
$$= i\varepsilon_{ijk}[i[(1 + ab)/4]J_k + [(a + b)/4]K_k] = \delta_{ab} i\varepsilon_{ijk} S_k^a \,. \tag{1.36}$$

Therefore the group algebra factorizes in a direct product of two $\mathrm{SU}(2)$ algebras (this is of course not true in terms of groups). We can express J_i and K_i in terms of $S_i^{\pm}$ as

$$i J_i = S_i^+ + S_i^- \,, \qquad K_i = S_i^+ - S_i^- \,. \tag{1.37}$$

Therefore Eq. (1.34) can be written as

$$\Lambda = \exp[s_i(S_i^+ - S_i^-) - i\varphi_i(S_i^+ + S_i^-)] = \exp[-i x_i S_i^+] \exp[-i x_i^* S_i^-]$$

with $x_i = \varphi_i + i s_i$.

Translations in space and time

The Casimir operators of S^+ and S^- can now be used to classify the representations of the restricted Lorentz group. These Casimir operators are, however, no invariants of representations of the complete Poincaré group since they do not commute with all translations of space and time. In this section we show that the spin of a massive particle is, nevertheless, a well-defined quantity.

We extend the Minkowski space by a fifth dimension so that we can express a general transformation of the Poincaré group, see Eq. (1.5), conveniently as

$$x' = \Gamma(\Lambda, T)x \tag{1.38}$$

with Lorentz transformation Λ, a four-dimensional translation vector (T_μ), $(x_\mu) = (x_0, x_1, x_2, x_3, 1)$, and

$$\Gamma(\Lambda, T) = \begin{pmatrix} \Lambda & (T_\mu) \\ 0 & 1 \end{pmatrix} \tag{1.39}$$

in block notation. The generators of translations in space and time P_μ are therefore given by the matrices

$$P_\mu = \begin{pmatrix} 0 & (\delta_{\mu\nu}) \\ 0 & 0 \end{pmatrix} \tag{1.40}$$

in block notation. A finite translation is given by

$$\Gamma(\mathbb{1}, T) = \exp\left[\sum_{\mu=0}^{3} T_\mu P_\mu\right]. \tag{1.41}$$

We can now determine the algebra of the complete Poincaré group,

$$\begin{aligned} &[P_\mu, P_\nu] = 0\,, && [P_0, J_i] = 0\,, && [P_0, K_i] = -P_i\,, \\ &[P_i, J_j] = \varepsilon_{ijk} P_k\,, && [P_i, K_j] = -\delta_{ij} P_0\,, && [K_i, K_j] = -\varepsilon_{ijk} J_k\,, \\ &[J_i, J_j] = \varepsilon_{ijk} J_k\,, && [K_i, J_j] = \varepsilon_{ijk} K_k\,. \end{aligned} \tag{1.42}$$

The Poincaré algebra has two Casimir operators. The first one is given by

$$C_1 = P_\mu P^\mu = P_0^2 - P_i^2\,. \tag{1.43}$$

We check explicitly that

$$[P_\mu, C_1] = 0\,, \tag{1.44}$$

$$\begin{aligned} [J_i, C_1] &= [J_i, P_0^2] - [J_i, P_j^2] = -[J_i, P_j]P_j - P_j[J_i, P_j] \\ &= 2\varepsilon_{ijk} P_k P_j = -2\varepsilon_{ijk} P_k P_j = 0\,, \end{aligned} \tag{1.45}$$

$$\begin{aligned} [K_i, C_1] &= [K_i, P_0]P_0 + P_0[K_i, P_0] - [K_i, P_j]P_j - P_j[K_i, P_j] \\ &= 2P_i P_0 - 2P_i P_0 = 0 \end{aligned} \tag{1.46}$$

for arbitrary i and μ. Let us pause at this point and ask what this means for a theory of a free particle with energy E and momentum $\vec{p}$. In quantum mechanics the generator of the translations in space, P_i, measures the ith component of the momentum, and the generator of the translations in time, P_0,

measures the energy. Therefore if we let C_1 act on a free particle state $|E,\vec{p}\rangle$ with energy E and momentum $\vec{p}$ we find

$$C_1\,|E,\vec{p}\rangle = (E^2-\vec{p}^2)\,|E,\vec{p}\rangle = m^2\,|E,\vec{p}\rangle\ , \tag{1.47}$$

where m is the mass of the particle. We can conclude that the mass of a particle is invariant under the Poincaré group and can be considered a well-defined property of a particle.

The second Casimir operator C_2 can be conveniently defined in terms of the *Pauli-Lubanski vector* W^μ with

$$W_0 = J_jP_j\,, \qquad W_i = P_0J_i - \varepsilon_{ijk}K_jP_k\,. \tag{1.48}$$

It is given by

$$C_2 = W^\mu W_\mu = (W_0)^2 - (W_i)^2\,. \tag{1.49}$$

In order to prove that C_2 is indeed a Casimir operator we first show that W_μ commutes with translations, i.e.,

$$[P_\mu, W_0] = [P_\mu, J_jP_j] = [P_\mu, J_j]P_j = (1-\delta_{\mu0})\varepsilon_{\mu jk}P_kP_j = 0\,, \tag{1.50}$$
$$[P_j, W_i] = P_0[P_j, J_i] - \varepsilon_{ilk}[P_j, K_l]P_k = P_0P_k(\varepsilon_{jik}+\varepsilon_{ijk}) = 0\,, \tag{1.51}$$
$$[P_0, W_i] = -\varepsilon_{ilk}[P_0, K_l]P_k = \varepsilon_{ilk}P_lP_k = 0\,. \tag{1.52}$$

Next we discuss the commutators of W_μ with boosts and calculate

$$\begin{aligned}[K_j, W_0] &= [K_j, J_iP_i] = [K_j, J_i]P_i + J_i[K_j, P_i] \\ &= \varepsilon_{jik}K_kP_i + J_jP_0 = W_j\end{aligned} \tag{1.53}$$

and

$$\begin{aligned}[K_j, W_i] &= [K_j, P_0J_i] - \varepsilon_{ilk}[K_j, K_lP_k] \\ &= P_0[K_j, J_i] + [K_j, P_0]J_i - \varepsilon_{ilk}K_l[K_j, P_k] - \varepsilon_{ilk}[K_j, K_l]P_k \\ &= \varepsilon_{jik}P_0K_k + P_jJ_i - \varepsilon_{ilj}K_lP_0 + \varepsilon_{ilk}\varepsilon_{jlr}J_rP_k \\ &= \varepsilon_{jik}[P_0, K_k] + P_jJ_i + (\delta_{ij}\delta_{kr} - \delta_{ir}\delta_{kj})J_rP_k \\ &= -\varepsilon_{jik}P_k + [P_j, J_i] + \delta_{ij}J_kP_k = -\varepsilon_{jik}P_k + \varepsilon_{jik}P_k + \delta_{ij}J_kP_k \\ &= \delta_{ij}W_0\,.\end{aligned} \tag{1.54}$$

We finally calculate the commutators of W_μ with rotations and find

$$\begin{aligned}[J_j, W_0] &= [J_j, J_iP_i] = [J_j, J_i]P_i + J_i[J_j, P_i] = \varepsilon_{jik}J_kP_i - \varepsilon_{ijk}J_iP_k \\ &= \varepsilon_{jik}J_kP_i - \varepsilon_{kji}J_kP_i = 0\,,\end{aligned} \tag{1.55}$$

$$\begin{aligned}[J_j, W_i] &= [J_j, P_0J_i] - \varepsilon_{ilk}[J_j, K_lP_k] \\ &= \varepsilon_{jik}P_0J_k - \varepsilon_{ilk}[J_j, K_l]P_k - \varepsilon_{ilk}K_l[J_j, P_k] \\ &= \varepsilon_{jik}P_0J_k + \varepsilon_{ilk}\varepsilon_{ljr}K_rP_k + \varepsilon_{ilk}\varepsilon_{kjr}K_lP_r \\ &= \varepsilon_{jik}P_0J_k + (\varepsilon_{ilk}\varepsilon_{ljr} + \varepsilon_{ljk}\varepsilon_{irl})K_rP_k \\ &= \varepsilon_{jik}P_0J_k + (\delta_{kj}\delta_{ir} - \delta_{jr}\delta_{ik})K_rP_k \\ &= \varepsilon_{jik}P_0J_k + \varepsilon_{lji}\varepsilon_{lkr}K_rP_k \\ &= \varepsilon_{jik}(P_0J_k + \varepsilon_{klr}K_rP_l) = \varepsilon_{jik}W_k\,.\end{aligned} \tag{1.56}$$

We observe that W_μ has the same commutation relations with the other parts of the algebra as P_μ, and therefore C_2 is also a Casimir operator.

For a massive particle we can calculate the action of C_2 in its rest frame, i.e.,

$$C_2 \left|m, 0\right\rangle = -m^2 J_i^2 \left|m, 0\right\rangle \ . \tag{1.57}$$

Therefore $|m, 0\rangle$ must also be an eigenstate of J_i^2 and the corresponding eigenvalues $s(s+1)$ correspond to the *spin* or intrinsic rotation of the point-like particle. In other words, massive particles can be classified according to their spin as defined by their behavior under the rotation group.

For a massless particle there is no rest frame and thus the situation is more complicated. It turns out that for massless particles the projection of the spin to the momentum,

$$\lambda = \vec{J} \cdot \hat{P} \,, \tag{1.58}$$

is a well-defined property and assumes the role of the spin of massive particles. This property is called *helicity*.

For a detailed discussion of the representation theory of the complete Poincaré group we refer to Refs. [1, 3, 5].

1.2 The Lagrangian of spin $1/2$ fields

In this section we construct a Lagrangian of massive spin $1/2$ particles that is invariant under orthochronous Lorentz transformations.

Spinor representations

Note that the sub-sectors $+$ and $-$ of the restricted Lorentz group both transform identically under rotations with

$$\Lambda = \exp[-i\varphi_i S_i^{\pm}] \,. \tag{1.59}$$

Since φ_i are the angles of a rotation in space and the S_i span the algebra of $\mathrm{SU}(2)$ the different representations of S correspond to different spin states. Possible representations of $S^+ \oplus S^-$ are

$$0 \oplus 0 \,, \qquad \frac{1}{2} \oplus 0 \,, \qquad 0 \oplus \frac{1}{2} \,, \qquad \frac{1}{2} \oplus \frac{1}{2} \,, \qquad \ldots \,. \tag{1.60}$$

As already outlined in the introductory paragraph of this chapter we aim to construct a theory of spin $1/2$ particles. To this end we first consider fields that transform in the $(1/2) \oplus 0$ representations of $S^+ \oplus S^-$. We set

$$S_i^+ = \frac{1}{2}\sigma_i \,, \qquad S_i^- = 0 \tag{1.61}$$

with Pauli matrices σ_i and consider two-dimensional spinors ψ^+ which transform as

$$\psi'^+ = \exp[(s_i - i\varphi_i)\sigma_i/2]\psi^+ \tag{1.62}$$

under the restricted Lorentz group.

Let us try to construct a Lagrangian with fields ψ^+. Each term in the Lagrangian has to satisfy the following properties: (i) Due to relativity each term has to be a Lorentz scalar. (ii) The Lagrangian has to be real. (iii) Each term has to have mass dimension of 4 (the action has to be dimensionless).

The mass term

One may be tempted to write down a simple mass term of the form

$$\mathcal{L}_{\text{mass}} = m(\psi^+)^\dagger \psi^+ \,. \tag{1.63}$$

Unfortunately, such a term does not satisfy (i) and is therefore not allowed in the Lagrangian. We discuss how a proper mass term can be constructed if we consider the representation $(1/2) \oplus (1/2)$ of $S^+ \oplus S^-$ below. This is the mass term relevant for QCD. It is, however, instructive to consider another way to construct an invariant mass term that involves only $(\psi^+)^T$ and ψ^+, the *Majorana* mass term $(\psi^+)^T \sigma_2 \psi^+$. First note that $\sigma_i^T = \sigma_i (-1)^{\delta_{i2}}$ with anticommutator $\{\sigma_i, \sigma_j\} = 2\delta_{ij}\,\mathbb{1}$, and therefore

$$\sigma_i^T \sigma_2 \sigma_i = (-1)^{\delta_{i2}} \sigma_i \sigma_2 \sigma_i = (-1)^{\delta_{i2}} (-\sigma_2 + 2\delta_{i2}\sigma_i) = -\sigma_2 \,, \tag{1.64}$$

where no sum over i is implied. Thus $\sigma_i^T \sigma_2 = -\sigma_2 \sigma_i$, and for infinitesimal transformations with coordinates $x_i \ll 1$ we find

$$\begin{aligned}(\psi^+)^T \sigma_2 \psi^+ \to & (\psi^+)^T (\mathbb{1} - i x_i \sigma_i^T/2) \sigma_2 (\mathbb{1} - i x_i \sigma_i/2) \psi^+ \\ & = (\psi^+)^T \sigma^2 \psi^+ - (i/2) x_i (\psi^+)^T (\sigma_i^T \sigma^2 + \sigma^2 \sigma_i) \psi^+ \\ & = (\psi^+)^T \sigma^2 \psi^+ \,. \end{aligned} \tag{1.65}$$

In order to make this term real we need to also include its complex conjugate. Since σ_2 is purely imaginary we write

$$\mathcal{L}_{\text{Majorana mass}} = im((\psi^+)^T \sigma^2 \psi^+ - (\psi^+)^\dagger \sigma^2 (\psi^+)^*) \,. \tag{1.66}$$

Note that for a two-component field $(\psi^+)^T = (a, b)$ we find $(\psi^+)^T \sigma^2 \psi^+ = i(ba - ab)$. Therefore if we consider a and b to be ordinary numbers, the Majorana mass term would vanish identically. However, in a quantized theory a and b anticommute since they correspond to fermions, and the Majorana mass term is nonzero.

The kinetic term

In this subsection we consider terms of the form

$$(\psi^+)^\dagger R \psi^+ \,, \tag{1.67}$$

where R contains objects that transform non-trivially under the restricted Lorentz group. We use the first non-trivial ansatz including Lorentz vectors

$$R = M_\mu v^\mu \,, \tag{1.68}$$

where v^μ is a contravariant vector, M_μ is a matrix in the two-dimensional spin space and the sum over μ is implied. Note that M_μ is not a Lorentz vector. Therefore under Lorentz transformations we find

$$R' = M_\mu v'^\mu = M_\mu \Lambda^\mu{}_\nu v^\nu \,. \tag{1.69}$$

In order to construct an invariant term we need

$$(\psi^+)^\dagger R \psi^+ = (\psi^+)^\dagger \exp[(s_i + i\varphi_i)\sigma_i/2] R' \exp[(s_i - i\varphi_i)\sigma_i/2] \psi^+ \,. \tag{1.70}$$

Let us first consider a infinitesimal boost in r direction, i.e., $\vec{\varphi} = 0$, $s_i = \delta_{ir} s$ with $s \ll 1$, and

$$v'^{\mu} = v^{\mu} + s K^{\mu}_{r\ \nu} v^{\nu} \,. \tag{1.71}$$

Now Eq. (1.70) gives

$$\begin{aligned} M_\mu v^\mu &\stackrel{!}{=} [\mathbb{1} + s\sigma_r/2] M_\mu v'^\mu [\mathbb{1} + s\sigma_r/2] \\ &= [\mathbb{1} + s\sigma_r/2] M_\mu [v^\mu + s K^{\mu}_{r\ \nu} v^\nu] [\mathbb{1} + s\sigma_r/2] \\ &= M_\mu v^\mu + s(M_\mu K^{\mu}_{r\ \nu} v^\nu + \sigma_r M_\mu v^\mu/2 + v^\mu M_\mu \sigma_r/2) \,. \end{aligned} \tag{1.72}$$

This has to hold for all v^μ so that we need

$$0 = M_\nu K^{\nu}_{r\ \mu} + \{\sigma_r, M_\mu\}/2 = M_0 \delta_{r\mu} + \delta_{\mu 0} M_r + \{\sigma_r, M_\mu\}/2 \,. \tag{1.73}$$

Now this means that

$$M_r = -\{\sigma_r, M_0\}/2 \,, \qquad M_0 \delta_{ri} = -\{\sigma_r, M_i\}/2 \,. \tag{1.74}$$

Next, we consider a rotation about the r axis, i.e., $\vec{s} = 0$, $\varphi_i = \delta_{ir}\varphi$ with $\varphi \ll 1$, and

$$v'^{\mu} = v^{\mu} + \varphi J^{\mu}_{r\ \nu} v^{\nu} \,. \tag{1.75}$$

Now Eq. (1.70) gives

$$\begin{aligned} M_\mu v^\mu &\stackrel{!}{=} M_\mu v'^\mu = [\mathbb{1} + i\varphi\sigma_r/2] M_\mu [v^\mu + \varphi J^{\mu}_{r\ \nu} v^\nu] [\mathbb{1} - i\varphi\sigma_r/2] \\ &= M_\mu v^\mu + \varphi(M_\nu J^{\nu}_{r\ \mu} v^\mu + i[\sigma_r/2, M_\mu] v^\mu) \,. \end{aligned} \tag{1.76}$$

This has to hold for all v^μ so that we need

$$0 = M_\nu J^{\nu}_{r\ \mu} + i[\sigma_r/2, M_\mu] = -\varepsilon_{\mu r i}(1 - \delta_{\mu 0}) M_i + i[\sigma_r/2, M_\mu] \,, \tag{1.77}$$

and thus

$$[\sigma_r, M_\mu] = i 2 \varepsilon_{r\mu i}(1 - \delta_{\mu 0}) M_i \,. \tag{1.78}$$

For $\mu = 0$ this means that $[\sigma_r, M_0] = 0$ for arbitrary r. This is only satisfied for

$$M_0 = c\,\mathbb{1} \ . \tag{1.79}$$

For $\mu = j$ with $j = 1, 2, 3$ this means that

$$[\sigma_r, M_j] = i 2 \varepsilon_{rji} M_i \,. \tag{1.80}$$

We know that this is satisfied by the Pauli matrices

$$M_j = \sigma_j \,. \tag{1.81}$$

We determine c from Eq. (1.74) and $\{\sigma_r, \sigma_i\} = 2\,\mathbb{1}\,\delta_{ri}$ and find $c = -1$. It is easy to check that if we would have considered the sector $-$ instead of $+$ the solution would be $c = 1$. We define $(M_\mu) = (\sigma^+_\mu) = (-\mathbb{1}, \sigma_1, \sigma_2, \sigma_3)$ and $(\sigma^\mu_+) = (-\mathbb{1}, -\sigma_1, -\sigma_2, -\sigma_3)$ so that

$$(\psi^+)^\dagger \sigma^+_\mu v^\mu \psi^+ = (\psi^+)^\dagger \sigma^+_\nu g^{\mu\nu} v_\mu \psi^+ = (\psi^+)^\dagger \sigma^\mu_+ v_\mu \psi^+ \tag{1.82}$$

is invariant under the restricted Lorentz group. While σ^μ_+ does not transform as a Lorentz vector, we can conclude that

$$(\psi^+)^\dagger \sigma^\mu_+ \psi^+ \tag{1.83}$$

does transform as a Lorentz vector. Note that the relevant matrices for the $-$ sector are $(\sigma^-_\mu) = (\mathbb{1}, \sigma_1, \sigma_2, \sigma_3)$ and $(\sigma^\mu_-) = (\mathbb{1}, -\sigma_1, -\sigma_2, -\sigma_3)$.

By substituting $v_\mu = \partial_\mu$ we can thus construct an invariant kinetic term that only involves $+$ fields.

Chirality

Let us consider all orthochronous Lorentz transformations, i.e, let us include the parity operator in addition to the restricted Lorentz transformations. The action of parity is defined by

$$\Lambda(s,\varphi)P = P^2\Lambda(s,\varphi)P = P\Lambda(-s,\varphi) \tag{1.84}$$

due to $P^2 = 1$, $PK_iP = -K_i$, and $PJ_iP = J_i$. Equation (1.84) has to hold for all representations, and therefore the action $D(\Lambda)$ of Lorentz transformations Λ on ψ_+ yields

$$\begin{aligned}(D(P)\psi'_+) &= D(P)D(\Lambda(s,\varphi))\psi_+ \\ &= D(\Lambda(-s,\varphi))(D(P)\psi_+)\end{aligned} \tag{1.85}$$

with $\psi'_+ = D(\Lambda(s,\varphi))\psi_+$. We observe that the field $D(P)\psi^+$ transforms according to the $1/2$ representation of S^-. Therefore if we want to construct a theory that is also invariant under parity, we need to include a spin $1/2$ representation of S^- as well. The twofold structure that emerges from the $(1/2)\oplus(1/2)$ representation of $S^+\oplus S^-$ is called *chirality*.

We consider a spinor

$$\psi = \begin{pmatrix}\psi_- \\ \psi_+\end{pmatrix}, \tag{1.86}$$

where $\psi_\pm$ transform according to the $1/2$ representation of $S^\pm$. The action of parity shall be given by

$$D(P)\psi = \begin{pmatrix}\psi_+ \\ \psi_-\end{pmatrix}, \tag{1.87}$$

in accordance with Eq. (1.85). We can write down a mass term

$$\mathcal{L}_{mass} = m\bar{\psi}\psi \tag{1.88}$$

with

$$\bar{\psi} = \begin{pmatrix}\psi_+^\dagger & \psi_-^\dagger\end{pmatrix} \tag{1.89}$$

that is invariant under orthochronous Lorentz transformations, see Eq. (1.38).

We already know that

$$(\psi^+)^\dagger\sigma_+^\mu\partial_\mu\psi^+ \tag{1.90}$$

and

$$(\psi^-)^\dagger\sigma_-^\mu\partial_\mu\psi^- \tag{1.91}$$

are both invariant under the restricted Lorentz group. Under parity we have $\psi^+ \leftrightarrow \psi^-$ and $\partial_i \to -\partial_i$ for $i = 1,2,3$ so that

$$\sigma_+^\mu\partial_\mu \leftrightarrow -\sigma_-^\mu\partial_\mu\,. \tag{1.92}$$

Therefore we can construct a real and Lorentz invariant kinetic term

$$\begin{aligned}\mathcal{L}_{kinetic} &= i[(\psi^-)^\dagger\sigma_-^\mu\partial_\mu\psi^- - (\psi^+)^\dagger\sigma_+^\mu\partial_\mu\psi^+] \\ &= \bar{\psi}i\gamma^\mu\partial_\mu\psi\end{aligned} \tag{1.93}$$

with

$$\gamma^\mu = \begin{pmatrix} 0 & -\sigma_+^\mu \\ \sigma_-^\mu & 0 \end{pmatrix}. \tag{1.94}$$

The factor i is needed since ∂_μ is anti-Hermitian, i.e.,

$$\begin{aligned} \langle\psi'|\,\partial_x\,|\psi\rangle &= \int dx\;\psi'^*(x)\partial_x\psi(x) = -\int dx(\partial_x\psi'^*(x))\psi(x) \\ &= -\,\langle\psi|\,\partial_\mu\,|\psi'\rangle^* \end{aligned} \tag{1.95}$$

for arbitrary fields ψ and ψ' with vanishing spacetime boundary contributions.

We write out the gamma matrices as

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \tag{1.96}$$

with $i = 1, 2, 3$ and note that

$$\bar\psi = \psi^\dagger\gamma^0\,. \tag{1.97}$$

The total Lagrangian of a noninteracting, massive spin $1/2$ particle of mass m is thus given by

$$\mathcal{L} = \bar\psi(i\gamma^\mu\partial_\mu - m)\psi\,. \tag{1.98}$$

It is apparent that this Lagrangian is also invariant under translations of space and time. The corresponding equation of motion is the *Dirac equation* of a free spin $1/2$ field

$$(i\gamma^\mu\partial_\mu - m)\psi = (i\not{\partial} - m)\psi = 0 \tag{1.99}$$

with *Dirac operator* $\not{\partial} = \gamma^\mu\partial_\mu$.

Note that we do not have to consider ψ_- and ψ_+ as independent fields. If we identify

$$\psi_- = i\sigma^2\psi_+^* \tag{1.100}$$

it follows from $\sigma_2\sigma_i^*\sigma_2 = -\sigma_i$, see Eq. (1.64), that under restricted Lorentz transformations

$$\begin{aligned} \psi'_- &= i\sigma^2[\exp[(s_i - i\varphi_i)\sigma_i/2]\psi_+]^* = \exp[(s_i + i\varphi_i)\sigma^2\sigma_i^*\sigma^2/2]i\sigma^2\psi_+^* \\ &= \exp[(-s_i - i\varphi_i)\sigma_i/2]\psi_-\,, \end{aligned} \tag{1.101}$$

in accordance with Eq. (1.85). The mass terms then become Majorana mass terms, and it can be shown that the fields ψ_+ become their own antiparticles. This, however, implies that they are not allowed to carry a nonzero charge and therefore excludes this scenario for the quarks of QCD.

Gamma matrices and Lorentz structure

Before we continue with the discussion of gauge symmetries a few notes about the algebra of gamma matrices are in order. The gamma matrices satisfy the *Clifford-algebra* relation

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}\,. \tag{1.102}$$

The parity operator can be written in terms of γ^0 as

$$D(P)\psi = \gamma^0\psi\,. \tag{1.103}$$

Furthermore, it is convenient to define

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} -\mathbb{1} & \\ & \mathbb{1} \end{pmatrix} \tag{1.104}$$

which allows to project on the $-$ and $+$ sectors by

$$P_\pm = \frac{\mathbb{1} \pm \gamma^5}{2}\,, \tag{1.105}$$

where $\mathbb{1}$ is the identity matrix in the respective space. The matrix γ^5 anticommutes with all other gamma matrices,

$$\{\gamma^5, \gamma^\mu\} = 0 \tag{1.106}$$

with $\mu = 0, 1, 2, 3$.

Note that the gamma matrices can be used to construct field bilinears that transform in a well-defined way under the orthochronous Lorentz group. Under restricted Lorentz transformations Λ we find

$$\begin{aligned} v^\mu = \bar\psi\gamma^\mu\psi &\quad\to\quad \Lambda^\mu{}_\nu v^\nu\,, \\ a^\mu = \bar\psi\gamma^\mu\gamma^5\psi &\quad\to\quad \Lambda^\mu{}_\nu a^\nu\,, \\ s = \bar\psi\psi &\quad\to\quad s\,, \\ p = \bar\psi\gamma^5\psi &\quad\to\quad p\,, \end{aligned} \tag{1.107}$$

see Eq. (1.83). The action of parity P on v, a, s and p is given by

$$\begin{aligned} v^\mu &\quad\to\quad -v^\mu + 2g^{0\mu}v^0\,, \\ a^\mu &\quad\to\quad a^\mu - 2g^{0\mu}a^0\,, \\ s &\quad\to\quad s\,, \\ p &\quad\to\quad -p\,. \end{aligned} \tag{1.108}$$

Therefore v^μ transforms as a vector, a^μ transforms as an axial vector, s transforms as a scalar and p transforms as a pseudoscalar.

1.3 Gauge symmetry

In the last section we have constructed a relativistically invariant Lagrangian of a massive spin $1/2$ field. Up to now the particles represented by the field do not interact with each other. In the following we add a local internal symmetry (or *gauge symmetry*) to the Lagrangian and show that such a modification introduces an interaction between the spin $1/2$ particles that is mediated by massless spin 1 particles.

Internal symmetries

Consider the Lagrangian of Eq. (1.98), i.e.,

$$\mathcal{L} = \bar\psi(i\gamma^\mu\partial_\mu - m)\psi \tag{1.98}$$

with fields ψ in spinor space. The operation of the matrices γ^μ on ψ is given by the matrix-vector multiplication in this space. The most trivial way to add an additional symmetry S_i is to choose a new symmetry group S that is a direct product of the Poincaré symmetry group S_p and S_i,

$$S = S_p \otimes S_i \,. \tag{1.109}$$

In such a modification we call S_i an *internal symmetry* of the Lagrangian. The fields ψ must transform in representations of the bigger symmetry group S and therefore live in a product space of the spinor space and the vector space of the internal symmetry.

Local symmetries

Let us choose S_i to consist of spacetime-dependent transformations of $\psi(x)$ with infinitesimal transformations $G(x)$ defined by

$$\psi(x) \to \psi(x) + iG(x)\psi(x) \,, \tag{1.110}$$

where the action of $G(x)$ on $\psi(x)$ is the matrix-vector multiplication in the internal symmetry space. We ignore terms of order G^2 throughout the remainder of this section. The mass term of Eq. (1.98),

$$\mathcal{L}_{\text{mass}} = m\bar{\psi}\psi \,, \tag{1.111}$$

is symmetric under Eq. (1.110) if

$$G(x)^\dagger = G(x) \,, \tag{1.112}$$

i.e., if $G(x)$ generates unitary transformations. The kinetic term

$$\mathcal{L}_{\text{kinetic}} = \bar{\psi}(i\gamma^\mu\partial_\mu)\psi \,, \tag{1.113}$$

however, transforms to

$$\mathcal{L}'_{\text{kinetic}} = \mathcal{L}_{\text{kinetic}} - \bar{\psi}(\partial_\mu G(x))\gamma^\mu\psi \tag{1.114}$$

under unitary transformations. An invariant term can only be constructed if we replace

$$\partial_\mu \to D_\mu \tag{1.115}$$

with

$$D_\mu \to [\mathbb{1} + iG(x)]D_\mu[\mathbb{1} - iG(x)^\dagger] \tag{1.116}$$

under Eq. (1.110), where $\mathbb{1}$ is the identity matrix. We call D_μ a *covariant derivative*. The covariant derivative has to generate a kinetic term for the spin $1/2$ fields, and therefore we use the ansatz

$$D_\mu = \partial_\mu + iA_\mu \,, \tag{1.117}$$

where A_μ has to transform under S_i in a way that satisfies Eq. (1.116). Note that A_μ can act non-trivially on the internal symmetry space. Since ∂_μ is an anti-Hermitian operator, we require $A = A^\dagger$ so that the Lagrangian is real. In accordance with Eq. (1.116) we request that the transformed A'_μ satisfies

$$\begin{aligned} \partial_\mu + iA'_\mu &= [\mathbb{1} + iG(x)](\partial_\mu + iA_\mu)[\mathbb{1} - iG(x)^\dagger] \\ &= \partial_\mu + iA_\mu - i(\partial_\mu G(x)) - [G(x), A_\mu] \,, \end{aligned} \tag{1.118}$$

where we used the Hermiticity of $G(x)$. Thus we can construct an invariant kinetic term if A_μ transforms as

$$A'_\mu = A_\mu - (\partial_\mu G(x)) + i[G(x), A_\mu]\,. \tag{1.119}$$

We conclude that we can construct a Lagrangian

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi - \bar{\psi}\gamma^\mu A_\mu \psi \tag{1.120}$$

that is invariant under the symmetry group S with internal symmetry S_i defined by the infinitesimal transformation

$$\begin{aligned} \psi(x) &\to \psi(x) + iG(x)\psi(x)\,, \\ A_\mu &\to A_\mu - (\partial_\mu G(x)) + i[G(x), A_\mu]\,. \end{aligned} \tag{1.121}$$

Note that the A_μ also transform in the fundamental representation of the restricted Lorentz symmetry group,

$$A_\mu \to \Lambda_\mu{}^\nu A_\nu \tag{1.122}$$

under Lorentz transformation Λ. The spin operator of the fundamental representation of the restricted Lorentz group is given by $S_j = iJ_j$ with $S^2 = s(s+1)$ and $s = 1$. Therefore we have introduced fields A_μ of spin 1 that interact with the spin $1/2$ fields due to the term

$$\mathcal{L}_{\text{interaction}} = -\bar{\psi}\gamma^\mu A_\mu \psi \tag{1.123}$$

in the Lagrangian. Since the Lagrangian has to be invariant under Eq. (1.121) the fields A_μ are not allowed to have a quadratic mass term and must therefore correspond to massless particles. They can, however, have a kinetic term that allows them to propagate in spacetime. To second order in $\partial_\mu A_\nu$ the only term that is invariant under S_i and S_p is proportional to

$$\mathcal{L}_{\text{YM}} \propto \text{Tr}[D_\mu, D_\nu][D^\mu, D^\nu]\,, \tag{1.124}$$

where the trace Tr acts on the internal symmetry space. This is the *Yang-Mills* term. The invariance under S_i is due to the covariance of

$$[D_\mu, D_\nu] \to [\mathbb{1} + iG(x)][D_\mu, D_\nu][\mathbb{1} - iG(x)^\dagger] \tag{1.125}$$

under Eq. (1.121). We define the *field-strength tensor*

$$F_{\mu\nu} = -i[D_\mu, D_\nu] = (\partial_\mu A_\nu) - (\partial_\nu A_\mu) + i[A_\mu, A_\nu] \tag{1.126}$$

and express the total Lagrangian conveniently as

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi + \text{Tr}\, F_{\mu\nu}F^{\mu\nu}\,. \tag{1.127}$$

Note that if the local symmetry group is not abelian, the term $[A_\mu, A_\nu]$ introduces a self-interaction between the massless spin 1 particles.

If we choose the first non-trivial unitary symmetry group $\text{U}(1)$, we recover the theory of electrodynamics coupled to a spin $1/2$ field. The photons are now given by the spin 1 fields A_μ. The equations of motion of the fields A_μ can readily be identified with Maxwell's equations of electrodynamics.

The Lagrangian of QCD

The internal symmetry group of QCD is given by $\mathrm{SU}(3)$. If we choose A_μ to live in the group algebra of $\mathrm{SU}(3)$, we can write

$$A_\mu = A_\mu^a \lambda_a \,, \tag{1.128}$$

where the matrices λ_a ($a = 1, \ldots, 8$) span the algebra of $\mathrm{SU}(3)$. The eight fields A_μ^a now correspond to eight independent gluons. The quarks live in the internal symmetry space of $\mathrm{SU}(3)$. Its fundamental representation is three-dimensional and therefore there are three different quark fields, or three different *colors* of quarks[1]. The bound states of quarks and anti-quarks, called *hadrons*, must transform as singlets of S_i and are therefore "color neutral". There are two types of hadrons: *mesons* and *baryons*. Mesons, such as the pion, are bosonic hadrons that consist of a quark and an anti-quark. Baryons, such as the proton or neutron, are fermionic hadrons that consist of three quarks.

Note that since $\mathrm{SU}(3)$ is non-abelian, gluons are self-interacting. This property can be shown to lead to the *asymptotic freedom* of QCD, i.e., for high energies the strength of the interaction becomes weaker [4].

We rescale the fields $A_\mu \to g A_\mu$ and change the prefactor of the kinetic term of gluons so that we can adjust the strength of the interaction of quarks and gluons explicitly. The Lagrangian of a quark coupled to the gluons then reads

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi + \mathrm{Tr}\, F_{\mu\nu} F^{\mu\nu} - g A_\mu^a \bar{\psi} \gamma^\mu \lambda_a \psi \tag{1.129}$$

with

$$F_{\mu\nu} = (\partial_\mu A_\nu) - (\partial_\nu A_\mu) + ig[A_\mu, A_\nu] \,. \tag{1.130}$$

It turns out that in nature there are more than one kind of quarks which differ by their mass and electromagnetic charge. One currently has experimental evidence for 6 different types of quarks, called different quark *flavors*, of which three have a fractional electromagnetic charge of $+2/3$ and three have a fractional electromagnetic charge of $-1/3$. Two quarks are very light and thus play an important role in the low-energy physics of QCD discussed in the remainder of this thesis. They are called *up* and *down* quarks (corresponding to their respective fractional electromagnetic charges $+2/3$ and $-1/3$). The next heavier quark is called *strange* quark and has a fractional electromagnetic charge of $-1/3$. Their masses are related approximately by

$$\frac{m_s}{m_d} \approx 20 \,, \qquad \frac{m_u}{m_d} \approx \frac{1}{2} \,, \tag{1.131}$$

where m_u, m_d, m_s are the masses of up, down and strange quark [6]. Note that these relations are only order-of-magnitude estimates. The total Lagrangian of QCD thus reads

$$\begin{aligned} \mathcal{L}_{\mathrm{QCD}} = &\sum_{f=1}^{6} \bar{\psi}_f (i\gamma^\mu \partial_\mu - m_f)\psi_f + \mathrm{Tr}\, F_{\mu\nu} F^{\mu\nu} \\ &- g \sum_{f=1}^{6} A_\mu^a \bar{\psi}_f \gamma^\mu \lambda_a \psi_f \,. \end{aligned} \tag{1.132}$$

We observe that, depending on the quark masses, the total Lagrangian has an additional symmetry in flavor space. This is exploited in the following chapter in order to construct an effective low-energy theory of QCD.

[1] The name quantum chromodynamics is due to this interpretation of the three different quark fields as different colors of quarks.

1.4 Euclidean field theory

In the remainder of this thesis we consider QCD and the low-energy effective theory of QCD at finite temperature in the *Euclidean formulation*. We replace the vector x_μ in Minkowski space by the Euclidean vector $\tilde{x}_\mu$ defined by

$$\tilde{x}_j = x_j\,, \qquad x_0 = -i\tilde{x}_0 \tag{1.133}$$

with $j = 1, 2, 3$. Therefore

$$\partial_0 = \frac{\partial}{\partial x_0} = i\frac{\partial}{\partial \tilde{x}_0} = i\tilde{\partial}_0\,, \qquad \int dx_0 = -i\int d\tilde{x}_0\,, \tag{1.134}$$

and the scalar product with Minkowski metric

$$x_\mu x^\mu = x_0^2 - x_j^2 = -(\tilde{x}_0)^2 - (\tilde{x}_j)^2 = -\tilde{x}_\mu\tilde{x}_\mu \tag{1.135}$$

is replaced by the scalar product with Euclidean metric. The same prescription for the time evolution operator $U(x_0)$ of a quantum system with Hamiltonian H yields

$$U(x_0) = \exp\left[-iHx_0\right] = \exp\left[-H\tilde{x}_0\right]. \tag{1.136}$$

This allows for the interpretation of

$$Z = \mathrm{Tr}\, U(x_0) \tag{1.137}$$

as the partition function at finite temperature $T = 1/\tilde{x}_0$. In Sec. 2.2 we shall express Eq. (1.137) for QCD in terms of a path integral with weight

$$\exp\left[i\int d^4x \mathcal{L}_{\mathrm{QCD}}\right]. \tag{1.138}$$

We have to replace

$$iS = i\int d^4x \mathcal{L}_{\mathrm{QCD}} = i\int d^4x \bar{\psi}(i\gamma^\mu D_\mu - m)\psi + iS_{\mathrm{YM}}\,, \tag{1.139}$$

where S_{YM} is the Yang-Mills action of the gluon fields, by

$$-\tilde{S} = \int d^4\tilde{x}\bar{\psi}(-\gamma^0(\tilde{\partial}_0 + gA_0) - i\gamma^j(\tilde{\partial}_j + igA_j) - m)\psi - \tilde{S}_{\mathrm{YM}}\,,$$

where $\tilde{S}_{\mathrm{YM}}$ is the Euclidean Yang-Mills action, and the sum over repeated indices $j = 1, 2, 3$ is implied. Note that we also need to replace

$$A_0 \to iA_0 \tag{1.140}$$

so that we can combine $\tilde{\partial}_0$ and A_0 in an anti-Hermitian operator $\tilde{D}_\mu$,

$$-\tilde{S} = -\int d^4\tilde{x}\bar{\psi}(\tilde{\gamma}_\mu\tilde{D}_\mu + m)\psi - \tilde{S}_{\mathrm{YM}} \tag{1.141}$$

with

$$(\tilde{\gamma}_\mu) = (\gamma^0, i\gamma^j)\,, \qquad (\tilde{D}_\mu) = (\tilde{\partial}_0 + igA_0, \tilde{\partial}_j + igA_j)\,. \tag{1.142}$$

The Euclidean gamma matrices satisfy

$$\{\tilde{\gamma}_\mu, \tilde{\gamma}_\nu\} = 2\delta_{\mu\nu}\,. \tag{1.143}$$

We define $\tilde{\gamma}^5$ in terms of Euclidean gamma matrices by

$$\tilde{\gamma}^5 = \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = -\tilde{\gamma}_0\tilde{\gamma}_1\tilde{\gamma}_2\tilde{\gamma}_3 \tag{1.144}$$

and the Euclidean Dirac operator by

$$\tilde{\not{D}} = \tilde{\gamma}_\mu \tilde{D}_\mu\,. \tag{1.145}$$

Note that the Euclidean gamma matrices are Hermitian, and therefore the Euclidean Dirac operator is anti-Hermitian. The Euclidean action can then be written as

$$\tilde{S} = \int d^4\tilde{x}\; \bar{\psi}(\tilde{\not{D}} + m)\psi + \tilde{S}_{\mathrm{YM}}\,. \tag{1.146}$$

As for $\tilde{S}_{\mathrm{YM}}$ we have to replace

$$\begin{aligned} F_{00} &\to -F_{00}\,, \qquad F_{0j} \to iF_{0j}\,, \\ F_{j0} &\to iF_{j0}\,, \qquad F_{jk} \to F_{jk}\,, \end{aligned} \tag{1.147}$$

where $j, k = 1, 2, 3$, according to Eq. (1.140).

In the remainder of this thesis we consider only Euclidean quantities and therefore drop the distinction between Minkowski and Euclidean spacetime.

Chapter 2

Construction of the low-energy effective theory of QCD

In this chapter we introduce the low-energy effective theory of QCD. The theory is formulated in terms of pions, the lightest hadrons of QCD. In fact, the pions are approximately four times lighter than the next heavier hadrons, the kaons (see Fig. 2.1 and Ref. [6]). Their small mass is due to the fact that they are the pseudo Nambu-Goldstone (NG) bosons of the spontaneously broken chiral symmetry, i.e., the symmetry of QCD with massless quarks under rotations in flavor space.

In the following chapter we explain the mechanism of spontaneous symmetry breaking and discuss the relevant flavor symmetries of QCD. We then derive the effective Lagrangian and describe a systematic perturbative expansion of the theory.

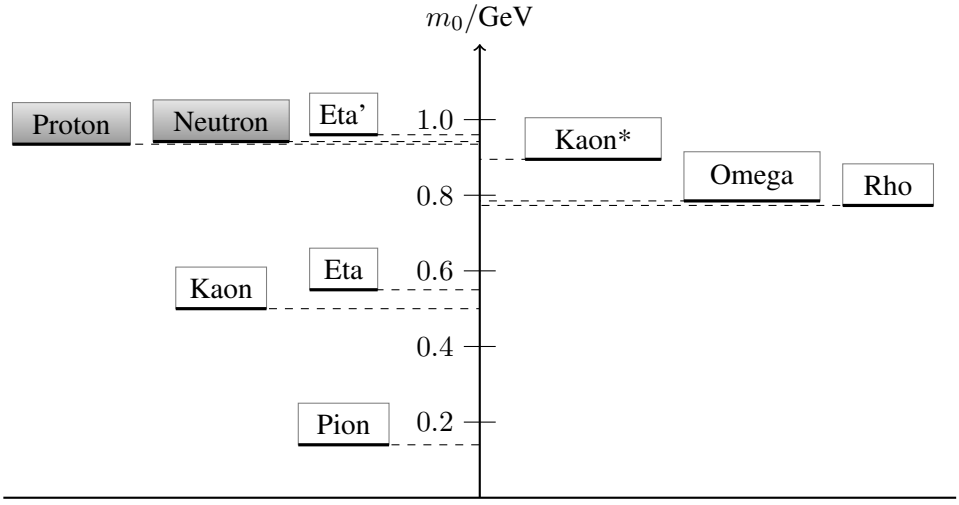


Figure 2.1: Rest mass m_0 of lightest mesons and baryons (shaded). Pseudoscalar (vector) mesons are shown left (right).

2.1 Spontaneous symmetry breaking

Consider the Lagrangian of N real scalar fields $\varphi_1, \ldots, \varphi_N$,

$$\mathcal{L} = (\partial_\mu \varphi_a)(\partial^\mu \varphi_a) - V(\varphi)\,, \tag{2.1}$$

where the sum over $a = 1, \ldots, N$ is implied. We define the *vacuum* configuration $\tilde{\varphi}$ by the minimum of the potential $V(\varphi)$, i.e.,

$$\frac{\partial V(\tilde{\varphi})}{\partial \varphi_a} = 0\,. \tag{2.2}$$

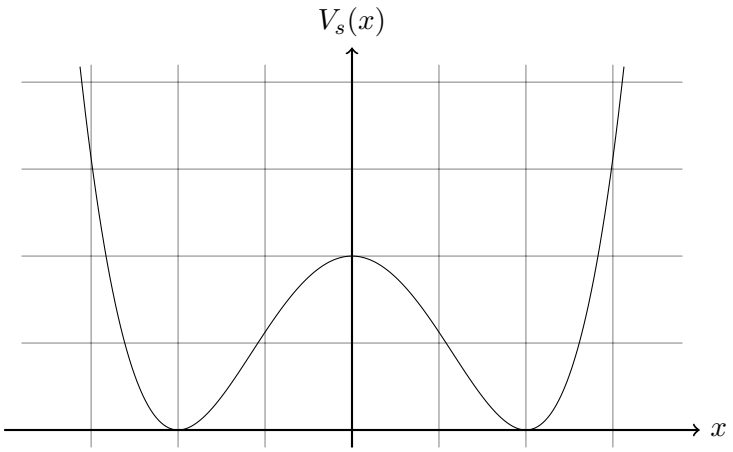


Figure 2.2: Mexican hat potential $V(\varphi) = V_s(|\varphi|)$ with $V_s(x) = (x^2 - 1)^2$.

For low energies the fields stay close to $\tilde{\varphi}$ and we can expand the fields as

$$\varphi_a = \tilde{\varphi}_a + \delta\varphi_a \,. \tag{2.3}$$

By ignoring higher terms in $\delta\varphi$ we obtain a low-energy effective theory. The potential $V(\varphi)$ is approximated by

$$V(\varphi) = V(\tilde{\varphi}) + \frac{1}{2}\delta\varphi_a \delta\varphi_b m_{ab}^2 + \mathcal{O}(\delta\varphi^3) \tag{2.4}$$

with

$$m_{ab}^2 = \frac{\partial^2 V(\tilde{\varphi})}{\partial\varphi_a \partial\varphi_b} \,. \tag{2.5}$$

If we keep terms to order $\delta\varphi^2$ and diagonalize the matrix m_{ab}^2, we observe that the eigenvectors of m_{ab}^2 correspond to low-energy excitations with masses given by the corresponding eigenvalues.

Now consider an infinitesimal linear transformation of φ_a defined by

$$T : \varphi_a \to \varphi_a + \varepsilon G_{ab}\varphi_b \tag{2.6}$$

with $N \times N$ matrix G and $\varepsilon \ll 1$. Let T be a symmetry of the Lagrangian with

$$G_{ab} = -G_{ba} \,, \tag{2.7}$$

so that the kinetic term is invariant under T, and

$$0 = \frac{\partial V(\varphi)}{\partial\varphi_a} G_{ab}\varphi_b \,, \tag{2.8}$$

so that the potential is invariant under T. In Fig. 2.2 we show a common example of a potential $V(\varphi)$ with a rotational symmetry for constant $|\varphi|^2 = \sum_a \varphi_a^2$.

We differentiate Eq. (2.8) with respect to φ_c and find

$$0 = \frac{\partial^2 V(\varphi)}{\partial\varphi_a \partial\varphi_c} G_{ab}\varphi_b + \frac{\partial V(\varphi)}{\partial\varphi_a} G_{ac} \,. \tag{2.9}$$

This can be evaluated at $\varphi = \tilde{\varphi}$ and yields

$$0 = m_{ac}^2 G_{ab} \tilde{\varphi}_b \,. \tag{2.10}$$

If the transformation T leaves $\tilde{\varphi}$ unchanged, i.e.,

$$G_{ab} \tilde{\varphi}_b = 0 \,, \tag{2.11}$$

this statement holds trivially.

If, however, $\tilde{\varphi}$ is not symmetric under T, the matrix m_{ac}^2 has a zero eigenvalue with eigenvector $(G_{ab}\tilde{\varphi}_b)$. This eigenvector corresponds to a massless particle called *Nambu-Goldstone particle*. Such a symmetry of the Lagrangian that does not leave the vacuum invariant is called a *spontaneously broken symmetry*. We conclude that for a classical field theory with Lagrangian $\mathcal{L}$ the following theorem holds.

Goldstone's theorem *A spontaneously broken symmetry leads to a massless particle.*

It can be shown that Goldstone's theorem remains valid after the theory is quantized [4].

2.2 Chiral symmetry of supersymmetric QCD

In this section we discuss the chiral symmetry of QCD, i.e., the symmetry of QCD in flavor space in the limit of massless quarks. This symmetry is spontaneously broken in QCD, and thus Goldstone's theorem applies. Physical quarks, however, have a nonzero mass so that chiral symmetry is only an approximate symmetry of nature. Therefore we do not find exactly massless particles in the hadronic mass spectrum but particles with a very small mass. These *pseudo-Nambu-Goldstone particles* of chiral symmetry breaking with massless up and down quarks are the pions.

One can also consider chiral symmetry breaking with massless up, down and strange quarks, where pions, kaons and the eta meson are the corresponding pseudo-Nambu-Goldstone bosons. This approximation, however, holds to a much smaller extent.

Supersymmetric extension of QCD

In the following we consider the partition function of QCD with $N_f + N_v$ quarks and N_v *bosonic quarks*. A bosonic quark field enters the Lagrangian in the same way a fermionic quark field does, but it is quantized as a boson. In nuclear physics and condensed matter physics these additional bosonic degrees of freedom are known from the supersymmetry method or Efetov method for quenched disorder [7]. In the context of QCD this idea was first used by Morel [8]. The additional N_v quarks are useful for the extraction of information about the eigenvalues of the *Dirac operator* $\not{D}$, see Sec. 3.4. For equal quark masses this extension of QCD leads to a supersymmetry that mixes fermionic and bosonic quarks.

The following discussion partly summarizes and clarifies the results of Bernard and Golterman [9], Osborn et. al. [10], Damgaard et. al. [11], Dalmazi and Verbaarschot [12], and Sharpe and Shoresh [13].

We separate the $N_f + N_v$ quarks in N_f *sea quarks* and N_v *valence quarks* and define the Euclidean partition function, see Sec. 1.4,

$$Z = \int d[A]\, e^{-S_{\text{YM}}} \left[\prod_{f=1}^{N_f} \det(\not{D} + m_f) \right] \left[\prod_{i=1}^{N_v} \frac{\det(\not{D} + m_{vi})}{\det(\not{D} + m'_{vi})} \right] , \tag{2.12}$$

where the integral is over all gluon fields A, m_1, ..., m_{N_f} are the masses of the sea quarks, m_{v1}, ..., m_{vN_v} are the masses of the fermionic valence quarks, and m'_{v1}, ..., m'_{vN_v} are the masses of the bosonic valence quarks. By setting the mass m_{vi} of a valence quark equal to the mass m'_{vi} of the corresponding bosonic quark, the ratio of determinants of this pair cancels and the flavor i is quenched.

Next we rewrite the determinants in terms of fermionic quark fields ψ and bosonic quark fields φ using

$$\det(\not{D} + m) = \int d[\bar{\psi}\psi]\, e^{-\int d^4x\, \bar{\psi}(\not{D}+m)\psi} \tag{2.13}$$

and

$$\frac{1}{\det(\not{D} + m)} = \int d[\bar{\varphi}\varphi]\, e^{-\int d^4x\, \bar{\varphi}(\not{D}+m)\varphi}\,, \tag{2.14}$$

where ψ and $\bar{\psi}$ are independent Grassmann variables with Berezin integral $\int d[\bar{\psi}\psi]$, and φ and $\bar{\varphi}$ are commuting complex fields related by complex conjugation,

$$\bar{\varphi} = \varphi^\dagger\,. \tag{2.15}$$

Note that the right-hand side of Eq. (2.14) only converges if all eigenvalues of $\not{D} + m$ have a positive real part. Since $\not{D}$ is anti-Hermitian this condition is satisfied as long as $\mathrm{Re}\, m > 0$. Thus

$$Z = \int d[A]\, d[\bar{\Psi}\Psi]\, e^{-S_{\mathrm{YM}} - \int d^4x\, \bar{\Psi}(\not{D}+M)\Psi} \tag{2.16}$$

with mass matrix $M = \mathrm{diag}(m_1, \ldots, m_{N_f}, m_{v1}, \ldots, m_{vN_v}, m'_{v1}, \ldots, m'_{vN_v})$ and fields

$$\bar{\Psi} = \begin{pmatrix} \bar{\psi} & \bar{\varphi} \end{pmatrix}, \qquad \Psi = \begin{pmatrix} \psi \\ \varphi \end{pmatrix}. \tag{2.17}$$

Transformation of the fields

Consider an infinitesimal transformation of the fields Ψ, $\bar{\Psi}$ defined by

$$\Psi \to (\mathbb{1} + iG_f \otimes G_s)\Psi\,, \qquad \bar{\Psi} \to \bar{\Psi}(\mathbb{1} - i\bar{G}_f \otimes \bar{G}_s)\,, \tag{2.18}$$

where G_f and $\bar{G}_f$ are $(N_f + N_v, N_v)$ supermatrices [7] in flavor space, and G_s and $\bar{G}_s$ are matrices in color and spinor space. Such a transformation leaves the Lagrangian of the massless theory

$$\mathcal{L}_0 = \bar{\Psi}(\mathbb{1} \otimes \not{D})\Psi \tag{2.19}$$

invariant if

$$\bar{G}_f \otimes (\bar{G}_s \not{D}) = G_f \otimes (\not{D} G_s)\,. \tag{2.20}$$

Therefore a symmetry of the Lagrangian has to satisfy $\bar{G}_f = G_f$ and $\bar{G}_s \not{D} = \not{D} G_s$. This holds for any linear combination of

$$G_s = \bar{G}_s = \mathbb{1} \tag{2.21}$$

and

$$G_s = -\bar{G}_s = \gamma^5 \,. \tag{2.22}$$

The former transformations are called *vector* symmetries, the latter transformations are called *axial* symmetries. We write G_f in fermion-boson block notation [7]

$$\bar{G}_f = G_f = \begin{pmatrix} G_{ff} & G_{fb} \\ G_{bf} & G_{bb} \end{pmatrix}, \tag{2.23}$$

so that the transformation of Eq. (2.18) in flavor space can be written as

$$\begin{pmatrix} \psi \\ \varphi \end{pmatrix} \to \begin{pmatrix} \psi \\ \varphi \end{pmatrix} + i \begin{pmatrix} G_{ff}\psi + G_{fb}\varphi \\ G_{bf}\psi + G_{bb}\varphi \end{pmatrix} \tag{2.24}$$

and

$$\begin{pmatrix} \bar{\psi} & \bar{\varphi} \end{pmatrix} \to \begin{pmatrix} \bar{\psi} & \bar{\varphi} \end{pmatrix} - i \begin{pmatrix} \bar{\psi}G_{ff} + \bar{\varphi}G_{bf} & \bar{\psi}G_{fb} + \bar{\varphi}G_{bb} \end{pmatrix}. \tag{2.25}$$

We conclude from Eqs. (2.15), (2.24), and (2.25) that only transformations with

$$G_{bb} = G_{bb}^\dagger \tag{2.26}$$

are allowed.

Let us consider the eigenmodes ψ_n of $\not{D}$ for fixed gauge fields A, where

$$\not{D}\psi_n = i\lambda_n \psi_n \,, \qquad \psi_n^\dagger \not{D} = -i\lambda_n \psi_n^\dagger \tag{2.27}$$

and n is allowed to be continuous. The fields $\psi_n(x)$ are complex functions and vectors in spinor and color space. We find

$$\not{D}(\gamma^5\psi_n) = -\gamma^5 \not{D}\psi_n = -i\lambda_n(\gamma^5\psi_n) \,, \tag{2.28}$$

and thus for each eigenmode ψ_n with eigenvalue $i\lambda_n$ there is an eigenmode $\gamma^5\psi_n$ with eigenvalue $-i\lambda_n$. We define

$$\psi_n^\pm = \psi_n \pm \gamma^5 \psi_n \tag{2.29}$$

with

$$\gamma^5 \psi_n^\pm = \pm \psi_n^\pm \tag{2.30}$$

since $(\gamma^5)^2 = \mathbb{1}$, i.e., the modes $\psi_n^\pm$ have definite *chirality* ± 1. The modes $\psi_n^\pm$ allow for the construction of a complete set of modes with definite chirality. Since ψ_n and $\gamma^5\psi_n$ are linearly independent, both vectors $\psi_n^\pm$ are nonzero. If ψ_n is a zeromode, i.e., an eigenmode with eigenvalue $\lambda_n = 0$, then $\psi_n^\pm$ are also eigenmodes of $\not{D}$ with

$$\not{D}\psi_n^\pm = 0 \,. \tag{2.31}$$

In the case of $\lambda_n = 0$ we can find $\psi_n = \pm\gamma^5\psi_n$ so that one of the modes in Eq. (2.29) vanishes identically, and thus the *topological charge* of the gauge field configuration $\nu = n_+ - n_-$ is nonzero in general, where n_+ (n_-) is the number of zeromodes with positive (negative) chirality.

Next we expand the gauge fields Ψ and $\bar{\Psi}$ in the path integral in terms of ψ_n as [14, 15]

$$\Psi(x) = \sum_n a_n \psi_n(x)\,, \qquad \bar{\Psi}(x) = \sum_n \bar{a}_n \psi_n^\dagger(x)\,, \tag{2.32}$$

where a_n and $\bar{a}_n$ are now supervectors [7] in flavor space. Note that for bosonic fields the ith components $\bar{\Psi}_i(x) = \Psi_i(x)^\dagger$, and therefore $\bar{a}_n^i = (a_n^i)^\dagger$ for $N_f + N_v < i \leq N_f + 2N_v$.

We can thus express the integration measure as

$$d[\bar{\Psi}\Psi] = \prod_{n,i} d\bar{a}_n^i da_n^i\,, \tag{2.33}$$

where for fermionic indices i the integral is over independent Grassmann variables $\bar{a}_n^i$ and a_n^i, and for bosonic indices i the integral is over the real and imaginary part of a_n^i. We invert the relation (2.32) as

$$a_n^i = \int d^4x \psi_n(x)^\dagger \Psi_i(x)\,, \qquad \bar{a}_n^i = \int d^4x \bar{\Psi}_i(x)\psi_n(x) \tag{2.34}$$

and express the transformation of Eq. (2.18) as

$$\begin{aligned} a_n^i \to a_n'^i &= a_n^i + iG_f^{ij} \int d^4x \psi_n(x)^\dagger G_s \Psi_j(x) \\ &= \left(\delta_{ij}\delta_{nm} + iG_f^{ij} \int d^4x \psi_n(x)^\dagger G_s \psi_m(x)\right) a_m^j\,, \end{aligned} \tag{2.35}$$

$$\begin{aligned} \bar{a}_n^i \to \bar{a}_n'^i &= \bar{a}_n^i - i \int d^4x \bar{\Psi}_j(x) \bar{G}_s \psi_n(x) \bar{G}_f^{ji} \\ &= \bar{a}_m^j \left(\delta_{ij}\delta_{nm} - i\bar{G}_f^{ji} \int d^4x \psi_m^\dagger(x) \bar{G}_s \psi_n(x)\right). \end{aligned} \tag{2.36}$$

The transformation of the integration measure is thus given by

$$\begin{aligned} d[\bar{\Psi}\Psi] \to d[\bar{\Psi}\Psi] &\left(1 + i(-1)^{\varepsilon_i} G_f^{ii} \int d^4x \psi_n(x)^\dagger G_s \psi_n(x)\right) \\ &\times \left(1 - i(-1)^{\varepsilon_i} \bar{G}_f^{ii} \int d^4x \psi_n(x)^\dagger \bar{G}_s \psi_n(x)\right) \end{aligned} \tag{2.37}$$

for infinitesimal G, where

$$\varepsilon_a = \begin{cases} 0 & \text{if } a \text{ corresponds to a bosonic index}\,, \\ 1 & \text{if } a \text{ corresponds to a fermionic index}\,. \end{cases} \tag{2.38}$$

Note that there are no anomalous contributions from Efetov-Wegner terms [16, 17] if we introduce an infinitesimal mass term, so that the integrand vanishes at the boundary of the bosonic field integrals.

We can express Eq. (2.37) as

$$d[\bar{\Psi}\Psi] \to d[\bar{\Psi}\Psi] \left(1 + i\,\mathrm{Str}(G_f)\hat{\mathrm{Tr}}(G_s) - i\,\mathrm{Str}(\bar{G}_f)\hat{\mathrm{Tr}}(\bar{G}_s)\right) \tag{2.39}$$

with

$$\hat{\mathrm{Tr}}(A) = \int d^4x \psi_n(x)^\dagger A \psi_n(x)\,. \tag{2.40}$$

A symmetry transformation of the Lagrangian satisfies $G_f = \bar{G}_f$, so that

$$d[\bar{\Psi}\Psi] \to d[\bar{\Psi}\Psi] \left(1 + i \operatorname{Str}(G_f)\hat{\operatorname{Tr}}(G_s - \bar{G}_s)\right). \tag{2.41}$$

A vector symmetry satisfies $G_s = \bar{G}_s$ and therefore leaves the integral measure invariant. Such a symmetry of the Lagrangian that leaves the measure invariant is called a *non-anomalous* symmetry. An axial symmetry satisfies $G_s = -\bar{G}_s = \gamma^5$, and therefore

$$d[\bar{\Psi}\Psi] \to d[\bar{\Psi}\Psi] \left(1 + 2i \operatorname{Str}(G_f)\hat{\operatorname{Tr}}(\gamma^5)\right). \tag{2.42}$$

A symmetry of the Lagrangian that does not leave the measure invariant is called an *anomalous* symmetry. Let us calculate $\hat{\operatorname{Tr}}\gamma^5$ explicitly. We separate the zeromodes and write

$$\begin{aligned}
\hat{\operatorname{Tr}}(\gamma^5) &= \sum_{\lambda_n>0} \int d^4x \left[\psi_n(x)^\dagger \gamma^5 \psi_n(x) + (\gamma^5\psi_n(x))^\dagger \gamma^5 (\gamma^5 \psi_n(x))\right] \\
&\quad + \sum_{\lambda_n=0} \int d^4x \psi_n(x)^\dagger \gamma^5 \psi_n(x) \\
&= \frac{1}{2} \sum_{\lambda_n>0} \int d^4x \left[\psi_n^+(x)^\dagger \gamma^5 \psi_n^+(x) + \psi_n^-(x)^\dagger \gamma^5 \psi_n^-(x)\right] \\
&\quad + \sum_{\lambda_n=0} \int d^4x \psi_n(x)^\dagger \gamma^5 \psi_n(x)\,.
\end{aligned} \tag{2.43}$$

Now the states $\psi_n^\pm$ as well as the zeromodes are eigenstates of γ^5. Therefore

$$\hat{\operatorname{Tr}}(\gamma^5) = \sum_{\lambda_n=0} \int d^4x \psi_n(x)^\dagger \gamma^5 \psi_n(x) = n_+ - n_- = \nu \tag{2.44}$$

and the measure transforms as

$$d[\bar{\Psi}\Psi] \to d[\bar{\Psi}\Psi](1 + 2i \operatorname{Str}(G_f)\nu) \tag{2.45}$$

under Eq. (2.18). Since the topological charge ν is nonzero in general, an axial flavor symmetry of the supersymmetric partition function needs to satisfy

$$\operatorname{Str}(G_f) = 0\,. \tag{2.46}$$

The flavor symmetry group is thus given by

$$\hat{\operatorname{Gl}}(N_f + N_v|N_v)_{\text{vector}} \otimes \operatorname{S}\hat{\operatorname{Gl}}(N_f + N_v|N_v)_{\text{axial}}\,, \tag{2.47}$$

where $\hat{\operatorname{Gl}}(N_f + N_v|N_v)$ is the supermanifold [18] with base

$$\operatorname{Gl}(N_f + N_v) \otimes [\operatorname{Gl}(N_v)/\operatorname{U}(N_v)] \tag{2.48}$$

and $\operatorname{S}\hat{\operatorname{Gl}}(N_f + N_v|N_v)$ is the restriction of $\hat{\operatorname{Gl}}(N_f + N_v|N_v)$ to elements with unit superdeterminant.

A comment about a different representation of $\hat{\operatorname{Tr}}\gamma^5$ is in order. We can write

$$\begin{aligned}
\hat{\operatorname{Tr}}(\gamma^5) &= \int d^4x \psi_n(x)^\dagger \gamma^5 \psi_n(x) = \lim_{M\to\infty} \int d^4x \psi_n(x)^\dagger \gamma^5 \exp[-\lambda_n^2/M^2]\psi_n(x) \\
&= \lim_{M\to\infty} \int d^4x \psi_n(x)^\dagger \gamma^5 \exp[\not{D}^2/M^2]\psi_n(x)\,,
\end{aligned} \tag{2.49}$$

where we introduce a gauge-invariant regulator $\not{D}$ that suppresses large eigenvalues of $\not{D}$. The trace can be reformulated as

$$\begin{aligned}\hat{\mathrm{Tr}}(\gamma^5) &= \lim_{M\to\infty} \int d^4x \psi_n(x)^\dagger \gamma^5 \exp[\not{D}^2/M^2]\psi_n(x) \\ &= \lim_{M\to\infty} \int d^4x \int \frac{d^4k}{(2\pi)^4} \langle k| \,\mathrm{Tr}\left[\gamma^5 \exp[\not{D}^2/M^2]\right] |k\rangle \ , \end{aligned} \tag{2.50}$$

where the trace Tr is in color and spinor space, and $\{|k\rangle\}$ is a complete set of momentum eigenstates. Next we express the regulator in terms of gauge fields

$$\begin{aligned}\not{D}^2 &= \gamma^\mu\gamma^\nu D_\mu D_\nu = \frac{1}{2}\left[\{\gamma^\mu,\gamma^\nu\} + [\gamma^\mu,\gamma^\nu]\right] D_\mu D_\nu \\ &= D_\mu^2 + \frac{1}{4}[\gamma^\mu,\gamma^\nu]\left[[D_\mu,D_\nu] + \{D_\mu,D_\nu\}\right] \\ &= D_\mu^2 + \frac{i}{4}[\gamma^\mu,\gamma^\nu]F_{\mu\nu}\,, \end{aligned} \tag{2.51}$$

and therefore

$$\exp[\not{D}^2/M^2]\,|k\rangle = |k\rangle \exp[-(-k_\mu + gA_\mu)^2/M^2] \exp\left[\frac{i}{4}[\gamma^\mu,\gamma^\nu]F_{\mu\nu}/M^2\right]. \tag{2.52}$$

We scale $k_\mu \to k_\mu M$ and keep only terms in leading order in $1/M$, i.e.,

$$\hat{\mathrm{Tr}}(\gamma^5) = -\frac{1}{32}\int d^4x \int \frac{d^4k}{(2\pi)^4} \exp[-k_\mu^2]\,\mathrm{Tr}_c[F_{\mu\nu}F_{\rho\sigma}]\,\mathrm{Tr}_s\left[\gamma^5[\gamma^\mu,\gamma^\nu][\gamma^\rho,\gamma^\sigma]\right], \tag{2.53}$$

where Tr_c (Tr_s) is the trace in color (spinor) space. All positive powers of M vanish since

$$\mathrm{Tr}_s\,\gamma^5 = 0\,, \qquad \mathrm{Tr}_s\,\gamma^5[\gamma^\mu,\gamma^\nu] = 0\,. \tag{2.54}$$

We integrate over the momenta and express the remaining trace by

$$\mathrm{Tr}_s[\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma\gamma^5] = -4\varepsilon^{\mu\nu\rho\sigma}\,, \tag{2.55}$$

where $\varepsilon^{\mu\nu\rho\sigma}$ is the completely antisymmetric tensor of rank 4, and write

$$\hat{\mathrm{Tr}}(\gamma^5) = \frac{1}{32\pi^2}\int d^4x \varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}_c[F_{\mu\nu}F_{\rho\sigma}]\,. \tag{2.56}$$

We compare this result to Eq. (2.44) and conclude that

$$\nu = \frac{1}{32\pi^2}\int d^4x \varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}_c[F_{\mu\nu}F_{\rho\sigma}]\,. \tag{2.57}$$

This is the celebrated *Atiyah-Singer index theorem*.

Symmetry breaking pattern

We define the *chiral condensate* Σ by the vacuum expectation value

$$\Sigma = \left\langle \bar\Psi\Psi \right\rangle = \left\langle \bar\Psi_R\Psi_L + \bar\Psi_L\Psi_R \right\rangle . \tag{2.58}$$

It is symmetric only under vector transformations. Therefore the chiral symmetry of QCD is broken spontaneously if Σ assumes a nonzero value. If we consider only fermionic quarks, we know that at low temperatures the chiral condensate is indeed nonzero [19, 20]. Next we investigate the effects of bosonic quarks.

Consider the matrix Ω defined by the vacuum expectation value

$$\tilde{\Omega}_{ba} = \left\langle \Psi_b \bar{\Psi}_a \right\rangle . \tag{2.59}$$

It transforms under vector transformations V to

$$\tilde{\Omega}'_{ba} = \left\langle V_{bb'} \Psi_{b'} \bar{\Psi}_{a'} V^{-1}_{a'a} \right\rangle = V_{bb'} \tilde{\Omega}_{b'a'} V^{-1}_{a'a} \tag{2.60}$$

or in matrix form

$$\tilde{\Omega} \to V \tilde{\Omega} V^{-1} . \tag{2.61}$$

The Vafa-Witten theorem states that vector symmetries cannot be spontaneously broken in vector-like gauge symmetries [21], and therefore we must find

$$\tilde{\Omega}' = \tilde{\Omega} , \tag{2.62}$$

and thus

$$\tilde{\Omega} = \omega \, \mathbb{1} \tag{2.63}$$

with $\omega \in \mathbb{C}$ since otherwise $\tilde{\Omega}$ would be an order parameter of the spontaneously broken vector symmetry. In the fermionic quark sector we find

$$\Sigma \propto \operatorname{Tr} \tilde{\Omega} , \tag{2.64}$$

and therefore we conclude that $\omega \neq 0$. This implies that the axial symmetry is spontaneously broken in the complete theory as well. The *symmetry breaking pattern* is therefore given by

$$\left[\hat{\mathrm{Gl}}(N_f + N_v | N_v)_{\text{vector}} \otimes \mathrm{S}\hat{\mathrm{Gl}}(N_f + N_v | N_v)_{\text{axial}} \right] \to \hat{\mathrm{Gl}}(N_f + N_v | N_v)_{\text{vector}} \tag{2.65}$$

with *Nambu-Goldstone manifold*

$$\mathrm{S}\hat{\mathrm{Gl}}(N_f + N_v | N_v)_{\text{axial}} \tag{2.66}$$

defined by all non-anomalous symmetry generators that act non-trivially on the vacuum.

Ward identities

The flavor symmetries of QCD have important implications in QCD apart from their role in spontaneous symmetry breaking. Let us consider an infinitesimal local transformation

$$\begin{aligned} \Psi(x) &\to \Psi'(x) = \Psi(x) + i\varepsilon(x) G \Psi(x) , \\ \bar{\Psi}(x) &\to \bar{\Psi}'(x) = \bar{\Psi}(x) - i\varepsilon(x) \bar{\Psi}(x) \bar{G} , \end{aligned} \tag{2.67}$$

where G and $\bar{G}$ are matrices in flavor and spinor space, and $\varepsilon(x)$ is a real-valued function of spacetime coordinate x with $\varepsilon(x) \ll 1$. We ignore terms of order $\mathcal{O}(\varepsilon^2)$ in the following. The action of massless QCD can be written as

$$S[\bar{\Psi}, \Psi] = \int d^4x \bar{\Psi}(x) D_\mu \gamma^\mu \Psi(x) , \tag{2.68}$$

where D_μ is a linear differential operator in x, and transforms under Eq. (2.67) to

$$\begin{aligned}
S[\bar{\Psi}', \Psi'] &= \int d^4x \bar{\Psi}(x)(1 - i\varepsilon(x)\bar{G})(\partial_\mu + igA_\mu)\gamma^\mu(1 + i\varepsilon(x)G)\Psi(x) \\
&= S[\bar{\Psi}, \Psi] - i\int d^4x \varepsilon(x)\bar{\Psi}(x)\bar{G}(\partial_\mu + igA_\mu)\gamma^\mu\Psi(x) \\
&\quad + i\int d^4x \varepsilon(x)\bar{\Psi}(x)(\partial_\mu + igA_\mu)\gamma^\mu G\Psi(x) \\
&\quad + i\int d^4x \bar{\Psi}(x)(\partial_\mu\varepsilon(x))\gamma^\mu G\Psi(x) \\
&= S[\bar{\Psi}, \Psi] - i\int d^4x \varepsilon(x)\bar{\Psi}(x)(\bar{G}\gamma^\mu - \gamma^\mu G)D_\mu\Psi(x) \\
&\quad - i\int d^4x \varepsilon(x)\partial_\mu(\bar{\Psi}(x)\gamma^\mu G\Psi(x))\,,
\end{aligned} \tag{2.69}$$

where we require that the boundary contribution of $\Psi(x)$ vanishes. We again consider the theory with infinitesimal mass, so that the measure transforms as

$$d[\bar{\Psi}\Psi] \to d[\bar{\Psi}'\Psi'] = d[\bar{\Psi}\Psi]\left(1 + i\int d^4x \varepsilon(x)\mathcal{A}(x)\right) \tag{2.70}$$

with *anomaly function* $\mathcal{A}(x)$. Let us further consider an arbitrary local operator

$$\mathcal{O}(y) = \langle O(y)\rangle \tag{2.71}$$

with

$$\langle O(y)\rangle = \int d[\bar{\Psi}\Psi]O(y)e^{-S[\bar{\Psi},\Psi]}\,. \tag{2.72}$$

Under Eq. (2.67) the operator shall transform to

$$O'(y) = O(y) + \varepsilon(y)\Delta O(y)\,. \tag{2.73}$$

Now the operator $\mathcal{O}$ has to be the same when calculated in terms of the transformed fields Ψ' and $\bar{\Psi}'$. Therefore

$$\begin{aligned}
\langle O(y)\rangle &= \int d[\bar{\Psi}\Psi]O(y)e^{-S[\bar{\Psi},\Psi]} = \int d[\bar{\Psi}'\Psi']O'(y)e^{-S[\bar{\Psi}',\Psi']} \\
&= \int d[\bar{\Psi}\Psi]e^{-S[\bar{\Psi},\Psi]}\left[O(y) + \int dx\varepsilon(x)\Delta O(x)\delta(x-y)\right] \\
&\quad \times\left(1 + i\int d^4x \varepsilon(x)\bar{\Psi}(x)(\bar{G}\gamma^\mu - \gamma^\mu G)D_\mu\Psi(x)\right. \\
&\qquad \left. + i\int d^4x \varepsilon(x)\partial_\mu(\bar{\Psi}(x)\gamma^\mu G\Psi(x)) + i\int d^4x \varepsilon(x)\mathcal{A}(x)\right)\,.
\end{aligned} \tag{2.74}$$

This has to hold for arbitrary $\varepsilon(x)$, and therefore we must find

$$\begin{aligned}
i\delta(x-y)\langle\Delta O(y)\rangle &= \langle O(y)\mathcal{A}(x)\rangle + \partial_\mu\left\langle O(y)j^\mu_G(x)\right\rangle \\
&\quad + \left\langle O(y)\bar{\Psi}(x)(\bar{G}\gamma^\mu - \gamma^\mu G)D_\mu\Psi(x)\right\rangle\,.
\end{aligned} \tag{2.75}$$

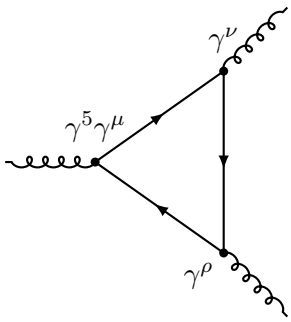


Figure 2.3: Vector–vector–axial vector (VVA) triangle diagram.

with

$$j^\mu_G(x) = \bar{\Psi}(x)\gamma^\mu G\Psi(x)\,. \tag{2.76}$$

If the Lagrangian is invariant under Eq. (2.67) and we set $O(y) = 1$, we find

$$\partial_\mu \left\langle j^\mu_G(x)\right\rangle = -\left\langle \mathcal{A}(x)\right\rangle\ . \tag{2.77}$$

We note that if the transformation G is non-anomalous, we have a conserved *Noether current* j^μ_G. In case of an axial transformation $G = G_f \otimes \gamma^5$ we find

$$\mathcal{A}(x) = \frac{1}{16\pi^2}\,\mathrm{Str}(G_f)\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{Tr}_c[F_{\mu\nu}(x)F_{\rho\sigma}(x)]\,, \tag{2.78}$$

see Eqs. (2.45) and (2.56). This is the generalization of the well-known anomaly of the axial current of QCD. Perturbatively it is related to the triangle diagram shown in Fig. 2.3.

If the Lagrangian is invariant under a non-anomalous transformation G and we use an arbitrary local operator $\mathcal{O}(y)$, Eq. (2.75) states that

$$i\delta(x-y)\left\langle \Delta O(y)\right\rangle = \partial_\mu \left\langle O(y) j^\mu_G(x)\right\rangle\ . \tag{2.79}$$

This is a *Dyson-Schwinger equation* with local contact term. It is also referred to as the *Ward identity* of the transformation (2.67) and the operator $\mathcal{O}(y)$.

Low-energy poles from symmetries

In the following we discuss the low-energy effective theory from a different perspective. In order to determine the relevant degrees of freedom for a low-energy effective theory, we investigate correlation functions of pseudoscalar densities with axial currents, i.e., the Noether currents corresponding to the axial flavor symmetries. If the correlator exhibits long-range correlations we must include the relevant fields in the effective theory.[1]

We define the pseudoscalar density

$$\varphi_G(0) = \bar{\Psi}(0)(G\otimes\gamma^5)\Psi(0) \tag{2.80}$$

and the axial current

$$j^\mu_{G'}(x) = \bar{\Psi}(x)(G'\otimes\gamma^\mu\gamma^5)\Psi(x)\,, \tag{2.81}$$

[1] This section is based on Sec. IIIB of Ref. [13]. We refer the interested reader to Ref. [13] for more details.

where G and G' are generators of an axial flavor symmetry, see Eq. (2.22), and G' is non-anomalous, i.e., $\operatorname{Str} G' = 0$. Let us consider the correlator

$$C^{\mu}_{GG'}(x) = \left\langle j^{\mu}_{G'}(x)\varphi_G(0)\right\rangle . \tag{2.82}$$

The Ward identity of $\varphi_G(0)$ and the infinitesimal transformation with G' yields

$$i\delta(x)\left\langle \Delta\varphi_G(0)\right\rangle = \partial_\mu \left\langle \varphi_G(0) j^{\mu}_{G'}(x)\right\rangle \tag{2.83}$$

with

$$\begin{aligned}\Delta\varphi_G(0) &= \bar\Psi(0)(1+iG'\gamma^5)G\gamma^5(1+iG'\gamma^5)\Psi(0) - \bar\Psi(0)G\gamma^5\Psi(0)\\ &= i\bar\Psi(0)(G'G+GG')\Psi(0) + \mathcal{O}(G'^2)\,.\end{aligned} \tag{2.84}$$

Now Eqs. (2.59) and (2.63) state that

$$\left\langle \bar\Psi_a \Psi_b\right\rangle = (-1)^{\varepsilon_a}\omega\delta_{ab} \tag{2.85}$$

which can also be formulated locally (for each spacetime coordinate x with a $\omega(x)$) so that

$$\left\langle \bar\Psi_a(x) T^{ab}\Psi_b(x)\right\rangle = (-1)^{(\varepsilon_a+\varepsilon_b)\varepsilon_b+\varepsilon_a}\omega(x)\delta_{ab}T^{ab} = \omega(x)\operatorname{Str} T\,, \tag{2.86}$$

where T is a matrix in flavor space. Therefore

$$\left\langle \Delta\varphi_G(0)\right\rangle = 2i\omega(0)\operatorname{Str}(GG') \tag{2.87}$$

and

$$\partial_\mu C^{\mu}_{GG'}(x) = -2\omega(0)\delta(x)\operatorname{Str}(GG')\,. \tag{2.88}$$

It is instructive to consider Eq. (2.88) in Fourier space. The correlator $C^{\mu}_{GG'}(x)$ transforms as a Lorentz vector so that its Fourier representation must be of the form

$$C^{\mu}_{GG'}(p) = p^\mu F_{GG'}(p^2) \tag{2.89}$$

with complex function $F_{GG'}$. Therefore Eq. (2.88) is given in Fourier space by

$$p^2 F_{GG'}(p^2) = -2\omega(0)\operatorname{Str}(GG')\,. \tag{2.90}$$

Thus a non-vanishing right-hand side implies that the correlator has a pole at $p^2 = 0$. Therefore the current of G' couples to pseudoscalars G via long-range interactions, and the fields corresponding to G and G' must be included in the low-energy effective theory.

Nambu-Goldstone manifold

Now all off-diagonal generators $G' \in \mathrm{S\hat{G}l}$ and $G \in \hat{\mathrm{G}}\mathrm{l}$ give rise to light poles and do not mix with diagonal generators. For a *partially quenched theory* with $N_f > 0$ all non-anomalous diagonal generators give rise to light poles and do not mix with anomalous generators. A special case is

$$G' = \begin{pmatrix} N_v\,\mathbb{1}_{N_f+N_v} & 0\\ 0 & (N_f+N_v)\,\mathbb{1}_{N_v}\end{pmatrix}, \tag{2.91}$$

which is diagonal in the fermion and boson sector but non-anomalous. Furthermore $\mathrm{Str}\, G'^2 \neq 0$, so that G' is relevant for the low-energy effective theory. Since the symmetries in the bosonic quark sector must be non-compact, see Eq. (2.26), this generator can only enter as

$$i\lambda G' \,, \tag{2.92}$$

where $\lambda \in \mathbb{R}$. Note that not all generators of $\hat{\mathrm{SGl}}$ lead to new Ward identities. In fact, since Gl is the complexification of U, we can restrict the NG manifold to

$$\xi = \begin{pmatrix} \pi & \bar{\kappa}^T \\ \kappa & i\pi' \end{pmatrix} + \frac{i\varphi}{\sqrt{(N_f+N_v)N_vN_f}} \begin{pmatrix} N_v\, \mathbb{1}_{N_f+N_v} & 0 \\ 0 & (N_f+N_v)\, \mathbb{1}_{N_v} \end{pmatrix}, \tag{2.93}$$

where $\pi = \pi^\dagger$ and $\pi' = \pi'^\dagger$ are traceless Hermitian matrices of dimension $N_f + N_v$ and N_v, respectively, $\varphi \in \mathbb{R}$, and $\mathbb{1}_n$ is the n-dimensional identity matrix.

In the *fully quenched theory* with $N_f = 0$ also the diagonal matrix

$$G' = \mathbb{1}_{N_f+2N_v} \tag{2.94}$$

is non-anomalous. It couples to the anomalous generator

$$G = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \tag{2.95}$$

with $\mathrm{Str}(G'G) \neq 0$, and therefore also G needs to be included. The particle corresponding to G is the generalization of the singlet particle η'. Unless stated otherwise, we restrict the discussion to the case of $N_f > 0$ in the remainder of this thesis.

2.3 The effective Lagrangian

In this section we construct a Lagrangian $\mathcal{L}_{\text{eff}}$ of the low-energy effective theory of QCD. The Lagrangian $\mathcal{L}_{\text{eff}}$ has to transform under rotations in flavor space in the same way as the Lagrangian of QCD. This is the guiding principle that we use to construct the components of $\mathcal{L}_{\text{eff}}$ in the following.[2]

A local symmetry of QCD in flavor space

The Lagrangian of QCD without gauge fields is given by

$$\mathcal{L}_0 = \bar{\Psi}_R M_{RL} \Psi_L + \bar{\Psi}_L M_{LR} \Psi_R + \bar{\Psi}_R (\partial_\mu \sigma^\mu) \Psi_R + \bar{\Psi}_L (\partial_\mu \bar{\sigma}^\mu) \Psi_L \,, \tag{2.96}$$

where M_{RL} and M_{LR} are arbitrary mass matrices, the right-handed (left-handed) fields Ψ_R, $\bar{\Psi}_R$ (Ψ_L, $\bar{\Psi}_L$) correspond to parity sectors $-$ ($+$) and

$$\sigma^\mu = (\mathbb{1}, -i\sigma^i) \,, \qquad \bar{\sigma}^\mu = (\mathbb{1}, i\sigma^i) \,. \tag{2.97}$$

We add source terms $L_\mu(x)$ and $R_\mu(x)$,

$$\begin{aligned} \mathcal{L}_0 = {} & \bar{\Psi}_R M_{RL} \Psi_L + \bar{\Psi}_L M_{LR} \Psi_R + \bar{\Psi}_R (\partial_\mu \sigma^\mu + R_\mu \sigma^\mu) \Psi_R \\ & + \bar{\Psi}_L (\partial_\mu \bar{\sigma}^\mu + L_\mu \bar{\sigma}^\mu) \Psi_L \,, \end{aligned} \tag{2.98}$$

[2] Parts of the following discussion are published in [22].

so that we can introduce a nonzero chemical potential with

$$R_\nu = L_\nu = -\delta_{0\nu}\,\mathrm{diag}(\mu_1,\ldots,\mu_{N_f},\mu_{v1},\ldots,\mu_{vN_v},\mu'_{v1},\ldots,\mu'_{vN_v})\,, \tag{2.99}$$

where $\mu_1,\ldots,\mu_{N_f}$ are the chemical potentials corresponding to sea quarks, and $\mu_{v1},\ldots,\mu_{vN_v}$ (μ'_{v1}, …, μ'_{vN_v}) are the chemical potentials corresponding to fermionic (bosonic) valence quarks.

Let us define a local transformation of right-handed and left-handed fields by

$$\begin{aligned}
&\Psi_L(x) \to V_L(x)\Psi_L(x)\,, && \Psi_R(x) \to V_R(x)\Psi_R(x)\,,\\
&\bar\Psi_L(x) \to \bar\Psi_L(x)V_L^{-1}(x)\,, && \bar\Psi_R(x) \to \bar\Psi_R(x)V_R^{-1}(x)\,,\\
&L_\mu(x) \to L'_\mu(x)\,, && R_\mu(x) \to R'_\mu(x)\,,\\
&M_{LR} \to M'_{LR}(x)\,, && M_{RL} \to M'_{RL}(x)\,,
\end{aligned} \tag{2.100}$$

where $V_L(x)$, $V_R(x)$ are matrix functions of the spacetime coordinate x in flavor space, and L'_μ, R'_μ, M'_{LR}, M'_{RL} are determined below such that Eq. (2.100) leaves the Lagrangian $\mathcal{L}_0$ invariant. Note that we allow for local mass matrices. The mass term of $\mathcal{L}_0$ is symmetric under the transformation if

$$M'_{RL} = V_R M_{RL} V_L^{-1}\,, \qquad M'_{LR} = V_L M_{LR} V_R^{-1}\,. \tag{2.101}$$

The kinetic term $\mathcal{L}_0^k$ of $\mathcal{L}_0$ transforms to

$$\mathcal{L}'^{k}_0 = \bar\Psi_R V_R^{-1}(\partial_\mu\sigma^\mu + R'_\mu\sigma^\mu)V_R\Psi_R + \bar\Psi_L V_L^{-1}(\partial_\mu\bar\sigma^\mu + L'_\mu\bar\sigma^\mu)V_L\Psi_L\,. \tag{2.102}$$

Therefore we request

$$\begin{aligned}
\mathcal{L}'^{\,k}_0 - \mathcal{L}^k_0 = {}& \bar\Psi_R(V_R^{-1}(\partial_\mu V_R) + V_R^{-1}R'_\mu V_R - R_\mu)\sigma^\mu\Psi_R\\
&+ \bar\Psi_L(V_L^{-1}(\partial_\mu V_L) + V_L^{-1}L'_\mu V_L - L_\mu)\bar\sigma^\mu\Psi_L \overset{!}{=} 0\,,
\end{aligned} \tag{2.103}$$

and thus

$$\begin{aligned}
L'_\mu &= V_L[L_\mu - V_L^{-1}(\partial_\mu V_L)]V_L^{-1} = V_L L_\mu V_L^{-1} - (\partial_\mu V_L)V_L^{-1}\,,\\
R'_\mu &= V_R[R_\mu - V_R^{-1}(\partial_\mu V_R)]V_R^{-1} = V_R R_\mu V_R^{-1} - (\partial_\mu V_R)V_R^{-1}\,.
\end{aligned} \tag{2.104}$$

As we shall see below the invariance under this local flavor symmetry can be enforced in the low-energy effective theory as well. This is sufficient to determine the components of $\mathcal{L}_{\text{eff}}$.

Components of the effective Lagrangian

In the following we construct the components of the low-energy effective Lagrangian with fields

$$U(x) = \exp\left[i\xi(x)\right], \tag{2.105}$$

where $U(x)$ is given by the NG manifold and the coordinates π, π', κ, $\bar\kappa$, and φ in Eq. (2.93) are promoted to fields. The partition function of the low-energy effective theory has to be invariant under Eq. (2.100), i.e.,

$$\begin{aligned}
&M_{RL} \to V_R M_{RL} V_L^{-1}\,, && L_\mu \to V_L L_\mu V_L^{-1} - (\partial_\mu V_L)V_L^{-1}\,,\\
&M_{LR} \to V_L M_{LR} V_R^{-1}\,, && R_\mu \to V_R R_\mu V_R^{-1} - (\partial_\mu V_R)V_R^{-1}\,,\\
&U \to U'\,,
\end{aligned} \tag{2.106}$$

where we allow for the transformation of U to U', and U' is determined below. Therefore the integral measure has to satisfy

$$d[U] = d[U'] \,. \tag{2.107}$$

Furthermore, the Lagrangian has to be real and a Lorentz scalar.

To lowest order in M_{LR}, M_{RL}, and U the mass term must be proportional to

$$\mathrm{Str}[UM_{LR} + U^{-1}M_{RL}] \tag{2.108}$$

which transforms under (2.106) to

$$\mathrm{Str}[V_R^{-1}U'V_L M_{LR} + V_L^{-1}U'^{-1}V_R M_{RL}] \,. \tag{2.109}$$

Therefore the mass term is invariant under (2.106) if

$$U' = V_R U V_L^{-1} \,. \tag{2.110}$$

Note that Eq. (2.107) states that the integral measure needs to satisfy

$$d[U'] = d[V_R U V_L^{-1}] = d[U] \,. \tag{2.111}$$

We discuss how to obtain such an integral measure in Sec. 2.5.

The construction of the lowest-order kinetic term is more delicate. Since we impose a local transformation, we need a covariant derivative. The partial derivative of $\partial_\mu U$ transforms under Eq. (2.106) as

$$\begin{aligned} \partial_\mu U &\to (\partial_\mu V_R)UV_L^{-1} + V_R(\partial_\mu U)V_L^{-1} + V_R U(\partial_\mu V_L^{-1}) \\ &= (\partial_\mu V_R)UV_L^{-1} + V_R(\partial_\mu U)V_L^{-1} - V_R U V_L^{-1}(\partial_\mu V_L)V_L^{-1} \,. \end{aligned} \tag{2.112}$$

We add a counter term proportional to L_μ, so that

$$\begin{aligned} \partial_\mu U - UL_\mu \to{}& (\partial_\mu V_R)UV_L^{-1} + V_R(\partial_\mu U)V_L^{-1} - V_R U V_L^{-1}(\partial_\mu V_L)V_L^{-1} \\ & - V_R U V_L^{-1}(V_L L_\mu V_L^{-1} - (\partial_\mu V_L)V_L^{-1}) \\ ={}& (\partial_\mu V_R)UV_L^{-1} + V_R[(\partial_\mu U) - UL_\mu]V_L^{-1} \,. \end{aligned} \tag{2.113}$$

The remaining term can be absorbed in a term proportional to R_μ as

$$\begin{aligned} \partial_\mu U - UL_\mu + R_\mu U \to{}& (\partial_\mu V_R)UV_L^{-1} + V_R[(\partial_\mu U) - UL_\mu]V_L^{-1} \\ & + (V_R R_\mu V_R^{-1} - (\partial_\mu V_R)V_R^{-1})V_R U V_L^{-1} \\ ={}& V_R[(\partial_\mu U) - UL_\mu + R_\mu U]V_L^{-1} \,. \end{aligned} \tag{2.114}$$

Therefore we define the covariant derivative

$$\begin{aligned} \nabla_\mu U &= \partial_\mu U - UL_\mu + R_\mu U \,, \\ \nabla_\mu U^{-1} &= \partial_\mu U^{-1} - U^{-1}R_\mu + L_\mu U^{-1} \end{aligned} \tag{2.115}$$

which transforms under Eq. (2.106) as

$$\begin{aligned} \nabla_\mu U &\to V_R \nabla_\mu U V_L^{-1} \,, \\ \nabla_\mu U^{-1} &\to V_L \nabla_\mu U^{-1} V_R^{-1} \,. \end{aligned} \tag{2.116}$$

The kinetic term to lowest-order in $\partial_\mu U$ must therefore be proportional to

$$\mathrm{Str}\,\nabla_\mu U \nabla_\mu U^{-1}\,. \tag{2.117}$$

For a vector source

$$V_\mu = L_\mu = R_\mu \tag{2.118}$$

the covariant derivative has the simple form

$$\nabla_\mu U = \partial_\mu U - [U, V_\mu]\,, \qquad \nabla_\mu U^{-1} = \partial_\mu U^{-1} - [U^{-1}, V_\mu]\,. \tag{2.119}$$

The low-energy effective theory at fixed vacuum angle

In accordance with the conventions for the non-supersymmetric effective theory (see, e.g., Refs. [23, 24]) we define the effective Lagrangian to leading order in $U(x)$, $\partial_\rho U(x)$, and M as

$$\mathcal{L}_{\text{eff}} = \frac{F^2}{4}\,\mathrm{Str}\left[\nabla_\rho U(x)^{-1}\nabla_\rho U(x)\right] - \frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger U(x) + U(x)^{-1}M\right], \tag{2.120}$$

where F and Σ are low-energy constants, $M = M_{RL}$, $M^\dagger = M_{LR}$. The theory in a θ-vacuum [2] is then obtained by rotating the sea quark masses,

$$\begin{aligned}\mathcal{L}_{\text{eff}}(\theta) = {}& \frac{F^2}{4}\,\mathrm{Str}\left[\nabla_\rho U(x)^{-1}\nabla_\rho U(x)\right] \\ & - \frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger e^{-i\bar\theta/N_f} U(x) + U(x)^{-1} e^{i\bar\theta/N_f} M\right],\end{aligned} \tag{2.121}$$

where

$$\bar\theta = \theta \begin{pmatrix} \mathbb{1}_{N_f} & 0 \\ 0 & 0 \end{pmatrix} \tag{2.122}$$

is an $(N_f + 2N_v)$-dimensional matrix that projects onto the sea-quark sector. The partition function of the effective theory at fixed θ is thus given by

$$Z_{\text{eff}}(\theta) = \int d[U]\, e^{-\int d^4x\, \mathcal{L}_{\text{eff}}(\theta)}\,, \tag{2.123}$$

where $d[U]$ is the invariant integration measure. We restrict the discussion to the effective theory in the remainder of this thesis and thus drop the subscript in the following.

The low-energy effective theory at fixed topology

The partition function at fixed θ-angle is given by the Fourier series

$$Z(\theta) = \sum_{\nu=-\infty}^{\infty} e^{i\theta\nu} Z_\nu\,, \tag{2.124}$$

and thus the partition function at fixed topological charge ν is obtained by the Fourier transform

$$Z_\nu = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{-i\theta\nu} Z(\theta)\,. \tag{2.125}$$

For the partition function defined in Eq. (2.123) this means

$$Z_\nu = \int d\theta \int d[U]\ \exp\left\{-i\theta\nu - \int d^4x \left(\frac{F^2}{4}\,\mathrm{Str}\left[\nabla_\rho U(x)^{-1}\nabla_\rho U(x)\right] - \frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger e^{-i\bar{\theta}/N_f}U(x) + U(x)^{-1}e^{i\bar{\theta}/N_f}M\right]\right)\right\}. \tag{2.126}$$

If we separate the constant mode U_0 from $U(x)$ by the ansatz

$$U(x) = U_0 \exp\bigl(i\xi(x)\bigr) \tag{2.127}$$

with $\int d^4x\,\xi(x) = 0$ and $U_0 = \exp(i\xi^0)$, we can absorb θ in U_0 by

$$\pi_0 \to \tilde{\pi}_0 = \pi_0 - \frac{\theta}{N_f}\begin{pmatrix}\mathbb{1}_{N_f} & 0\\ 0 & 0\end{pmatrix}, \tag{2.128}$$

where π_0 is the constant mode of the pion fields in the fermionic quark sector of ξ^0. To avoid confusion with (2.122) we mention that the matrix in (2.128) has dimension $N_f + N_v$. Note that we absorb the θ-angle only in the sea sector of the theory. This yields

$$Z_\nu = \int d[U]\ \mathrm{Sdet}^\nu(U_0)\exp\left\{-\int d^4x \left(\frac{F^2}{4}\,\mathrm{Str}\left[\nabla_\rho U(x)^{-1}\nabla_\rho U(x)\right] - \frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger U(x) + U(x)^{-1}M\right]\right)\right\}, \tag{2.129}$$

where the integration manifold for the constant mode is changed from (2.93) to

$$\xi^0 = \begin{pmatrix}\tilde{\pi}_0 & \bar{\kappa}_0^T\\ \kappa_0 & i\pi_0'\end{pmatrix} + \frac{i\varphi_0}{\sqrt{(N_f+N_v)N_vN_f}}\begin{pmatrix}N_v\,\mathbb{1}_{N_f+N_v} & 0\\ 0 & (N_f+N_v)\,\mathbb{1}_{N_v}\end{pmatrix}, \tag{2.130}$$

in which $\tilde{\pi}_0$ now generates $\mathrm{U}(N_f+N_v)$ instead of $\mathrm{SU}(N_f+N_v)$[3] while π_0', $\bar{\kappa}_0$, κ_0, and φ_0 are defined in the same way as their counterparts in Eq. (2.93). Note that this parametrization of the constant mode is different from the parametrization used previously in the literature [10, 11]. In section 3.3 we show that this parametrization is consistent with the universality of QCD at small quark masses.

2.4 The effective theory in a finite volume

In the remainder of this thesis the fields shall be confined to a box of volume $V = L_0L_1L_2L_3$. The temporal extent of the box is given by L_0, and thus the temperature of the system is $T = 1/L_0$.

Note that hadronic states h of mass m_h enter the Euclidean partition function of QCD approximately as

$$Z = \sum_h \exp[-m_hL_0]\,. \tag{2.131}$$

The pseudo-NG particles dominate the theory if

$$\exp[-\Delta m L_0] \ll 1\,, \tag{2.132}$$

where Δm is the mass gap between the pseudo-NG particles and the next heavier hadrons of QCD. Therefore the low-energy effective theory can be applied if

$$T \ll \Delta m\,. \tag{2.133}$$

[3] The addition of $\mathbb{1}_{N_f}$ to the generators of $\mathrm{SU}(N_f+N_v)$ suffices to generate $\mathrm{U}(N_f+N_v)$. The normalization of θ in Eq. (2.128) yields the correct integration domain.

Boundary conditions

The quark fields of QCD have to be anti-periodic in the temporal dimension so that the partition function describes the physical system at finite temperature T. The boundary conditions in the spatial dimensions are arbitrary.

Let us consider the general case of boundary conditions defined by

$$\bar{\Psi}_i(x+l^\mu) = (s_\mu^i)^* \bar{\Psi}_i(x)\,, \qquad \Psi_i(x+l^\mu) = s_\mu^i \Psi_i(x)\,, \tag{2.134}$$

where $s_\mu^i \in \mathbb{C}$, $(l^\mu)_\nu = L_\mu \delta_{\mu\nu}$, $i = 1, \ldots, N_f + 2N_v$, and $\mu, \nu = 0, 1, 2, 3$. Therefore the pseudoscalar (PS) and scalar (S) correlators

$$\chi_{ij}^{\mathrm{PS}}(x) = \left\langle \bar{\Psi}_i(x)\gamma^5 \Psi_j(x) \bar{\Psi}(0)\gamma^5 \Psi(0) \right\rangle\,, \qquad \chi_{ij}^{\mathrm{S}}(x) = \left\langle \bar{\Psi}_i(x) \Psi_j(x) \bar{\Psi}(0) \Psi(0) \right\rangle \tag{2.135}$$

satisfy

$$\chi_{ij}^{\mathrm{PS/S}}(x+l^\mu) = (s_\mu^i)^* s_\mu^j \, \chi_{ij}^{\mathrm{PS/S}}(x)\,. \tag{2.136}$$

We use

$$\begin{aligned} \chi_{ij}^{\mathrm{PS/S}}(x) = (-1)^{\varepsilon_i(1+\varepsilon_j)} & \left[\frac{\delta}{\delta(M_{RL}(x))_{ij}} \mp \frac{\delta}{\delta(M_{LR}(x))_{ij}} \right] \\ & \times \sum_k \left[\frac{\delta}{\delta(M_{RL}(0))_{kk}} \mp \frac{\delta}{\delta(M_{LR}(0))_{kk}} \right] Z\,, \end{aligned} \tag{2.137}$$

where the upper (lower) sign is for the pseudoscalar (scalar) case, to calculate $\chi^{\mathrm{PS/S}}$ in the effective theory. The contribution of M_{LR} and M_{RL} to the leading-order Lagrangian of Eq. (2.120) is

$$\mathcal{L}_M = -\frac{\Sigma}{2} \operatorname{Str}\left[M_{LR}(x) U(x) + M_{RL}(x) U(x)^{-1} \right]\,, \tag{2.138}$$

and therefore

$$\begin{aligned} \chi_{ij}^{\mathrm{PS}}(x) &= \frac{\Sigma^2 (-1)^{\varepsilon_i \varepsilon_j}}{4} \left\langle (U(x)_{ji} - U(x)_{ji}^{-1}) \operatorname{Str}\left[U(0) - U(0)^{-1} \right] \right\rangle \\ &= -\Sigma^2 (-1)^{\varepsilon_i \varepsilon_j} \left\langle [\sin \xi(x)]_{ji} \operatorname{Str}\left[\sin \xi(0) \right] \right\rangle\,, \\ \chi_{ij}^{\mathrm{S}}(x) &= \frac{\Sigma^2 (-1)^{\varepsilon_i \varepsilon_j}}{4} \left\langle (U(x)_{ji} + U(x)_{ji}^{-1}) \operatorname{Str}\left[U(0) + U(0)^{-1} \right] \right\rangle \\ &= \Sigma^2 (-1)^{\varepsilon_i \varepsilon_j} \left\langle [\cos \xi(x)]_{ji} \operatorname{Str}\left[\cos \xi(0) \right] \right\rangle\,, \end{aligned} \tag{2.139}$$

where

$$U(x) = \exp[i\xi(x)]\,. \tag{2.140}$$

We conclude that $\chi_{ij}^{\mathrm{PS/S}}$ has to obey the same boundary conditions as the (j,i)-component of any odd/even power of ξ. If all quark flavors obey the same boundary conditions[4], i.e.,

$$s_\mu^i = s_\mu\,, \tag{2.141}$$

[4] One can also consider more complex scenarios, see, e.g., Refs. [25, 26].

we find

$$\chi_{ij}(x + l^\mu) = |s_\mu|^2 \chi_{ij}(x)\,. \tag{2.142}$$

The boundary conditions of ξ are therefore defined by

$$\sin(\xi(x + l^\mu)) = |s_\mu|^2 \sin(\xi(x))\,, \qquad \cos(\xi(x + l^\mu)) = |s_\mu|^2 \cos(\xi(x))\,, \tag{2.143}$$

see Eq. (2.139). This can only be satisfied for

$$U(x + l^\mu) = U(x)\,, \qquad |s_\mu| = 1\,, \tag{2.144}$$

i.e., the fields ξ are periodic in all four dimensions.

Finite-volume Lagrangian

At finite volume the effective Lagrangian may contain terms that break Lorentz invariance but vanish in the infinite-volume limit such as

$$(\nabla_2 U^{-1} \nabla_2 U)/L_1^2\,. \tag{2.145}$$

It was shown in Ref. [27] for ordinary QCD without bosonic quarks that the leading-order Lagrangian defined in Eq. (2.120) is not modified by terms such as (2.145). For higher orders in M, U, and $\nabla_\mu U$ the following argument can be made. The only modifications of a theory at finite temperature, in terms of the Euclidean partition function, are appropriate boundary conditions for the fields in temporal direction. Therefore low-energy constants are not allowed to depend on temperature. This excludes all terms which depend on L_0. If the boundary conditions for the fields of QCD are chosen in the same way for all four dimensions, the system has a permutation symmetry that forbids the dependence on L_1, L_2, L_3 as well. In such a setup the Lagrangian at finite volume is equal to the infinite-volume Lagrangian. The only dependence on the volume arises from the finite-volume propagators of fields ξ.

Systematic finite-volume expansion

Let us redefine the NG manifold with a different normalization of the fields by

$$U(x) = U_0 \exp\!\left(\frac{i\sqrt{2}}{F}\xi(x)\right), \tag{2.146}$$

where ξ is defined in Eq. (2.93), and U_0 is defined below. We expand the leading-order Lagrangian of Eq. (2.120) with $R_\mu = L_\mu = 0$ to second order in ξ and find

$$\exp\left[-\int d^4x \mathcal{L}\right] = \exp\left[-S_1 - S_2 - S_3 + \mathcal{O}(\xi^3)\right] \tag{2.147}$$

with

$$\begin{aligned}
S_1 &= \frac{1}{2}\int d^4x\, \mathrm{Str}\left[\partial_\rho \xi(x) \partial_\rho \xi(x)\right], \\
S_2 &= \frac{\Sigma}{2F^2}\int d^4x\, \mathrm{Str}\left[M^\dagger U_0 \xi(x)^2 + \xi(x)^2 U_0^{-1} M\right], \\
S_3 &= -\frac{V\Sigma}{2}\,\mathrm{Str}\left[M^\dagger U_0 + U_0^{-1} M\right].
\end{aligned} \tag{2.148}$$

We separate the constant mode of ξ in U_0, and thus $\int d^4x\, \xi(x) = 0$. The lowest momenta in S_1 contribute as

$$\partial_\rho \xi(x) \propto \frac{1}{L_\rho} \xi(x) \tag{2.149}$$

and suppress fluctuations of ξ with $\sqrt{V}\xi^2 \gg 1$, so that

$$\sqrt{V}\xi^2 = \mathcal{O}(1)\,. \tag{2.150}$$

We express U_0 in terms of its algebra as

$$U_0 = \exp\left(\frac{i\sqrt{2}}{F}\xi_0\right), \tag{2.151}$$

expand U_0 to second order in ξ_0, and find

$$\begin{aligned} S_3 = &-\frac{V\Sigma}{2}\,\mathrm{Str}\left[M^\dagger + M\right] - i\frac{V\Sigma}{\sqrt{2}F}\,\mathrm{Str}\left[(M^\dagger - M)\xi_0\right] \\ &+ \frac{V\Sigma}{2F^2}\,\mathrm{Str}\left[(M^\dagger + M)\xi_0^2\right] + \mathcal{O}(\xi_0^3)\,. \end{aligned} \tag{2.152}$$

Therefore S_3 suppresses fluctuations in ξ_0 with

$$\frac{m\Sigma V\xi_0^2}{F^2} \gg 1\,, \tag{2.153}$$

and we can count

$$\frac{m\Sigma V\xi_0^2}{F^2} = \mathcal{O}(1)\,, \tag{2.154}$$

where m is a typical quark mass. For $m\Sigma V \gg 1$ the constant mode U_0 stays close to $\mathbb{1}$. In this case S_2 leads to a suppression for ξ, and

$$\frac{m\Sigma V\xi^2}{F^2} = \mathcal{O}(1)\,. \tag{2.155}$$

Therefore we can treat ξ_0 on the same footing as ξ, i.e., we can treat U_0 perturbatively as well. Equations (2.150) and (2.155) can be combined to

$$\frac{m\Sigma\sqrt{V}}{F^2} = \mathcal{O}(1)\,. \tag{2.156}$$

Note that we can identify the pion mass m_π from S_2 with

$$m_\pi^2 = \frac{2m\Sigma}{F^2}\,. \tag{2.157}$$

This is the well-known *Gell-Mann–Oakes–Renner relation*. In terms of the pion mass Eq. (2.156) states that

$$\sqrt{V}m_\pi^2 = \mathcal{O}(1)\,. \tag{2.158}$$

	$m\Sigma V$	constant mode	propagator
p expansion	$\gg 1$	perturbative	massive
mixed expansion	≥ 1	non-perturbative	massive
ε expansion	$\mathcal{O}(1)$	non-perturbative	massless

Table 2.1: Systematic finite-volume expansions.

We conclude that a consistent power counting is given by

$$\xi^4 \sim \frac{1}{V} \sim m^2 \sim \partial_\rho^4 \sim p^4 \,. \tag{2.159}$$

The corresponding systematic expansion in powers of p is the *p expansion* introduced in Ref. [28].

If we use Eq. (2.159) and treat U_0 non-perturbatively, we obtain the *mixed expansion* introduced in Ref. [24]. This expansion interpolates between $m\Sigma V \gg 1$ and $m\Sigma V = \mathcal{O}(1)$.

In the case of $m\Sigma V = \mathcal{O}(1)$ we have to treat U_0 non-perturbatively, see Eq. (2.154). There is no suppression due to the mass term S_2 since U_0 has an arbitrary phase. A consistent power counting in this case is given by

$$\xi^4 \sim \frac{1}{V} \sim m \sim \partial_\rho^4 \sim \varepsilon^4 \,. \tag{2.160}$$

The corresponding systematic expansion in powers of ε is the *ε expansion* introduced in Ref. [29]. Note that the mass term is of order ε^2, while the kinetic term is of order ε^0. Therefore the mass of the fields ξ is treated as a perturbation, and the fields ξ have a massless propagator. We summarize the different expansions in Tab. 2.1.

2.5 Invariant integration

In this section we calculate the invariant integral measure for the parametrization

$$\begin{aligned} U(x) &= U_0 U_1 = \exp\left[i\varphi\right] \exp\left[i\xi(x)\right] \\ &= \exp\left[i\varphi^a \lambda_a\right] \exp\left[i\xi^{a,n} \lambda_a g_n(x)\right] \end{aligned} \tag{2.161}$$

to second order in $\xi(x)$. We restrict the discussion to fermionic quarks for simplicity. The matrices λ_a with $a = 1, \ldots, (N_f^2 - 1)$ span the group algebra of SU(N_f). They are traceless and Hermitian and satisfy

$$\begin{aligned} &\operatorname{Tr} \lambda_a \lambda_b = C\delta_{ab} \,, && [\lambda_a, \lambda_b] = i h_{abc} \lambda_c \,, \\ &h_{acd} h_{bcd} = 2N_f C \delta_{ab} \end{aligned} \tag{2.162}$$

with $C \in \mathbb{C}$ and $h_{abc} \in \mathbb{R}$. The functions $g_n(x)$ form a basis of periodic functions on a 4-torus with

$$\int d^4x \; g_n(x) = 0 \,, \tag{2.163}$$

and the coefficients $\xi^{a,n}$ and φ^a are the coordinates on the group manifold.

In order to avoid formal manipulations we work on a discretized spacetime with N points in each dimension and choose the basis of the discrete Fourier transform

$$g_n^p = e^{2\pi i \vec{n} \cdot \vec{p}/N} \tag{2.164}$$

with

$$\frac{1}{N^4}\sum_p g_n^{p*} g_m^p = \delta_{mn}\,, \tag{2.165}$$

where $p_1,\ldots,p_4 = 1,\ldots,N$ and $n_1,\ldots,n_4 = 1,\ldots,N$. We therefore replace

$$g_n(x) \to g_n^p\,, \qquad \xi(x) \to \xi_p\,. \tag{2.166}$$

Note that

$$g_n^* = g_{\tilde{N}-n}\,, \qquad \xi^{a,n*} = \xi^{a,\tilde{N}-n}\,, \tag{2.167}$$

where $\tilde{N} = (N,N,N,N)$. Furthermore $\xi^{a,\tilde{N}} = 0$ due to Eq. (2.163). The variable transformation from complex $\xi^{a,n}$ to independent real degrees of freedom is orthogonal. Therefore it suffices to calculate the invariant measure w.r.t. the complex degrees of freedom $\xi^{a,n}$ and to treat them as independent variables.

The line element

$$ds^2 = \frac{1}{N^4}\sum_p \mathrm{Tr}[dU_p^{-1} dU_p] = \frac{1}{N^4}\sum_p \mathrm{Tr}[dU_p^\dagger dU_p] \tag{2.168}$$

is invariant under Eq. (2.107). Therefore the corresponding volume element is also invariant under Eq. (2.107). We use the ansatz

$$ds^2 = \begin{pmatrix} d\varphi^\dagger & d\xi^\dagger \end{pmatrix} G \begin{pmatrix} d\varphi & d\xi \end{pmatrix}^T\,, \tag{2.169}$$

where $d\varphi$ and $d\xi$ are infinitesimal vectors corresponding to the coordinates φ^a and $\xi^{a,n}$. The matrix

$$G = \begin{pmatrix} G^{pp} & G^{px} \\ (G^{px})^\dagger & G^{xx} \end{pmatrix} \tag{2.170}$$

is determined below. The corresponding volume element is given by

$$d[U] = \sqrt{\det G}\prod_a d\varphi^a \prod_{b,n} d\xi^{b,n}\,. \tag{2.171}$$

We use the identity

$$\det\begin{pmatrix} A & B \\ B^\dagger & C \end{pmatrix} = \det(A)\det(C - B^\dagger A^{-1} B) \tag{2.172}$$

to separate the invariant measure $d[U_0]$ of the collective coordinates φ^a,

$$\begin{aligned} d[U] &= \left[\sqrt{\det(G^{pp})}\prod_a d\varphi^a\right]\sqrt{\det(G^{xx} - (G^{px})^\dagger (G^{pp})^{-1} G^{px})}\prod_{b,n} d\xi^{b,n} \\ &= d[U_0]\sqrt{\det(G^{xx} - (G^{px})^\dagger (G^{pp})^{-1} G^{px})}\prod_{b,n} d\xi^{b,n}\,. \end{aligned} \tag{2.173}$$

We separate the trace of infinitesimals as

$$\begin{aligned} \mathrm{Tr}(dU^\dagger dU) &= \mathrm{Tr}((dU_0 U_1 + U_0 dU_1)^\dagger (dU_0 U_1 + U_0 dU_1)) \\ &= \mathrm{Tr}(\delta U_0^\dagger \delta U_0 + \delta U_0^\dagger \delta U_1 + \delta U_1^\dagger \delta U_0 + \delta U_1^\dagger \delta U_1)\,, \end{aligned} \tag{2.174}$$

where

$$\begin{aligned} \delta U_0 &= U_0^\dagger dU_0\,, & \delta U_0^\dagger &= dU_0^\dagger U_0\,, \\ \delta U_1 &= dU_1 U_1^\dagger\,, & \delta U_1^\dagger &= U_1 dU_1^\dagger\,. \end{aligned} \tag{2.175}$$

The three independent components are calculated below. We expand

$$\delta U_1 = dU_1 U_1^\dagger = \left[U_1(\xi^{a,n} + d\xi^{a,n}) - U_1(\xi^{a,n})\right] U_1(\xi^{a,n})^\dagger \tag{2.176}$$

to leading order in $d\xi$ and to second order in ξ and calculate

$$ds_{xx}^2 = \frac{1}{CN^4}\sum_p \mathrm{Tr}\left[\delta U_1^\dagger \delta U_1\right] = d\xi^{a,n} d\xi^{b,m\,*} G^{xx}_{a,n;b,m}\,, \tag{2.177}$$

where

$$G^{xx}_{a,n;b,m} = \delta_{nm}\delta_{ab} - \frac{1}{12N^4}\xi^{d,j}\xi^{c,i} h_{aed} h_{bec} \sum_p g_n^p g_j^p g_i^p g_m^{p\,*}\,. \tag{2.178}$$

The variation δU_0 lives in the algebra of $\mathrm{SU}(N_f)$, and thus

$$\delta U_0 = m(\varphi^a)_c^b \lambda_b d\varphi^c \tag{2.179}$$

with unknown coefficients m_c^b that depend on the coordinates φ^a. In terms of m_c^b we find

$$\begin{aligned} ds_{px}^2 &= \frac{1}{CN^4}\sum_p \mathrm{Tr}\left[\delta U_1^\dagger \delta U_0\right] = d\xi^{b,m} d\varphi^i G^{px}_{i;b,m}\,, \\ ds_{pp}^2 &= \frac{1}{CN^4}\sum_p \mathrm{Tr}\left[\delta U_0^\dagger \delta U_0\right] = d\varphi^a d\varphi^c G^{pp}_{ac}\,, \end{aligned} \tag{2.180}$$

where

$$G^{px}_{i;a,n} = \frac{i}{2} h_{ajb} m_i^j \xi^*_{b,n}\,, \qquad G^{pp}_{ab} = m_b^{c*} m_a^c = -(M^T M)_{ab}\,, \tag{2.181}$$

$M_{ab} = m_b^a$, and we used that $m_a^{b\,*} = -m_a^b$. We combine the contributions of δU_0 in

$$\left[(G^{px})^\dagger (G^{pp})^{-1} G^{px}\right]_{a,n;b,m} = \frac{1}{4}\delta_{yn}\delta_{xm}\xi^*_{c,x}\xi^{d,y} h_{cbl} h_{dal}\,. \tag{2.182}$$

Note that the dependence on M has canceled. Therefore

$$\begin{aligned} &\left[G^{xx} - (G^{px})^\dagger (G^{pp})^{-1} G^{px}\right]_{a,n;b,m} \\ &= \delta_{nm}\delta_{ab} - \xi^*_{c,i}\xi^{d,j} h_{aed} h_{bec}\left[\frac{1}{12}\frac{1}{N^4}\sum_p g_n^p g_j^p g_i^{p*} g_m^{p\,*} + \frac{1}{4}\delta_{jn}\delta_{im}\right]. \end{aligned} \tag{2.183}$$

We use the identity

$$\det(\mathbb{1} + \varepsilon M) = 1 + \varepsilon\,\mathrm{Tr}\,M + \mathcal{O}(\varepsilon^2) \tag{2.184}$$

and expand the determinant to second order in ξ. The result is given by

$$\begin{aligned}\mathcal{J}(\xi) &= \sqrt{\det\left[G^{xx} - (G^{px})^\dagger (G^{pp})^{-1} G^{px}\right]} \\ &= 1 - N_f \left[\frac{1}{12}N^4 + \frac{1}{6}\right]\left(\frac{1}{N^4}\sum_p \operatorname{Tr}\xi_p^2\right),\end{aligned} \tag{2.185}$$

and therefore

$$d[U] = d[U_0]\mathcal{J}(\xi)\prod_{b,n} d\xi^{b,n}\,. \tag{2.186}$$

Note that the measure contains a term proportional to N^4. This power divergence is absent if the calculation is performed in dimensional regularisation, see Refs. [30, 31].

Part II

The epsilon expansion

Chapter 3

The universal limit

To leading order in the ε expansion, the partition function of the effective theory is defined by two low-energy constants Σ and F, which are of great phenomenological importance. In this chapter we show that the partition function of the low-energy effective theory to lowest order in the ε expansion is equal to the partition function of the chiral unitary ensemble of random matrix theory (RMT). We can therefore determine the low-energy constants by fitting analytical results from RMT to numerical data for the eigenvalue spectrum of the Dirac operator obtained from lattice QCD simulations. In chapters 4 and 5 we calculate the effect of the finite volume on the distribution of eigenvalues. In chapter 6 we use data obtained from lattice QCD simulations of JLQCD [32] to determine Σ and F.

3.1 The effective theory to leading order in ε

In this section we calculate the partition function of the effective theory to leading order in ε. We restrict the vector sources L_μ and R_μ to the case of imaginary chemical potential, see Eq. (2.99). In this case the corresponding Dirac operator is anti-Hermitian and can therefore be calculated efficiently in lattice QCD simulations, see Refs. [33, 34]. For nonzero imaginary chemical potential the Lagrangian of the effective theory is given by

$$\mathcal{L} = \frac{F^2}{4}\,\mathrm{Str}\left[\nabla_\rho U(x)^{-1}\nabla_\rho U(x)\right] - \frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger U(x) + U(x)^{-1}M\right] \tag{3.1}$$

with

$$\nabla_\rho U(x) = \partial_\rho U(x) - i\delta_{\rho 0}[C, U(x)]\,, \tag{3.2}$$

where $C = \mathrm{diag}(\mu_1, \ldots, \mu_{N_f}, \mu_{v1}, \ldots, \mu_{vN_v}, \mu'_{v1}, \ldots, \mu'_{vN_v})$, and $i\mu_i$ is the imaginary chemical potential of quark flavor i. We use the ε expansion power counting defined in Eq. (2.160) and count

$$\mu \sim \varepsilon^2\,, \tag{3.3}$$

so that the kinetic term and the chemical potential term in $\nabla_\rho U$ are of the same order. To leading order in ε^2 the Lagrangian is given by

$$\begin{aligned}\mathcal{L}_0 = {} & \frac{1}{2}\,\mathrm{Str}\left[\partial_\rho\xi(x)\partial_\rho\xi(x)\right] - \frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger U_0 + U_0^{-1}M\right] \\ & - \frac{F^2}{4}\,\mathrm{Str}\,[C, U_0^{-1}][C, U_0]\,.\end{aligned} \tag{3.4}$$

The partition function for fixed topological charge ν to the same order in ε is

$$Z_\nu = \int d[U_0]\ \mathrm{Sdet}^\nu(U_0)\exp\Big(-\int d^4x\mathcal{L}_0\Big)\,. \tag{3.5}$$

We observe that the dependence on F is only non-trivial if C is not diagonal. One possible choice that leads to a non-trivial coupling to F is a vanishing chemical potential for the sea quarks and a nonzero chemical potential for the valence quarks. In this setup one can use existing lattice QCD configurations that were generated without chemical potential.

3.2 The partition function of chiral random matrix theory

Equation (3.4) shows that only the constant mode U_0 couples to the external sources C and M to this order in ε, and thus the low-energy effective theory is zero-dimensional. Therefore it is described by chiral random matrix theory [35, 36, 37, 38]. In this section we introduce the corresponding chiral unitary ensemble with imaginary chemical potential defined by

$$Z_\nu = \int d[V]d[W] \left[\prod_{f=1}^{N_f} \det(D(\mu_f^r) + m_f^r)\right] \left[\prod_{i=1}^{N_v} \frac{\det(D(\mu_{vi}^r + m_{vi}^r)}{\det(D(\mu_{vi}'^r + m_{vi}'^r)}\right] \times \exp\left[-N \operatorname{Tr}(W^\dagger W + V^\dagger V)\right], \tag{3.6}$$

where m_1^r, ..., $m_{N_f}^r$ (μ_1^r, ..., $\mu_{N_f}^r$) are the masses (chemical potentials) of the sea quarks, m_{v1}^r, ..., $m_{vN_v}^r$ (μ_{v1}^r, ..., $\mu_{vN_v}^r$) are the masses (chemical potentials) of the fermionic valence quarks, and $m_{v1}'^r$, ..., $m_{vN_v}'^r$ ($\mu_{v1}'^r$, ..., $\mu_{vN_v}'^r$) are the masses (chemical potentials) of the bosonic valence quarks, see Refs. [34, 39] and Ref. [40] for the case of real chemical potential. The integral is over the real and imaginary part of the elements of the complex $N \times (N + \nu)$ matrices W and V. The matrix Dirac operator is defined by

$$D(\mu_f^r) = \begin{pmatrix} 0 & iV + i\mu_f^r W \\ iV^\dagger + i\mu_f^r W^\dagger & 0 \end{pmatrix} \tag{3.7}$$

which has ν zeromodes. Therefore ν is interpreted as the topological charge. Note that m_f^r and μ_f^r are dimensionless quantities. They have to be mapped to physical quantities by comparison with the low-energy effective theory of QCD. It was shown in Ref. [39] that in the limit $N \to \infty$ Eq. (3.6) can be written as

$$Z_\nu = \int_{\hat{\mathrm{Gl}}(N_f+N_v|N_v)} d[U] \operatorname{Sdet}(U)^\nu \exp\left[-N \operatorname{Str}\left[M_r(U + U^{-1})\right]\right] \times \exp\left[-N \operatorname{Str}\left[C_r U C_r U^{-1}\right]\right], \tag{3.8}$$

where $M_r = \operatorname{diag}(m_1^r, \ldots, m_{N_f}^r, m_{v1}^r, \ldots, m_{vN_v}^r, m_{v1}'^r, \ldots, m_{vN_v}'^r)$, and $C_r = \operatorname{diag}(\mu_1^r, \ldots, \mu_{N_f}^r, \mu_{v1}^r, \ldots, \mu_{vN_v}^r, \mu_{v1}'^r, \ldots, \mu_{vN_v}'^r)$. In Sec. 3.3 we show for $C_r = 0$ that the integral over $\hat{\mathrm{Gl}}$ used previously in the literature [10, 11] is equal to the integral over U_0 defined in Sec. 2.3. Therefore we match Eq. (3.8) with Eqs. (3.4) and (3.5) and find

$$\hat{m}_f = m_f V \Sigma = 2N m_f^r, \qquad \hat{\mu}_f^2 = \mu_f^2 F^2 V = 2N(\mu_f^r)^2, \tag{3.9}$$

where f denotes an arbitrary quark flavor. Note that Refs. [34] and [39] use a different notation for the dimension of the matrix Dirac operator. We observe that the low-energy constants Σ and F appear in random matrix theory only as the scales of the masses and chemical potentials. The quantities $\hat{m}_f$ and $\hat{\mu}_f$ are often referred to as *microscopic scaling quantities* due to the limit $N \to \infty$.

3.3 Proof of equivalence

In the following we show that the integral over the parametrization of U_0 described in Sec. 2.3 is equal to the integral over $\hat{\mathrm{Gl}}$ used previously in the literature [10, 11]. This proof is published in Ref. [22]. For simplicity we restrict ourselves to the case of vanishing imaginary chemical potential, $C = 0$. The leading-order partition function for fixed topological charge ν is given by

$$Z_\nu = \int d[U_0]\ \mathrm{Sdet}^\nu(U_0) \exp\left(\frac{\Sigma V}{2}\,\mathrm{Str}\left[M^\dagger U_0 + U_0^{-1} M\right]\right), \tag{3.10}$$

where the integration manifold is specified in Eq. (2.130). There are different methods to calculate integrals over supermanifolds, see, e.g., [41, 42, 43]. In our case it is sufficient to choose an explicit parametrization and reduce the integral to ordinary group integrals. For convenience we use a slightly different notation and calculate

$$Z_\nu = \int d[U]\ \mathrm{Sdet}^\nu(U) \exp\Big(\mathrm{Str}\left[M^\dagger U + U^{-1} M\right]\Big) \tag{3.11}$$

with integration manifold given by

$$U = \begin{pmatrix} V e^{N_v \varphi} & 0 \\ 0 & V' e^{(N_f+N_v)\varphi} \end{pmatrix} \exp\begin{pmatrix} 0 & \bar\kappa^T \\ \kappa & 0 \end{pmatrix} = U_c U_g\,, \tag{3.12}$$

where $V \in \mathrm{U}(N_f + N_v)$, $V' \in \mathrm{Gl}(N_v)/\,\mathrm{U}(N_v)$ with $\det V' = 1$, and $\varphi \in \mathbb{R}$. Thus we have

$$\mathrm{Sdet}\, U = \det V = e^{i\theta} \tag{3.13}$$

with $\theta \in [0, 2\pi)$. This is the zero-mode integral following from the parametrization used in the perturbative calculation above. In the literature a similar integral was computed to determine the static limit of the low-energy effective theory [10, 11] that amounts to replacing U_c by

$$U_c \to \begin{pmatrix} V & 0 \\ 0 & V' e^{\varphi/N_v} \end{pmatrix}. \tag{3.14}$$

Note first that a parametrization such as $U = U_c U_g$ above leads to factorization of the corresponding measure as

$$d[U] = d[U_c] d[U_g]\,. \tag{3.15}$$

This is due to the fact that the invariant length element is

$$\begin{aligned} ds^2 &= \mathrm{Str}\left[dU d(U^{-1})\right] = \mathrm{Str}\left[dU_c d(U_c^{-1}) + dU_g d(U_g^{-1}) - 2U_c^{-1} dU_c dU_g U_g^{-1}\right] \\ &= \mathrm{Str}\left[dU_c d(U_c^{-1}) + dU_g d(U_g^{-1})\right] \end{aligned} \tag{3.16}$$

since

$$dU_g U_g^{-1} = \begin{pmatrix} 0 & d\bar\kappa^T \\ d\kappa & 0 \end{pmatrix}, \tag{3.17}$$

$U_c^{-1} dU_c$ is block diagonal, and therefore

$$\mathrm{Str}[U_c^{-1} dU_c dU_g U_g^{-1}] = 0\,. \tag{3.18}$$

In both parametrizations the measure of V, V', and φ also factorizes. Thus

$$d[U] = d[U_g]d[V]d[V']d\varphi \tag{3.19}$$

in both cases. Note that this parametrization has no contributions from Efetov-Wegner terms, as was discussed in a special case in the literature [11]. Introducing the short-hand notation

$$U_g M^\dagger = \begin{pmatrix} X_{\text{ff}} & X_{\text{fb}} \\ X_{\text{bf}} & X_{\text{bb}} \end{pmatrix}, \qquad M U_g^{-1} = \begin{pmatrix} Y_{\text{ff}} & Y_{\text{fb}} \\ Y_{\text{bf}} & Y_{\text{bb}} \end{pmatrix}, \tag{3.20}$$

we find for the first parametrization

$$\begin{aligned} \operatorname{Str}\left[M^\dagger U + M U^{-1}\right] &= \operatorname{Str}\left[M^\dagger U_c U_g + M U_g^{-1} U_c^{-1}\right] = \operatorname{Str}\left[U_c X + U_c^{-1} Y\right] \\ &= \operatorname{Tr}\left[V e^{N_v \varphi} X_{\text{ff}} - V' e^{(N_f+N_v)\varphi} X_{\text{bb}} + V^{-1} e^{-N_v\varphi} Y_{\text{ff}} - V'^{-1} e^{-(N_f+N_v)\varphi} Y_{\text{bb}}\right]. \end{aligned} \tag{3.21}$$

Next we use a result of [44],

$$\begin{aligned} &\int_{\mathrm{U}(p)} d[U] \det{}^\nu(U) \exp\left[\operatorname{Tr}(AU + BU^{-1})\right] \\ &\qquad = c_p \det(BA^{-1})^{\nu/2} \frac{\det\left[\mu_i^{j-1} I_{\nu+j-1}(2\mu_i)\right]}{\Delta(\mu^2)}, \end{aligned} \tag{3.22}$$

where c_p is a constant, $\Delta(\mu^2)$ is the Vandermonde determinant, and the μ_i^2 are the eigenvalues of AB. Thus the integral over V results in

$$e^{-N_v(N_f+N_v)\nu\varphi} \det(Y_{\text{ff}} X_{\text{ff}}^{-1})^{\nu/2} \frac{\det\left[\mu_i^{j-1} I_{\nu+j-1}(2\mu_i)\right]}{\Delta(\mu^2)} \tag{3.23}$$

with μ_i^2 the eigenvalues of $X_{\text{ff}} Y_{\text{ff}}$. In the second parametrization we find

$$\operatorname{Str}\left[M^\dagger U + M U^{-1}\right] = \operatorname{Tr}\left[V X_{\text{ff}} - V' e^{\varphi/N_v} X_{\text{bb}} + V^{-1} Y_{\text{ff}} - V'^{-1} e^{-\varphi/N_v} Y_{\text{bb}}\right]. \tag{3.24}$$

Note that in this parametrization we also have an additional factor of $e^{-\varphi\nu}$ from the superdeterminant. Thus the integral over V leads to

$$e^{-\nu\varphi} \det(Y_{\text{ff}} X_{\text{ff}}^{-1})^{\nu/2} \frac{\det\left[\mu_i^{j-1} I_{\nu+j-1}(2\mu_i)\right]}{\Delta(\mu^2)} \tag{3.25}$$

with μ_i^2 already defined above. Now we let $\varphi \to \varphi N_v(N_f + N_v)$ in order to have the same prefactor of V' and V'^{-1} in the supertrace. In both parametrizations the resulting integral is

$$\begin{aligned} \int d[U_g]d[V'] \int_{-\infty}^{\infty} d\varphi\, e^{-\nu\varphi(N_f+N_v)N_v} \det(Y_{\text{ff}} X_{\text{ff}}^{-1})^{\nu/2} \frac{\det\left(\mu_i^{j-1} I_{\nu+j-1}(2\mu_i)\right)}{\Delta(\mu^2)} \\ \times \exp\left(-\operatorname{Tr}\left[V' e^{(N_f+N_v)\varphi} X_{\text{bb}} + V'^{-1} e^{-(N_f+N_v)\varphi} Y_{\text{bb}}\right]\right). \end{aligned} \tag{3.26}$$

This completes the matching with Refs. [10, 11] and is sufficient to show that the parametrization of the NG manifold used in this thesis leads to the correct universal limit.

In order to extend this proof to the general case of $C \neq 0$ we would need to calculate the group integral

$$\int_{\mathrm{U}(p)} d[U] \det{}^\nu(U) \exp\left[\operatorname{Tr}(AU + BU^{-1}) + \operatorname{Tr}(DUDU^{-1})\right], \tag{3.27}$$

where A, B, and D are arbitrary complex $p \times p$-matrices. This, however, is beyond the scope of this thesis.

3.4 Dirac eigenvalues

The vacuum expectation value of an operator $\mathcal{O}$ in QCD is given by

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int d[A]\, d[\bar{\Psi}\Psi]\, \mathcal{O}\, e^{-S_{\rm YM} - \int d^4x\, \bar{\Psi}(\not{D}+M)\Psi}\,, \tag{3.28}$$

where the Dirac operator $\not{D}$, the mass matrix M, and the fields $\bar{\Psi}$, Ψ are defined in Sec. 2.2. The spectral density (or one-point function) of the Dirac operator $\not{D}$ can be related to the trace of the Dirac propagator with imaginary mass,

$$\rho(\lambda) = \left\langle \mathrm{Tr}\, \delta(\not{D} - i\lambda) \right\rangle = \lim_{\varepsilon \to 0} \frac{1}{\pi} \mathrm{Re} \left\langle \mathrm{Tr} (\not{D} - i\lambda + \varepsilon)^{-1} \right\rangle . \tag{3.29}$$

In order to calculate the Dirac propagator with mass $i\lambda$ we need to introduce a valence quark with mass $i\lambda$ to the theory. In other words, the flavor corresponding to mass $i\lambda$ has to be quenched.

A relatively simple method to obtain such a *partially quenched* theory is to introduce n replicated flavors in the unquenched theory and then to analytically continue in the discrete number of quark flavors to zero. This *replica trick* was first used in the theory of disordered systems [45]. It is well known that the replica trick fails for some observables since the analytic continuation from an isolated set of points is not uniquely defined [46]. Recently important progress has been made in the understanding of how to make the replica trick work [47, 48], and several publications have used the replica trick for perturbative calculations while borrowing exact result for the non-perturbative part of the theory from RMT [49, 50, 51, 24].

In this thesis we use an alternative way to obtain the partially quenched theory that does not suffer from the potential problems of the replica trick and can therefore be used to check and extend previous results. The additional bosonic quarks introduced in Sec. 2.2 allow for the discussion of valence quarks with arbitrary mass. A single Dirac propagator with mass m can be obtained from the partition function of Sec. 2.2 with $N_v = 1$ by

$$\left\langle \mathrm{Tr} (\not{D} + m)^{-1} \right\rangle = \frac{\partial}{\partial m_v} \log Z(m_1, \ldots, m_{N_f}; m_v, m'_v) \Big|_{m_v = m'_v = m} . \tag{3.30}$$

Analogously, higher-order spectral correlation functions can be obtained using $N_v = k$, where k is the desired order. From these k-point functions we can also compute individual eigenvalue distributions [52].

The partition function without chemical potential

The partition function of Eq. (3.6) without chemical potential was calculated explicitly in the limit of $N \to \infty$ in Refs. [48, 53]. The result is given by

$$Z = \frac{\det(Q)}{\Delta(\hat{m}_1^2, \ldots, \hat{m}_{N_f}^2, \hat{m}_{v1}^2, \ldots, \hat{m}_{vN_v}^2) \Delta((\hat{m}'_{v1})^2, \ldots, (\hat{m}'_{vN_v})^2)}\,, \tag{3.31}$$

where $\hat{m}_f$ with arbitrary flavor f is defined in Eq. (3.9), K_ν and I_ν are modified Bessel functions and $\Delta(x_1, \ldots, x_n)$ is the Vandermonde determinant

$$\Delta(x_1, \ldots, x_n) = \prod_{j>i} (x_j - x_i)\,. \tag{3.32}$$

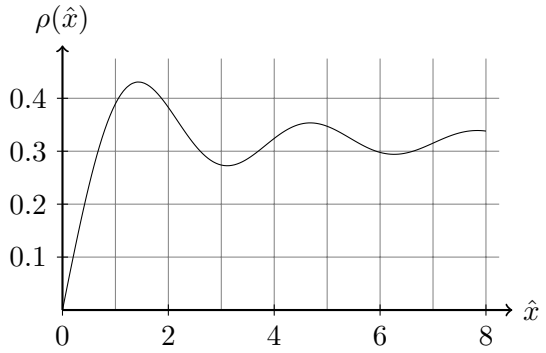


Figure 3.1: Spectral density for $N_f = 0$.

The matrix Q is defined as

$$Q = \begin{pmatrix} K_0(\hat{m}'_{v1}) & -\hat{m}'_{v1}K_1(\hat{m}'_{v1}) & (\hat{m}'_{v1})^2K_2(\hat{m}'_{v1}) & \dots \\ \vdots & \vdots & \vdots & \\ K_0(\hat{m}'_{vN_v}) & -\hat{m}'_{vN_v}K_1(\hat{m}'_{vN_v}) & (\hat{m}'_{vN_v})^2K_2(\hat{m}'_{vN_v}) & \dots \\ I_0(\hat{m}_1) & \hat{m}_1 I_1(\hat{m}_1) & (\hat{m}_1)^2 I_2(\hat{m}_1) & \dots \\ \vdots & \vdots & \vdots & \\ I_0(\hat{m}_{N_f}) & \hat{m}_{N_f} I_1(\hat{m}_{N_f}) & (\hat{m}_{N_f})^2 I_2(\hat{m}_{N_f}) & \dots \\ I_0(\hat{m}_{v1}) & \hat{m}_{v1} I_1(\hat{m}_{v1}) & (\hat{m}_{v1})^2 I_2(\hat{m}_{v1}) & \dots \\ \vdots & \vdots & \vdots & \\ I_0(\hat{m}_{vN_v}) & \hat{m}_{vN_v} I_1(\hat{m}_{vN_v}) & (\hat{m}_{vN_v})^2 I_2(\hat{m}_{vN_v}) & \dots \end{pmatrix} . \tag{3.33}$$

The partition function for $N_f = 0$ and $N_v = 1$ is thus given by

$$Z = \hat{m}_v K_0(\hat{m}'_v) I_1(\hat{m}_v) + \hat{m}'_v K_1(\hat{m}'_v) I_0(\hat{m}_v) \,, \tag{3.34}$$

where we used the identities

$$\partial_{\hat{m}} \hat{m}^\nu I_\nu(\hat{m}) = \hat{m}^\nu I_{\nu-1}(\hat{m}) \,, \qquad \partial_{\hat{m}} \hat{m}^\nu K_\nu(\hat{m}) = -\hat{m}^\nu K_{\nu-1}(\hat{m}) \,. \tag{3.35}$$

Therefore

$$\partial_{\hat{m}_v} Z\big|_{\hat{m}'_v = \hat{m}_v} = \hat{m}_v (K_0(\hat{m}_v) I_0(\hat{m}_v) + K_1(\hat{m}_v) I_1(\hat{m}_v)) \tag{3.36}$$

and

$$\rho(\hat{x}) = \frac{1}{\pi} \operatorname{Re} \partial_{\hat{m}_v} Z\big|_{\hat{m}'_v = \hat{m}_v = -i\hat{x}+\varepsilon} = \frac{\hat{x}}{2} (J_0(\hat{x})^2 + J_1(\hat{x})^2) \,, \tag{3.37}$$

where J_ν is the Bessel function of the first kind. We plot the spectral density $\rho(\hat{x})$ in Fig. 3.1.

Eigenvalue shift due to chemical potential

The eigenvalue correlation functions for the random matrix model defined by Eqs. (3.6) and (3.7) in the limit of $N \to \infty$ were calculated by Akemann et al. [34]. In this section we consider the case of $N_f = 2$, $N_v = 2$, and

$$\begin{aligned} \hat{m}_{v1} &= \hat{m}'_{v1} = -i\hat{x} + \varepsilon \,, & \hat{m}_{v2} &= \hat{m}'_{v2} = -i\hat{y} + \varepsilon \,, \\ \hat{m}_1 &= \hat{m}_u \,, & \hat{m}_2 &= \hat{m}_d \,, \\ \hat{\mu}_1 &= \hat{\mu}_2 = \hat{\mu}_{v1} = \hat{\mu}'_{v1} = 0 \,, & \hat{\mu}_{v2} &= \hat{\mu}'_{v2} = \hat{\delta} \,. \end{aligned} \tag{3.38}$$

In other words we consider the case of two sea quarks u and d with masses $\hat{m}_u$ and $\hat{m}_d$ at zero chemical potential and eigenvalues $\hat{x}$ at zero chemical potential and $\hat{y}$ at chemical potential $\hat{\delta}$. We define the two-point correlator

$$\rho^{(2)}_{(1,1)}(\hat{x},\hat{y}) = \left\langle \sum_{n,m} \delta(\hat{x}-\hat{\lambda}_n(\hat{\mu}=0))\delta(\hat{y}-\hat{\lambda}_m(\hat{\mu}=\delta)) \right\rangle , \tag{3.39}$$

where $\hat{\lambda}_n = 2N\lambda_n$ and the sum is over all eigenvalues λ_n of the matrix Dirac operator at chemical potential $\hat{\mu}=0$ and $\hat{\mu}=\hat{\delta}$. This correlator allows for a discussion of the shift of Dirac eigenvalues due to the imaginary chemical potential $\hat{\delta}$. Equation (3.39) is calculated in Ref. [34]. The result is given by

$$\begin{aligned}\rho^{(2)}_{(1,1)}(\hat{x},\hat{y}) = \hat{x}\,\hat{y}\,\det \begin{bmatrix} J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d)\end{bmatrix}^{-2} \\ \times \det \begin{bmatrix} \Upsilon_{11} & \Upsilon_{12} \\ \Upsilon_{21} & \Upsilon_{22}\end{bmatrix},\end{aligned} \tag{3.40}$$

where

$$\begin{aligned}\Upsilon_{11} &= \begin{vmatrix} \mathcal{I}^0(\hat{x},i\hat{m}_u) & J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ \mathcal{I}^0(\hat{x},i\hat{m}_d) & J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d) \\ \mathcal{I}^0(\hat{x},\hat{x}) & J_\nu(\hat{x}) & \hat{x}J_{\nu+1}(\hat{x})\end{vmatrix}, \\ \Upsilon_{12} &= \begin{vmatrix} \mathcal{I}^0(\hat{x},i\hat{m}_u) & J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ \mathcal{I}^0(\hat{x},i\hat{m}_d) & J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d) \\ -\tilde{\mathcal{I}}^-(\hat{x},\hat{y}) & e^{-\hat{\delta}^2/2}J_\nu(\hat{y}) & e^{-\hat{\delta}^2/2}G_\nu(\hat{y},\hat{\delta})\end{vmatrix},\end{aligned} \tag{3.41}$$

and

$$\begin{aligned}\Upsilon_{21} &= \begin{vmatrix} \mathcal{I}^+(\hat{y},i\hat{m}_u) & J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ \mathcal{I}^+(\hat{y},i\hat{m}_d) & J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d) \\ \mathcal{I}^+(\hat{y},\hat{x}) & J_\nu(\hat{x}) & \hat{x}J_{\nu+1}(\hat{x})\end{vmatrix}, \\ \Upsilon_{22} &= \begin{vmatrix} \mathcal{I}^+(\hat{y},i\hat{m}_u) & J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ \mathcal{I}^+(\hat{y},i\hat{m}_d) & J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d) \\ \mathcal{I}^0(\hat{y},\hat{y}) & e^{-\hat{\delta}^2/2}J_\nu(\hat{y}) & e^{-\hat{\delta}^2/2}G_\nu(\hat{y},\hat{\delta})\end{vmatrix}\end{aligned} \tag{3.42}$$

with

$$\begin{aligned}\mathcal{I}^0(\hat{x},\hat{y}) &= \frac{1}{2}\int_0^1 dt\; J_\nu(\hat{x}\sqrt{t})J_\nu(\hat{y}\sqrt{t}) \\ &= \frac{\hat{x}J_{\nu+1}(\hat{x})J_\nu(\hat{y}) - \hat{y}J_{\nu+1}(\hat{y})J_\nu(\hat{x})}{\hat{x}^2-\hat{y}^2}\,, \\ \mathcal{I}^\pm(\hat{x},\hat{y}) &= \frac{1}{2}\int_0^1 dt\; e^{\pm\hat{\delta}^2 t/2}J_\nu(\hat{x}\sqrt{t})J_\nu(\hat{y}\sqrt{t})\,, \\ \tilde{\mathcal{I}}^-(\hat{x},\hat{y}) &= \frac{1}{\hat{\delta}^2}\exp\left(-\frac{\hat{x}^2+\hat{y}^2}{2\hat{\delta}^2}\right) I_\nu\left(\frac{\hat{x}\hat{y}}{\hat{\delta}^2}\right) - \mathcal{I}^-(\hat{x},\hat{y})\,, \\ G_\nu(\hat{y},\hat{\delta}) &= \hat{y}J_{\nu+1}(\hat{y}) + \hat{\delta}^2 J_\nu(\hat{y})\,.\end{aligned} \tag{3.43}$$

In the limit of small chemical potential $\hat{\delta}^2 \ll 1$ the term proportional to $\hat{\delta}^{-2}$ in $\tilde{\mathcal{I}}^-$ dominates. Furthermore, we can perform a large argument expansion of the Bessel function in $\tilde{\mathcal{I}}^-$ and ignore all terms of order $\hat{\delta}^2$, so that

$$\rho^{(2)}_{(1,1)}(\hat{x},\hat{y}) = H_\nu(\hat{x},\hat{y},\hat{m}_u,\hat{m}_d)\frac{1}{\sqrt{2\pi\hat{\delta}^2}}\exp\left(-\frac{(\hat{x}-\hat{y})^2}{2\hat{\delta}^2}\right), \tag{3.44}$$

where

$$H_\nu(\hat{x},\hat{y},\hat{m}_u,\hat{m}_d) = \sqrt{\hat{x}\hat{y}}\frac{\begin{vmatrix} \mathcal{I}^0(\hat{y},i\hat{m}_u) & J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ \mathcal{I}^0(\hat{y},i\hat{m}_d) & J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d) \\ \mathcal{I}^0(\hat{y},\hat{x}) & J_\nu(\hat{x}) & \hat{x}J_{\nu+1}(\hat{x}) \end{vmatrix}}{\det\begin{bmatrix} J_\nu(i\hat{m}_u) & i\hat{m}_u J_{\nu+1}(i\hat{m}_u) \\ J_\nu(i\hat{m}_d) & i\hat{m}_d J_{\nu+1}(i\hat{m}_d) \end{bmatrix}}. \tag{3.45}$$

Note that the prefactor H_ν is independent of $\hat{\delta}$. Let us define a correlator that measures the shift of the eigenvalues due to the chemical potential $\hat{\delta}$ up to a cutoff $\hat{x}_c$,

$$\begin{aligned} P_d(\hat{d},\hat{x}_c) &= \int_0^{\hat{x}_c} d\hat{x}\,\rho^{(2)}_{(1,1)}(\hat{x},\hat{x}+\hat{d}) \\ &= \tilde{H}_\nu(\hat{d},\hat{x}_c,\hat{m}_u,\hat{m}_d)\frac{1}{\sqrt{2\pi\hat{\delta}^2}}\exp\left(-\frac{\hat{d}^2}{2\hat{\delta}^2}\right) \end{aligned} \tag{3.46}$$

with

$$\tilde{H}_\nu(\hat{d},\hat{x}_c,\hat{m}_u,\hat{m}_d) = \int_0^{\hat{x}_c} d\hat{x}\,H_\nu(\hat{x},\hat{x}+\hat{d},\hat{m}_u,\hat{m}_d)\,. \tag{3.47}$$

The Gaussian factor peaks strongly at $\hat{d}=0$, and thus we can expand $\tilde{H}_\nu$ about $\hat{d}=0$ to linear order in $\hat{d}$. The constant term in the expansion is fixed by the normalization

$$\int d\hat{d}\,P_d(\hat{d},\hat{x}_c) = 1 \tag{3.48}$$

for $\hat{\delta}^2 \to 0$. Without knowing the details of $\tilde{H}_\nu$ we can write

$$\begin{aligned} P_d(\hat{d},\hat{x}_c) &= \frac{1}{\sqrt{2\pi\hat{\delta}^2}}\exp\left(-\frac{\hat{d}^2}{2\hat{\delta}^2}\right)(1+c_1\hat{d}+\mathcal{O}(\hat{\delta}^2)) \\ &= \frac{1}{\sqrt{2\pi\hat{\delta}^2}}\exp\left(-\frac{(\hat{d}-c_1\hat{\delta}^2)^2}{2\hat{\delta}^2}+\mathcal{O}(\hat{\delta}^2)\right), \end{aligned} \tag{3.49}$$

where only the constant c_1 depends on $\hat{x}_c$. This quantity is well-suited to determine $\hat{\delta}$ and therefore F from a fit to eigenvalue spectra obtained in lattice QCD simulations, see chapter 6. For a related discussion with imaginary isospin chemical potential we refer to Ref. [54].

Distribution of lowest eigenvalue

In Ref. [52] the distribution of the lowest Dirac eigenvalue $\hat{y}$ at chemical potential $\hat{\mu}$ was calculated analytically. We use the notation of Ref. [52] and define

$$\begin{aligned} Q_S(\hat{y},\hat{m};t) = \frac{1}{2}\int_0^1 dr\,e^{r(t/2)\hat{\delta}^2}I_0(\sqrt{rt}\,\hat{m})\sqrt{\frac{t}{1-r}}\,\hat{y}\,I_1(\sqrt{(1-r)t}\,\hat{y}) \\ + e^{(t/2)\hat{\delta}^2}I_0(\sqrt{t}\,\hat{m})\,. \end{aligned} \tag{3.50}$$

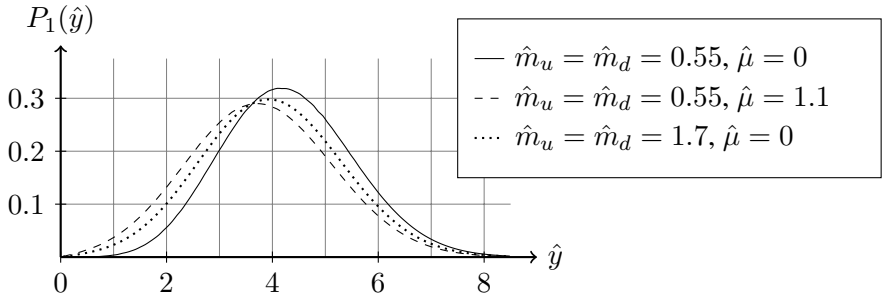


Figure 3.2: Distribution of lowest Dirac eigenvalue.

The gap probability with two sea quarks at masses $\hat{m}_u$ and $\hat{m}_d$ is given by

$$E_{0,0}^{(0+2)}(\hat{y},0) = \frac{2\det\begin{bmatrix} Q_S(\hat{y},\hat{m}_u;t=1) & \partial_t Q_S(\hat{y},\hat{m}_u;t)|_{t=1} \\ Q_S(\hat{y},\hat{m}_d;t=1) & \partial_t Q_S(\hat{y},\hat{m}_d;t)|_{t=1} \end{bmatrix}}{\hat{m}_d I_0(\hat{m}_u) I_1(\hat{m}_d) - \hat{m}_u I_0(\hat{m}_d) I_1(\hat{m}_u)} \times \exp\left(-\frac{1}{4}\hat{y}^2 - \hat{\delta}^2\right). \tag{3.51}$$

The distribution of the lowest eigenvalue is related to the gap probability by

$$P_1(\hat{y}) = -\partial_{\hat{y}} E_{0,0}^{(0+2)}(\hat{y},0)\,. \tag{3.52}$$

In Fig. 3.2 we display $P_1(\hat{y})$ for different values of $\hat{\mu}$ and $\hat{m}_u = \hat{m}_d$. Note that the dependence on $\hat{\mu}$ and $\hat{m}_u$ is entangled, and therefore it is not practical to use this quantity to determine both Σ and F from a fit to numerical data. Nevertheless, the distribution of the lowest eigenvalue is well-suited to determine the scale of $\hat{y}$ for $\hat{\mu} = 0$ and therefore Σ, see chapter 6.

Chapter 4

Leading-order corrections

In this chapter we account for the finite volume of lattice QCD simulations and calculate the partition function at next-to-leading order (NLO) in the ε expansion. We thus obtain the leading-order finite-volume corrections to the universal result of chapter 3. An important question is to what extent the finite-volume effects in the determination of a particular quantity, such as Σ or F, are universal in the sense that different methods used to determine this quantity give rise to the same finite-volume effects. In general the effects of the finite volume depend on the method, see, e.g., the finite-volume effects in the determination of F in Ref. [55]. We show that at next-to-leading order in the ε expansion the partially quenched partition function is equal to its infinite-volume counterpart with Σ and F replaced by effective values Σ_{eff} and F_{eff}. Since the knowledge of the analytic form of the partially quenched partition function suffices to determine all spectral correlation functions of the Dirac operator $\not{D}$, we find that all quantities that can be expressed in terms of spectral correlation functions of $\not{D}$ give rise to the same finite-volume corrections to Σ and F. We comment on how to minimize these corrections in lattice simulations of QCD by an optimal choice of lattice geometry.

The results of this chapter are published in Ref. [22]. A related calculation without bosonic quarks is performed in Refs. [23, 56].

4.1 The partition function

The next-to-leading order terms in the effective Lagrangian are given by

$$\mathcal{L}_2 = \mathcal{L}_2^M + \mathcal{L}_2^C + \mathcal{L}_2^N \tag{4.1}$$

with

$$\mathcal{L}_2^M = \frac{\Sigma}{2F^2}\,\mathrm{Str}\left[M^\dagger U_0 \xi(x)^2 + \xi(x)^2 U_0^{-1} M\right], \tag{4.2}$$

$$\begin{aligned}\mathcal{L}_2^C = &-\frac{1}{2}\,\mathrm{Str}\,U_0^{-1} C U_0 [\xi(x),[C,\xi(x)]] \\ &-\frac{i}{2}\,\mathrm{Str}\left(U_0^{-1} C U_0 + C\right)[\xi(x),\partial_0\xi(x)]\,,\end{aligned} \tag{4.3}$$

$$\begin{aligned}\mathcal{L}_2^N = &\frac{1}{12F^2}\,\mathrm{Str}\,[\partial_\rho\xi(x),\xi(x)][\partial_\rho\xi(x),\xi(x)] \\ &-\frac{1}{3\sqrt{2}F}\,\mathrm{Str}\;U_0^{-1}[C,U_0][\xi(x),[\partial_0\xi(x),\xi(x)]]\,.\end{aligned} \tag{4.4}$$

In this section we integrate out the fluctuations in ξ in order to obtain an effective finite-volume partition function. The term $\mathcal{L}_2^M$ couples to U_0 and M and thus corrects the leading-order mass term. In section 4.3 we discuss its effect on the low-energy constant Σ. The term $\mathcal{L}_2^C$ couples to U_0 and C and corrects the leading-order chemical potential term. Its effect on the low-energy constant F is discussed in section 4.4. The first term in $\mathcal{L}_2^N$ can be ignored since it does not couple to U_0

and therefore only amounts to an overall factor in the effective finite-volume partition function. The second term in $\mathcal{L}_2^N$ can be ignored at the order at which we are working since it does not give rise to leading-order corrections to Σ or F.

The integration measure for the parametrization of Eq. (2.146) is of the form

$$d[U] = d[U_0]d[\xi]\mathcal{J}(\xi)\,, \tag{4.5}$$

where $d[U_0]$ is the invariant measure for the constant-mode integral, $d[\xi]$ is the flat path integral measure of the fields ξ, and $\mathcal{J}(\xi)$ is the Jacobian corresponding to the change of variables of Eq. (2.146). Since ξ does not contain constant modes, the kinetic term in Eq. (3.4) suppresses large fluctuations in ξ, and thus the integrand vanishes at the integration boundaries of the π- and π'-fields. Therefore the invariant integration measure is well-defined and there are no anomalous contributions by Efetov-Wegner terms [16, 17]. The Jacobian must be of the form

$$\mathcal{J}(\xi) = 1 + \mathcal{O}(\varepsilon^2) \tag{4.6}$$

since there can be no contribution from a linear term in ξ because of $\int d^4x\,\xi(x) = 0$. Thus, at next-to-leading order the Jacobian only contributes an overall factor to the effective finite-volume partition function.

4.2 The propagator

The kinetic term of the Lagrangian in terms of the fields π, π', φ, $\bar{\kappa}$, and κ is given by

$$\begin{aligned}\frac{1}{2}\,\mathrm{Str}\,[(\partial_\rho\xi)(\partial_\rho\xi)] = \frac{1}{2}\,\mathrm{Tr}\,[(\partial_\rho\pi)(\partial_\rho\pi)] + \frac{1}{2}\,\mathrm{Tr}\,\left[(\partial_\rho\pi')(\partial_\rho\pi')\right] \\ + \frac{1}{2}\,\mathrm{Tr}\,[(\partial_\rho\varphi)(\partial_\rho\varphi)] + (\partial_\rho\bar{\kappa}_{ji})(\partial_\rho\kappa_{ji})\,.\end{aligned} \tag{4.7}$$

Since the mass term $\mathcal{L}_2^M$ of the Lagrangian, see (4.2), is of order $\mathcal{O}(\varepsilon^2)$, the fields are effectively massless. The massless propagator without zero modes, $\bar{G}(x)$, is finite in dimensional regularization [30]. In appendix A we give explicit expressions for the relevant propagators used in this chapter. For the pion fields π and π' the propagators are given by [57, 23]

$$\begin{aligned}\langle\pi(x)_{ab}\pi(y)_{cd}\rangle_0 &= \bar{G}(x-y)\left[\delta_{ad}\delta_{bc} - \frac{1}{N_f+N_v}\delta_{ab}\delta_{cd}\right], \\ \left\langle\pi'(x)_{ab}\pi'(y)_{cd}\right\rangle_0 &= \bar{G}(x-y)\left[\delta_{ad}\delta_{bc} - \frac{1}{N_v}\delta_{ab}\delta_{cd}\right],\end{aligned} \tag{4.8}$$

where the average is defined by

$$\langle\mathcal{O}[\xi]\rangle_0 = \frac{\int d[\xi]\;\mathcal{O}[\xi]\;e^{-\int d^4x\,\mathcal{L}_0}}{\int d[\xi]\;e^{-\int d^4x\,\mathcal{L}_0}}\,. \tag{4.9}$$

For the scalar field φ and for the fermionic field κ the propagators are easily shown to be

$$\begin{aligned}\langle\bar{\kappa}(x)_{ab}\kappa(y)_{cd}\rangle_0 &= -\bar{G}(x-y)\delta_{ac}\delta_{bd}\,, \\ \langle\varphi(x)\varphi(y)\rangle_0 &= \bar{G}(x-y)\,.\end{aligned} \tag{4.10}$$

Using the identities

$$\begin{aligned}\frac{1}{N_f+N_v}+\frac{N_v^2}{(N_f+N_v)N_fN_v}&=\frac{1}{N_f}\,,\\ -\frac{1}{N_v}+\frac{(N_f+N_v)^2}{(N_f+N_v)N_fN_v}&=\frac{1}{N_f}\,,\end{aligned}\tag{4.11}$$

we thus find the propagator of the composite field ξ to be

$$\langle\xi(x)_{ab}\xi(y)_{cd}\rangle_0=\bar{G}(x-y)\left[\delta_{ad}\delta_{bc}(-1)^{\varepsilon_b}-\frac{1}{N_f}\delta_{ab}\delta_{cd}\right]\tag{4.12}$$

with

$$\varepsilon_b=\begin{cases}0 & \text{for } 1\le b\le N_f+N_v\,,\\ 1 & \text{for } N_f+N_v<b\le N_f+2N_v\,.\end{cases}\tag{4.13}$$

Note that there is no explicit dependence on the number N_v of valence quarks in this propagator.

4.3 Finite-volume corrections to Σ

We now integrate out the fluctuations in the $\mathcal{O}(\varepsilon^2)$ mass term $\mathcal{L}_2^M$ to obtain the finite-volume corrections to the leading-order mass term in $\mathcal{L}_0$. Using Eq. (4.12) it is straightforward to show that

$$\langle\mathrm{Str}[A\xi(x)B\xi(y)]\rangle_0=\bar{G}(x-y)\left[\mathrm{Str}\,A\,\mathrm{Str}\,B-\frac{1}{N_f}\,\mathrm{Str}\,AB\right].\tag{4.14}$$

By expanding the action we find that the term

$$\int d^4x\,\left\langle\frac{\Sigma}{2F^2}\,\mathrm{Str}\left[M^\dagger U_0\xi(x)^2+\xi(x)^2U_0^{-1}M\right]\right\rangle_0\tag{4.15}$$

corrects the leading-order mass term in the Lagrangian,

$$-\frac{\Sigma}{2}\,\mathrm{Str}\left[M^\dagger U_0+U_0^{-1}M\right],\tag{4.16}$$

to

$$-\frac{\Sigma}{2}\left[1-\frac{N_f^2-1}{N_fF^2}\bar{G}(0)\right]\mathrm{Str}\left[M^\dagger U_0+U_0^{-1}M\right].\tag{4.17}$$

Thus at next-to-leading order we can read off an effective low-energy constant Σ_{eff} given by

$$\frac{\Sigma_{\text{eff}}}{\Sigma}=1-\frac{N_f^2-1}{N_fF^2}\bar{G}(0)\,.\tag{4.18}$$

This is the same result as previously derived for the unquenched partition function [23, 56]. Note that the one-loop propagator $\bar{G}(0)$ is of the order

$$\frac{1}{4\pi}\tag{4.19}$$

and scales with

$$\frac{1}{\sqrt{V}}\,. \tag{4.20}$$

Therefore the leading-order corrections to Σ are of the order

$$\frac{1}{4\pi F^2\sqrt{V}}\,. \tag{4.21}$$

In Sec. 4.5 we discuss the magnitude of the finite-volume corrections quantitatively.

4.4 Finite-volume corrections to F

The calculation of the finite-volume corrections to F is slightly more involved. The non-vanishing corrections to the leading-order imaginary chemical potential term are given by Eq. (4.3). We first calculate the contribution of the first term in (4.3),

$$\begin{aligned}
-\frac{1}{2}\int d^4x\,\big\langle \mathrm{Str}\; U_0^{-1}CU_0[\xi(x),[C,\xi(x)]]\big\rangle_0 \\
&= -\frac{1}{2}\int d^4x\,\big\langle \mathrm{Str}\; U_0^{-1}CU_0[2\xi(x)C\xi(x)-\xi(x)^2C-C\xi(x)^2]\big\rangle_0 \\
&= -V\bar{G}(0)\left[(\mathrm{Str}\,C)^2 - N_f\,\mathrm{Str}\,U_0^{-1}CU_0C\right],
\end{aligned} \tag{4.22}$$

where we have used (4.14). The first term in (4.22) couples only to C^2 and thus amounts only to a prefactor in the effective finite-volume partition function. The correction to the leading-order Lagrangian obtained from (4.22) is thus given by

$$\frac{\bar{G}(0)}{2}N_f\,\mathrm{Str}\,[C,U_0^{-1}][C,U_0]\,. \tag{4.23}$$

The contribution of the second term in (4.3) is given by

$$-\frac{i}{2}\int d^4x\,\big\langle \mathrm{Str}\,(U_0^{-1}CU_0+C)[\xi(x),\partial_0\xi(x)]\big\rangle_0 \sim \partial_0\bar{G}(0)=0 \tag{4.24}$$

due to the symmetry $\bar{G}(x)=\bar{G}(-x)$. However, the square of this term gives a nonzero contribution. We need to calculate

$$\begin{aligned}
-\frac{1}{2}\Big\langle\Big(-\frac{i}{2}\int d^4x\;\mathrm{Str}\,(U_0^{-1}CU_0+C)[\xi(x),\partial_0\xi(x)]\Big)^2\Big\rangle_0 \\
&= \frac{1}{8}\int d^4x\int d^4y\,\big\langle \mathrm{Str}\big(Y[\xi(x),\partial_0\xi(x)]\big)\,\mathrm{Str}\big(Y[\xi(y),\partial_0\xi(y)]\big)\big\rangle_0
\end{aligned} \tag{4.25}$$

with $Y=U_0^{-1}CU_0+C$. After performing all relevant contractions using (4.12) we find

$$\begin{aligned}
&\big\langle \mathrm{Str}[Y\xi(x)\xi(x')]\,\mathrm{Str}[Y\xi(y)\xi(y')]\big\rangle_0 \\
&\quad= \bar{G}(x-x')\bar{G}(y-y')\Big[(\mathrm{Str}\,Y)^2N_f^2 - 2(\mathrm{Str}\,Y)^2 + \frac{1}{N_f^2}(\mathrm{Str}\,Y)^2\Big] \\
&\qquad+\bar{G}(x-y)\bar{G}(x'-y')\Big[(\mathrm{Str}\,Y)^2 - \frac{2}{N_f}\,\mathrm{Str}\,Y^2 + \frac{1}{N_f^2}(\mathrm{Str}\,Y)^2\Big] \\
&\qquad+\bar{G}(x-y')\bar{G}(x'-y)\Big[N_f\,\mathrm{Str}\,Y^2 - \frac{2}{N_f}\,\mathrm{Str}\,Y^2 + \frac{1}{N_f^2}(\mathrm{Str}\,Y)^2\Big]\,.
\end{aligned} \tag{4.26}$$

Since $\mathrm{Str}\, Y = 2\,\mathrm{Str}\, C$ does not couple to U_0 we only need to take into account the terms involving $\mathrm{Str}\, Y^2$. We denote the irrelevant terms by "..." and write

$$(4.26) = -\frac{\mathrm{Str}\, Y^2}{N_f}[2\bar{G}(x-y)\bar{G}(x'-y') + (2-N_f^2)\bar{G}(x-y')\bar{G}(x'-y)] + \dots \tag{4.27}$$

We need to calculate

$$\begin{aligned}(\partial_{x_0'} - \partial_{x_0})(\partial_{y_0'} - \partial_{y_0}) \left\langle \mathrm{Str}[Y\xi(x)\xi(x')]\,\mathrm{Str}[Y\xi(y)\xi(y')]\right\rangle_0 \Big|_{x=x',\, y=y'} \\ = -2N_f\,\mathrm{Str}\, Y^2\big[\big(\partial_0\bar{G}(x-y)\big)\big(\partial_0\bar{G}(x-y)\big) - \big(\partial_0^2\bar{G}(x-y)\big)\bar{G}(x-y)\big] + \dots\end{aligned} \tag{4.28}$$

Thus we find

$$(4.25) = -\frac{V}{2}N_f\,\mathrm{Str}\, Y^2 \int d^4x \left(\partial_0\bar{G}(x)\right)^2 + \dots\,, \tag{4.29}$$

where we have used the fact that the propagator is periodic in time. Therefore the corrections to the effective Lagrangian are given by

$$-N_f\,\mathrm{Str}\, CU_0^{-1}CU_0 \int d^4x \left(\partial_0\bar{G}(x)\right)^2. \tag{4.30}$$

Combining (4.23) and (4.30), we find that the fluctuations correct the leading-order contribution to the Lagrangian,

$$-\frac{F^2}{2}\,\mathrm{Str}\; CU_0^{-1}CU_0\,, \tag{4.31}$$

to

$$-\frac{F^2}{2}\,\mathrm{Str}\; CU_0^{-1}CU_0\left[1 - \frac{2N_f}{F^2}\Big(\bar{G}(0) - \int d^4x\big(\partial_0\bar{G}(x)\big)^2\Big)\right]. \tag{4.32}$$

Thus at next-to-leading order we find an effective low-energy constant F_{eff} given by

$$\frac{F_{\text{eff}}}{F} = 1 - \frac{N_f}{F^2}\Big(\bar{G}(0) - \int d^4x \left(\partial_0\bar{G}(x)\right)^2\Big). \tag{4.33}$$

This again agrees with the result for the unquenched partition function [23, 56].

4.5 The optimal lattice geometry

In Fig. 4.1 we show the finite-volume corrections at NLO to the low-energy constants Σ and F as a function of the box size L in a symmetric box. Note that the effects of the finite volume increase with the number of sea quark flavors N_f and that, depending on N_f, a box size of $3-5$ fm is necessary to reduce the effects of the finite volume at NLO to about 10%. The effects are calculated at $F = 90$ MeV. In Fig. 4.2 we show the effect of an asymmetric box with $N_f = 2$ and $L = 2$ fm. An important message of this figure is that the magnitude of the finite-volume corrections can be significantly reduced by choosing one large spatial dimension instead of a large temporal dimension. The reason for this behavior is that the chemical potential only affects the temporal direction, see

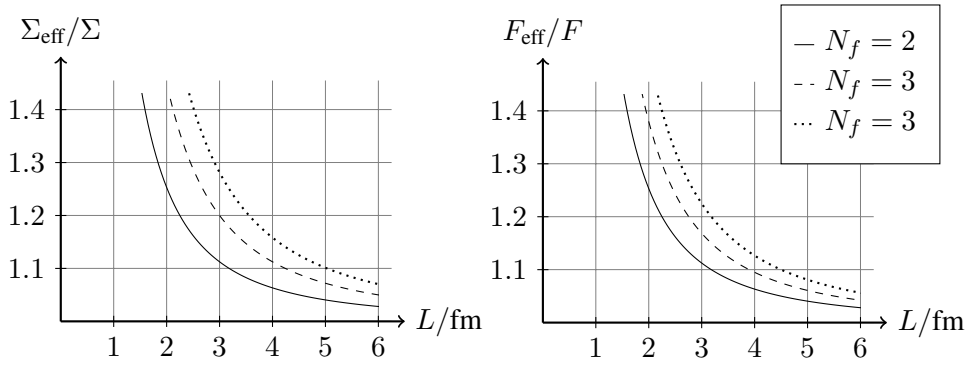


Figure 4.1: Volume-dependence at NLO of the low-energy constants Σ_{eff} (left) and F_{eff} (right) in a symmetric box with dimensions $L_0 = L_1 = L_2 = L_3 = L$ at $F = 90$ MeV.

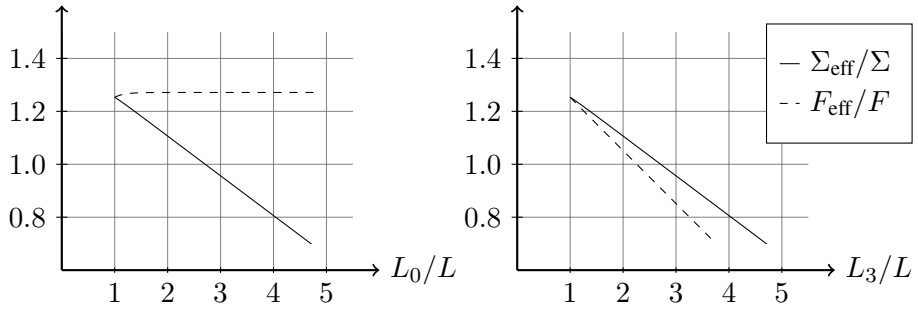


Figure 4.2: Effect of an asymmetric box with parameters $N_f = 2$, $L = 2$ fm, and $F = 90$ MeV. We compare a large temporal dimension L_0 with $L_1 = L_2 = L_3 = L$ (left) to a large spatial dimension L_3 with $L_0 = L_1 = L_2 = L$ (right).

Eq. (3.2), and therefore breaks the permutation symmetry of the four dimensions. This manifests itself in the propagator

$$\int d^4x \left(\partial_0 \bar{G}(x)\right)^2 \tag{4.34}$$

which, as shown in Eq. (A.70), contains a term proportional to $L_0^2/\sqrt{V}$, where L_0 is the size of the temporal dimension. This term leads to an enhancement of the corrections in case of a large temporal dimension. Choosing instead one large spatial dimension, the finite-volume corrections are reduced, unless the asymmetry is too large. For the parameters used in Fig. 4.2, the optimal value is $L_3/L \approx 2$.

This is good news. Many lattice simulations (at zero chemical potential) are performed with $L_1 = L_2 = L_3 = L$ and $L_0 = 2L$. To determine F, it suffices to introduce the imaginary chemical potential in the valence sector. Therefore, one can take a suitable set of existing dynamical configurations and redefine $L_0 \leftrightarrow L_3$ before adding the chemical potential. This will minimize the finite-volume corrections for both Σ and F, at least for the parameter values chosen in Fig. 4.2. Note that this procedure increases the temperature of the system by a factor of two. One needs to check that the system does not end up in the chirally restored phase, in which our results no longer apply.

Chapter 5

Next-to-leading-order corrections

In this chapter we calculate the partition function at next-to-next-to-leading order (NNLO) in the ε expansion. We allow for nonzero imaginary chemical potential and consider its contribution to leading order. In this way we obtain next-to-leading-order finite-volume corrections to the low-energy constants Σ and F. At this order 8 additional low-energy constants $L_1, \ldots, L_8$ need to be included.[1] In general the low-energy constants $L_1, \ldots, L_8$ are scale-dependent. We renormalize the theory and confirm that the scale dependence of the coupling constants $L_1, \ldots, L_8$ is the same as in the ordinary p expansion [58].

At NNLO in the ε expansion there are new terms in the finite-volume effective Lagrangian that are not present in the universal limit. We give their coefficients in terms of finite-volume propagators.

In the last section of this chapter we discuss the finite-volume corrections to Σ and F and the coefficients of the non-universal terms in the special case of $N_f = 2$ and an asymmetric box. This case is relevant for the numerical analysis of chapter 6.

A publication containing the results of this chapter is in preparation [59].

5.1 The partition function

In this section we express the partition function at NNLO in the ε expansion in terms of one-loop and two-loop propagators. For simplicity we restrict the discussion to the sea-quark sector $N_v = 0$. The terms at next-to-leading order in the Lagrangian with imaginary chemical potential, see Refs. [57] and [58], are given by

$$\begin{aligned}
\mathcal{L}_4 = &-L_1(\mathrm{Tr}[\nabla_\mu U^{-1}\nabla^\mu U])^2 - L_2\,\mathrm{Tr}[\nabla_\mu U^{-1}\nabla_\nu U]\,\mathrm{Tr}[\nabla^\mu U^{-1}\nabla^\nu U] \\
&- L_3\,\mathrm{Tr}[\nabla_\mu U^{-1}\nabla^\mu U\nabla_\nu U^{-1}\nabla^\nu U] \\
&+ \left(\frac{2\Sigma}{F^2}\right) L_4\,\mathrm{Tr}[\nabla_\mu U^{-1}\nabla^\mu U]\,\mathrm{Tr}[MU^{-1} + M^\dagger U] \\
&+ \left(\frac{2\Sigma}{F^2}\right) L_5\,\mathrm{Tr}[\nabla_\mu U^{-1}\nabla^\mu U(MU^{-1} + M^\dagger U)] \\
&- \left(\frac{2\Sigma}{F^2}\right)^2 L_6\big(\mathrm{Tr}[MU^{-1} + M^\dagger U]\big)^2 - \left(\frac{2\Sigma}{F^2}\right)^2 L_7\big(\mathrm{Tr}[MU^{-1} - M^\dagger U]\big)^2 \\
&- \left(\frac{2\Sigma}{F^2}\right)^2 L_8\,\mathrm{Tr}[MU^{-1}MU^{-1} + M^\dagger U M^\dagger U] - \left(\frac{2\Sigma}{F^2}\right)^2 H_2\,\mathrm{Tr}\,M^\dagger M\,,
\end{aligned} \tag{5.1}$$

where H_2 corresponds to a *contact term* that is needed in the renormalization of one-loop graphs. The field-strength tensors defined by L_μ and R_μ are not included since they vanish in the case of

[1] In order to distinguish the low-energy constants L_1, L_2, L_3 from the length of the corresponding spatial dimension, we rename the length L_i to L_i' with $i = 1, 2, 3$ in the remainder of this chapter.

imaginary chemical potential [58]. The invariant measure relevant to this order is given by

$$d[U] = d[U_0]d[\xi]\left(1 - \frac{N_f}{3F^2V}\int d^4x\,\mathrm{Tr}\left[\xi(x)^2\right]\right), \tag{5.2}$$

see Sec. 2.5. We perform the expansion in terms of fields ξ and average over the fields using computer algebra[2]. The resulting expression is given in terms of the massless finite-volume propagator in dimensional regularization defined in App. A,

$$\bar{G}(x) = \frac{1}{V}\sum_{k\neq 0}\frac{e^{ikx}}{k^2}, \tag{5.3}$$

where the sum is over all nonzero momenta. We use the identity

$$\partial_\rho^2\bar{G}(x)\big|_{x=0} = \frac{1}{V} \tag{5.4}$$

and finally express the result in terms of the propagators $P_1,\ldots,P_6$ defined below.

Propagators

The relevant propagators for the partition function at NNLO are defined as

$$\begin{aligned}
P_1 &= V\partial_0^2\bar{G}(0), & P_2 &= \sqrt{V}\bar{G}(0),\\
P_3 &= \sqrt{V}[\partial_0^2\bar{G}(x)]\bar{G}(x), & P_4 &= \bar{G}(x)^2,\\
P_5 &= [\partial_0^2\bar{G}(x+y)]\bar{G}(x)\bar{G}(y), & P_6 &= V[\partial_0^2\bar{G}(x)]\bar{G}(x)^2,
\end{aligned} \tag{5.5}$$

where the integral over open spacetime coordinates x, y, and z is implied. If we impose conservation of momentum and use

$$(\partial_{L'_\mu})L'_\mu\bar{G}_r = \frac{2\Gamma(r+1)}{V}\sum_{k\neq 0}\frac{k_\mu^2}{(k^2)^{r+1}}, \tag{5.6}$$

where $\partial_{L'_\mu}$ denotes the partial derivative w.r.t. L'_μ and no sum over μ is implied, we can relate the one-loop propagators $P_1,\ldots,P_5$ to $\bar{G}_r$ which is defined in App. A. We find

$$\begin{aligned}
P_1 &= -\frac{V}{2}(\partial_{L'_0})L'_0\bar{G}_0, & P_3 &= -\frac{\sqrt{V}}{2}(\partial_{L'_0})L'_0\bar{G}_1,\\
P_4 &= \bar{G}_2, & P_5 &= -\frac{1}{4}(\partial_{L'_0})L'_0\bar{G}_2.
\end{aligned} \tag{5.7}$$

For convenience we state the result of App. A explicitly as

$$\begin{aligned}
\bar{G}_r &= \lim_{m\to 0}\left[\frac{1}{(4\pi)^{d/2}}\Gamma(r-d/2)(m^2)^{d/2-r} + g_r - \frac{\Gamma(r)}{Vm^{2r}}\right],\\
Vg_0 &= \beta_0 + \beta_1 m^2\sqrt{V} + \frac{1}{2}\beta_2 m^4 V - \log(m^2\sqrt{V})\\
&\quad + \frac{Vm^4}{2(4\pi)^2}\left(\log(m^2\sqrt{V}) - \frac{1}{2}\right) + \mathcal{O}(m^6),\\
g_{r+1} &= -\frac{\partial g_r}{\partial(m^2)}
\end{aligned} \tag{5.8}$$

[2] We use a C++ library for tensor algebra developed by the author of this thesis.

with *shape coefficients* β_n. We express $\bar{G}_0$, $\bar{G}_1$, and $\bar{G}_2$ in terms of shape coefficients and find

$$\begin{aligned}
P_1 &= -\frac{1}{2}L_0'(\partial_{L_0'})\beta_0 + \frac{1}{4}\,, & P_2 &= -\beta_1\,,\\
P_3 &= \frac{1}{4}\beta_1 + \frac{1}{2}L_0'(\partial_{L_0'})\beta_1\,, & P_4 &= -2\lambda + \beta_2 + \frac{\log(\sqrt{V})}{(4\pi)^2}\,,\\
P_5 &= -\frac{1}{4}P_4 - \frac{1}{4}L_0'(\partial_{L_0'})\beta_2 - \frac{2}{(16\pi)^2}\,,
\end{aligned} \tag{5.9}$$

where we borrow the definition of λ from Ref. [58],

$$\lambda = \frac{1}{(4\pi)^2}\left[\frac{1}{d-4} - \frac{1}{2}\left[1 + \Gamma'(1) + \log(\mu^2) + \log(4\pi)\right]\right] \tag{5.10}$$

with number of spacetime dimensions d. We explicitly include the dependence on the scale μ which we define with positive mass dimension in this thesis. The two-loop propagator P_6 is calculated in Sec. 5.3. The result is given by

$$P_6 = P_6^r + \frac{1}{3}\lambda - \frac{10}{3}\lambda P_1\,, \tag{5.11}$$

where P_6^r is finite and depends only on the shape of the spacetime box.

The averaged Lagrangian at NNLO in the ε expansion and to leading order in the imaginary chemical potential C^2 can be written as

$$\begin{aligned}
\bar{\mathcal{L}} = &-\frac{\Sigma_{\text{eff}}}{2}\,\mathrm{Tr}\left[M^\dagger U_0 + U_0^{-1}M\right] - \frac{F_{\text{eff}}^2}{2}\,\mathrm{Tr}\; CU_0^{-1}CU_0 + \frac{\tilde{F}_{\text{eff}}^2}{2}\,\mathrm{Tr}\; C^2\\
&+ \bar{\mathcal{L}}_n(U_0, M, C)\,,
\end{aligned} \tag{5.12}$$

where $\bar{\mathcal{L}}_n$ contains new terms of order ε^8 that are not present in the universal limit,

$$\begin{aligned}
\bar{\mathcal{L}}_n = &\;\Upsilon_1 F^2\,\mathrm{Tr}[C]^2 + \Upsilon_2 V\Sigma^2(\mathrm{Tr}[M^\dagger U_0]^2 + \mathrm{Tr}[U_0^{-1}M]^2)\\
&+ \Upsilon_3 V\Sigma^2(\mathrm{Tr}[(M^\dagger U_0)^2] + \mathrm{Tr}[(U_0^{-1}M)^2])\\
&+ \Upsilon_4 V\Sigma^2\,\mathrm{Tr}[U_0^{-1}M]\,\mathrm{Tr}[M^\dagger U_0] + \Upsilon_5 V\Sigma^2\,\mathrm{Tr}[M^\dagger M]\\
&+ \Upsilon_6 V\Sigma F^2\,\mathrm{Tr}[U_0^{-1}CU_0C](\mathrm{Tr}[M^\dagger U_0] + \mathrm{Tr}[U_0^{-1}M])\\
&+ \Upsilon_7 V\Sigma F^2\,\mathrm{Tr}[C(M^\dagger CU_0 + U_0^{-1}CM)\\
&\qquad\qquad + U_0^{-1}CU_0(M^\dagger U_0 C + CU_0^{-1}M)]\\
&+ \Upsilon_8 V\Sigma F^2\,\mathrm{Tr}[C](\mathrm{Tr}[U_0\{M^\dagger, C\}] + \mathrm{Tr}[U_0^{-1}\{C, M\}])\\
&+ \Upsilon_9 V\Sigma F^2\,\mathrm{Tr}[C^2(\{U_0, M^\dagger\} + \{M, U_0^{-1}\})]\\
&+ \Upsilon_{10} V\Sigma F^2\,\mathrm{Tr}[C^2](\mathrm{Tr}[M^\dagger U_0] + \mathrm{Tr}[U_0^{-1}M])\,.
\end{aligned} \tag{5.13}$$

In the following we express Σ_{eff}, F_{eff}, $\tilde{F}_{\text{eff}}$, and $\Upsilon_1, \ldots, \Upsilon_{10}$ in terms of the propagators $P_1, \ldots, P_6$. Note that $\tilde{F}_{\text{eff}}$ and Υ_1 do not couple to U_0 and therefore have no physical effect. They are, however, needed in the renormalization of the coupling constants discussed in Sec. 5.2.

Finite-volume effective couplings

In the following we state the resulting expressions for Σ_{eff}, F_{eff}, $\tilde{F}_{\text{eff}}$, and $\Upsilon_1, \ldots, \Upsilon_{10}$. The effective chiral condensate is given by

$$\begin{aligned}\frac{\Sigma_{\text{eff}}}{\Sigma} &= 1 - \frac{P_2}{F^2\sqrt{V}}\left[N_f - N_f^{-1}\right] - \frac{1}{2}\left[1 - N_f^{-2}\right]\frac{P_2^2}{F^4V} \\ &\quad + \frac{P_4}{F^4V}\left[N_f^2 - 1\right] + \frac{8}{F^4V}\left[(N_f^2-1)L_4 + (N_f - N_f^{-1})L_5\right]\end{aligned} \tag{5.14}$$

which agrees with Eqs. (22) and (23) of Ref. [57]. The effective coupling constants

$$\begin{aligned}\frac{F_{\text{eff}}^2}{F^2} &= 1 - 2N_f\frac{P_2}{F^2\sqrt{V}} - 2N_f\frac{P_3}{F^2\sqrt{V}} + 2N_f^2\frac{P_2P_3}{F^4V} + 2N_f^2\frac{P_3^2}{F^4V} + N_f^2\frac{P_2^2}{F^4V} \\ &\quad + N_f^2\frac{(2P_4 + 4P_5 + P_6)}{F^4V} + \frac{16}{F^4V}\left[(N_f^2-1)L_1 + L_2 + (N_f - N_f^{-1})L_3\right] \\ &\quad + \frac{16P_1}{F^4V}\left[2L_1 + N_f^2L_2 + (N_f - 2N_f^{-1})L_3\right]\end{aligned} \tag{5.15}$$

and

$$\begin{aligned}\frac{\tilde{F}_{\text{eff}}^2}{F^2} &= 1 + 2N_f\frac{P_3}{F^2\sqrt{V}} - 2N_f^2\frac{P_2P_3}{F^4V} - 2N_f^2\frac{P_3^2}{F^4V} + N_f^2\frac{(P_6 - 4P_5)}{F^4V} \\ &\quad + \frac{16}{F^4V}\left[(N_f^2-1)L_1 + L_2 + (N_f - N_f^{-1})L_3\right] \\ &\quad + \frac{16P_1}{F^4V}\left[2L_1 + N_f^2L_2 + (N_f - 2N_f^{-1})L_3\right]\end{aligned} \tag{5.16}$$

contain the two-loop propagator P_6. The effective coupling constants of the non-universal terms are given by

$$\begin{aligned}\Upsilon_1 &= -\frac{(P_2 + 2P_3)}{F^2\sqrt{V}} + \frac{N_f}{2}\frac{(P_2^2 + 4P_3^2)}{F^4V} + N_f\frac{(P_4 + 4P_5)}{F^4V} + 2N_f\frac{P_2P_3}{F^4V}\,, \\ \Upsilon_2 &= -\frac{1}{8}\left[1 + 2N_f^{-2}\right]\frac{P_4}{F^4V} - \frac{4(L_6 + L_7)}{F^4V}\,, \\ \Upsilon_3 &= \frac{1}{2}\left[N_f^{-1} - \frac{1}{4}N_f\right]\frac{P_4}{F^4V} - \frac{4L_8}{F^4V}\,, \\ \Upsilon_4 &= -\frac{1}{4}\left[1 + 2N_f^{-2}\right]\frac{P_4}{F^4V} - \frac{8(L_6 - L_7)}{F^4V}\,,\end{aligned} \tag{5.17}$$

and

$$\begin{aligned}\Upsilon_5 &= \left[N_f^{-1} - \frac{1}{4}N_f\right]\frac{P_4}{F^4V} - \frac{4H_2}{F^4V}\,, & \Upsilon_6 &= -\frac{1}{2}\frac{(P_4 + 2P_5)}{F^4V} - \frac{4L_4}{F^4V}\,, \\ \Upsilon_7 &= -\frac{1}{4}N_f\frac{(P_4 + 2P_5)}{F^4V} - \frac{2L_5}{F^4V}\,, & \Upsilon_8 &= \frac{1}{2}\frac{P_4 + 4P_5}{F^4V}\,, \\ \Upsilon_9 &= -\frac{N_f}{2}\frac{P_5}{F^4V} + \frac{2L_5}{F^4V}\,, & \Upsilon_{10} &= -\frac{P_5}{F^4V} + \frac{4L_4}{F^4V}\,.\end{aligned} \tag{5.18}$$

In the next section we discuss how to absorb the infinities of P_4, P_5, and P_6.

5.2 Renormalization

All logarithmic divergences originate from P_4, P_5, and P_6. We separate their divergent parts as

$$\begin{aligned} P_4 &= P_4^r + \Phi_4\lambda\,, & P_5 &= P_5^r + \Phi_5\lambda\,, \\ P_6 &= P_6^r + \Phi_6\lambda + \Phi_6' P_1\lambda\,, \end{aligned} \tag{5.19}$$

where P_4^r, P_5^r, and P_6^r are finite and the coefficients are given by

$$\Phi_4 = -2\,, \qquad \Phi_5 = \frac{1}{2}\,, \qquad \Phi_6 = \frac{1}{3}\,, \qquad \Phi_6' = -\frac{10}{3}\,. \tag{5.20}$$

Furthermore, we separate the scale dependence of L_i and H_2 as

$$L_i = L_i^r + \Gamma_i\lambda\,, \qquad H_2 = H_2^r + \Delta_2\lambda \tag{5.21}$$

with $i = 1,\ldots,8$. The constants L_i^r and H_2^r are finite. For $N_f = 3$ Eqs. (5.14)-(5.18) yield the relations

$$\begin{aligned} \Gamma_4 &= \frac{1}{8}\,, & \Gamma_5 &= \frac{3}{8}\,, & \Gamma_6 &= \frac{11}{144}\,, \\ \Gamma_7 &= 0\,, & \Gamma_8 &= \frac{5}{48}\,, & \Delta_2 &= \frac{5}{24}\,, \end{aligned} \tag{5.22}$$

and

$$\frac{30}{16} = 16\Gamma_1 + 2\Gamma_2 + \frac{16}{3}\Gamma_3 = 2\Gamma_1 + 9\Gamma_2 + \frac{7}{3}\Gamma_3\,. \tag{5.23}$$

The coefficients $\Gamma_4,\ldots,\Gamma_8$, and Δ_2 are equal to the coefficients obtained in the one-loop expansion in the p power counting, see Ref. [58]. The renormalization conditions of Eq. (5.23) for $\Gamma_1,\Gamma_2,\Gamma_3$ are also compatible with the result of Ref. [58],

$$\Gamma_1 = \frac{3}{32}\,, \qquad \Gamma_2 = \frac{3}{16}\,, \qquad \Gamma_3 = 0\,. \tag{5.24}$$

Note that also the divergences in Υ_1 and Υ_8 cancel.

5.3 The two-loop propagator at finite volume

In this section we calculate the two-loop propagator P_6 defined by

$$P_6 = V[\partial_0^2\bar{G}(a)]\bar{G}(a)^2 = -\frac{1}{V}\sum_{k\neq 0}\frac{k_0^2}{k^2}\sum_{p\neq 0, p\neq -k}\frac{1}{p^2(p+k)^2}\,, \tag{5.25}$$

where the sum is over all nonzero momenta k and p. We first express the propagators without constant mode as the limit of ordinary, massive propagators,

$$P_6 = \lim_{m\to 0} P_6(m^2) = \lim_{m\to 0}\left[P_6^0(m^2) + P_6^1(m^2)\right] \tag{5.26}$$

with

$$\begin{aligned} P_6^0 &= \frac{2}{m^2 V}\sum_k \frac{k_0^2}{(k^2+m^2)^2}\,, \\ P_6^1 &= -\frac{1}{V}\sum_{k,p}\frac{k_0^2}{(p^2+m^2)((p+k)^2+m^2)(k^2+m^2)}\,. \end{aligned} \tag{5.27}$$

The terms P_6^0 and P_6^1 are calculated separately in the following.

The term P_6^0

We partition the term P_6^0 in its infinite-volume part and the finite-volume propagator g_1 defined in Eq. (5.8). We find

$$\begin{aligned} P_6^0 &= \frac{2}{m^2 V}\sum_k \frac{k_0^2}{(k^2+m^2)^2} = \frac{1}{m^2}(\partial_{L_0'})L_0'\frac{1}{V}\sum_k \frac{1}{k^2+m^2} \\ &= \frac{1}{m^2}\frac{1}{(4\pi)^{d/2}}\Gamma(1-d/2)(m^2)^{d/2-1} + \frac{1}{m^2}g_1(m^2) + \frac{1}{m^2}L_0'(\partial_{L_0'})g_1(m^2)\,, \end{aligned} \tag{5.28}$$

where

$$g_1(m^2) = \frac{1}{Vm^2} - \frac{\beta_1}{\sqrt{V}} - \frac{m^2\log m^2\sqrt{V}}{(4\pi)^2} - m^2\beta_2 + \mathcal{O}(m^4)\,. \tag{5.29}$$

Therefore we can express P_6^0 in terms of shape coefficients and λ as

$$\begin{aligned} P_6^0 = 2\lambda &- \frac{1}{m^2\sqrt{V}}L_0'(\partial_{L_0'})\beta_1 - \frac{\beta_1}{2m^2\sqrt{V}} - \frac{\log\sqrt{V}}{(4\pi)^2} \\ &- (\partial_{L_0'})(L_0'\beta_2) - \frac{1}{2(4\pi)^2} + \mathcal{O}(m^2)\,. \end{aligned} \tag{5.30}$$

The term P_6^1

The second term

$$P_6^1 = -\frac{1}{V}\sum_k \frac{k_0^2}{k^2+m^2}\sum_p \frac{1}{(p^2+m^2)((p+k)^2+m^2)} \tag{5.31}$$

is more involved. We use Poisson's summation formula, see App. A, and write

$$\begin{aligned} P_6^1 = -V\sum_{r,s}\int \frac{d^dk}{(2\pi)^d}\frac{d^dp}{(2\pi)^d}\exp\left[i\sum_j L_j'(r_jk_j+s_jp_j)\right] \\ \times \frac{k_0^2}{(p^2+m^2)((p+k)^2+m^2)(k^2+m^2)}\,, \end{aligned} \tag{5.32}$$

where the sum is over $r, s \in \mathbb{Z}^4$. We partition the sum over r and s in

$$\begin{aligned} &(A) \qquad r = 0 \wedge s = 0\,, \\ &(B) \qquad r \neq 0 \wedge s = 0\,, \\ &(C) \qquad r = 0 \wedge s \neq 0\,, \\ &(D) \qquad r \neq 0 \wedge s \neq 0 \wedge s = r\,, \\ &(E) \qquad r \neq 0 \wedge s \neq 0 \wedge s \neq r\,. \end{aligned} \tag{5.33}$$

Part (A) is given by the infinite-volume sunset diagram, see Ref. [60], which scales with Vm^d and therefore vanishes in the massless limit. The parts $P_6^{1B}, \ldots, P_6^{1E}$ are calculated in the following.

The term P_6^{1B}

Along the lines of Eqs. (A.10) and (A.11) of Ref. [61] we separate

$$P_6^{1B} = P_6^{1B1} + P_6^{1B2} \tag{5.34}$$

with

$$\begin{aligned} P_6^{1B1} &= -V \sum_{r\neq 0} \int \frac{d^dk}{(2\pi)^d} \frac{d^dp}{(2\pi)^d} \frac{k_0^2}{k^2+m^2} \frac{1}{(p^2+m^2)^2} \exp\left[i \sum_j L'_j r_j k_j \right], \\ P_6^{1B2} &= -V \sum_{r\neq 0} \int \frac{d^dk}{(2\pi)^d} \frac{d^dp}{(2\pi)^d} \frac{k_0^2}{k^2+m^2} \exp\left[i \sum_j L'_j r_j k_j \right] \\ &\quad \times \left[\frac{1}{(p^2+m^2)((p+k)^2+m^2)} - \frac{1}{(p^2+m^2)^2} \right]. \end{aligned} \tag{5.35}$$

The term P_6^{1B1} contains the ultraviolet divergence and can be calculated explicitly,

$$\begin{aligned} P_6^{1B1} &= -V \int \frac{d^dp}{(2\pi)^d} \frac{1}{(p^2+m^2)^2} \sum_{r\neq 0} \int \frac{d^dk}{(2\pi)^d} \frac{k_0^2}{k^2+m^2} \exp\left[i \sum_j L'_j r_j k_j \right] \\ &= -2\lambda P_1 - \frac{1+\log(m^2)}{(4\pi)^2} P_1 + \mathcal{O}(Vm^d), \end{aligned} \tag{5.36}$$

where P_1 is the one-loop propagator defined in Eq. (5.5). The term P_6^{1B2} is finite.

Numerical evaluation of P_6^{1B2}

After a tedious but straightforward calculation performing the same manipulations as in App. A we can express P_6^{1B2} as

$$P_6^{1B2} = -\frac{1}{(8\pi)^2} \sum_{r\neq 0} \int_0^\infty dxdydz\, K(x,y,z)\, \exp\left[-(x+y+z) \frac{m^2\sqrt{V}}{4\pi} \right] \tag{5.37}$$

with

$$\begin{aligned} K(x,y,z) &= \frac{1}{(xy+xz+yz)^3} \left[2(x+y) - \frac{({L'_0}^2/\sqrt{V})(2r_0(x+y))^2\pi}{(yz+xy+xz)} \right] \\ &\quad \times \exp\left[-\sum_j \frac{({L'_j}^2/\sqrt{V}) r_j^2 (x+y)\pi}{(yz+xy+xz)} \right] \\ &\quad - \frac{1}{(x+y)^2 z^3} \left(2 - ({L'_0}^2/\sqrt{V}) 4\pi r_0^2/z \right) \exp\left[-\sum_j ({L'_j}^2/\sqrt{V}) \pi \frac{r_j^2}{z} \right]. \end{aligned} \tag{5.38}$$

This expression is suitable for a numerical evaluation of P_6^{1B2} if we perform the integral over x, y and z in spherical coordinates.

The term P_6^{1C}

The method used to separate the divergent part of P_6^{1B} does not work for the integral over k since it has a power divergence. Nevertheless, we can calculate the divergent sub-diagram

$$I_{\mu\nu}(m,p) = \int \frac{d^dk}{(2\pi)^d} \frac{k_\mu k_\nu}{(k^2+m^2)((p+k)^2+m^2)} \tag{5.39}$$

explicitly. The result is given by [62]

$$\begin{aligned} I_{\mu\nu}(m,p) = g_{\mu\nu} &\int_0^1 dx \frac{(m^2+x(1-x)p^2)\log(m^2+x(1-x)p^2)}{2(4\pi)^2} \\ &- p_\mu p_\nu \int_0^1 dx \frac{x^2}{(4\pi)^2}[1+\log(m^2+x(1-x)p^2)] \\ &+ g_{\mu\nu}\lambda\left(\frac{1}{6}p^2+m^2\right) - \frac{2}{3}\lambda p_\mu p_\nu \,. \end{aligned} \tag{5.40}$$

We can thus separate the divergent part of

$$P_6^{1C} = -V\sum_{s\neq 0}\int \frac{d^dp}{(2\pi)^d}\frac{I_{00}(m,p)}{p^2+m^2}\exp\left[i\sum_j L'_j s_j p_j\right] \tag{5.41}$$

which is given by

$$\begin{aligned} (P_6^{1C})_{\text{UV}} &= -\frac{\lambda V}{6}\sum_{s\neq 0}\int \frac{d^dp}{(2\pi)^d}\frac{(p^2+m^2)+5m^2-4p_0^2}{p^2+m^2}\exp\left[i\sum_j L'_j s_j p_j\right] \\ &= -\frac{5}{6}\lambda - \frac{2}{3}\lambda P_1 \,. \end{aligned} \tag{5.42}$$

In the calculation of $(P_6^{1C})_{\text{UV}}$ we used the identities

$$\begin{aligned} V\sum_{s\neq 0}\int \frac{d^dp}{(2\pi)^d}\frac{1}{p^2+m^2}\exp\left[i\sum_j L'_j s_j p_j\right] &= \frac{1}{m^2}+\mathcal{O}(m^0)\,, \\ \sum_{s\neq 0}\int \frac{d^dp}{(2\pi)^d}\exp\left[i\sum_j L'_j s_j p_j\right] &= 0\,, \\ \sum_{s\neq 0}\int \frac{d^dp}{(2\pi)^d}\frac{p_0^2}{p^2+m^2}\exp\left[i\sum_j L'_j s_j p_j\right] &= -P_1+\mathcal{O}(m^d)\,. \end{aligned} \tag{5.43}$$

Note that the first two identities hold for arbitrary d. Thus there is no finite contribution from the product of these integrals with λ.

The finite contributions of P_6^{1C} are given by

$$(P_6^{1C})_{\text{finite}} = -\frac{V}{2(4\pi)^2}\sum_{s\neq 0} J'_s\,, \tag{5.44}$$

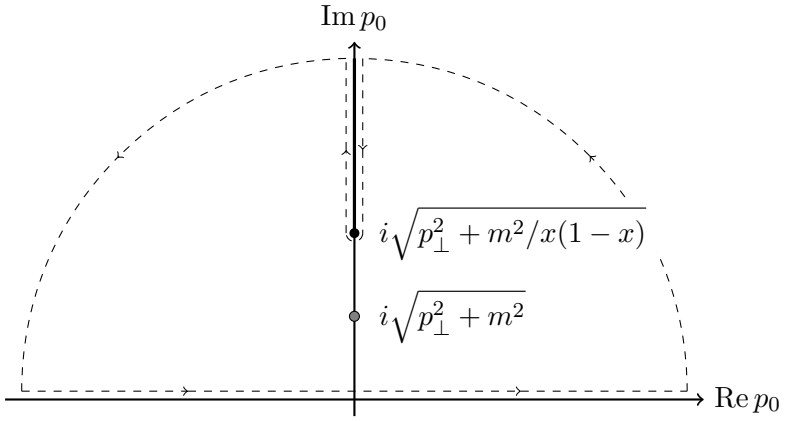


Figure 5.1: The complex plane of p_0.

where

$$J'_s = \int_0^1 dx \int \frac{d^4p}{(2\pi)^4} \exp\left[i \sum_j L'_j s_j p_j\right] \frac{\mathcal{F}_1(p^2) + \mathcal{F}_2(p^2)(\partial_{s_0})^2 / {L'_0}^2}{p^2 + m^2} \tag{5.45}$$

with

$$\begin{aligned} \mathcal{F}_1(p^2) &= (m^2 + x(1-x)p^2)\log(m^2 + x(1-x)p^2)\,, \\ \mathcal{F}_2(p^2) &= 2x^2[1 + \log(m^2 + x(1-x)p^2)]\,. \end{aligned} \tag{5.46}$$

We define $L_i^s = L'_i s_i$ and rotate the coordinate system of p such that

$$J'_s = \int_0^1 dx \int \frac{d^4p}{(2\pi)^4} \frac{\mathcal{F}_1(p^2) + \mathcal{F}_2(p^2)(\partial_{s_0})^2 / L_0^2}{p^2 + m^2} \exp\left[iL^s p_0\right] \tag{5.47}$$

with $(L^s)^2 = \sum_{n=0}^3 (L_n^s)^2$. After differentiating w.r.t. s_0 we find

$$J'_s = \int_0^1 dx \int \frac{d^4p}{(2\pi)^4} \frac{[\mathcal{F}_1(p^2) + \mathcal{F}_2(p^2)\mathcal{G}_s(p_0 V^{1/4})] \exp\left[iL^s p_0\right]}{\left[p_0 - i\sqrt{p_\perp^2 + m^2}\right]\left[p_0 + i\sqrt{p_\perp^2 + m^2}\right]} \tag{5.48}$$

with

$$\mathcal{G}_s(p_0 V^{1/4}) = \frac{ip_0}{L^s} - \frac{ip_0 s_0^2 (L'_0)^2}{(L^s)^3} - \frac{(L'_0)^2 p_0^2 s_0^2}{(L^s)^2} \tag{5.49}$$

and

$$p^2 = p_0^2 + p_\perp^2\,. \tag{5.50}$$

In Fig. 5.1 we sketch the structure of the integrand in the complex plane. There are two poles at $p_0 = \pm i\sqrt{p_\perp^2 + m^2}$ and a branch cut due to the logarithms in $\mathcal{F}_1(p^2)$ and $\mathcal{F}_2(p^2)$. We can close the integration contour in the upper half-plane and find

$$J'_s = (J'_s)_p + (J'_s)_c\,, \tag{5.51}$$

where $(J'_s)_p$ is the contribution of the pole and $(J'_s)_c$ is the contribution of the branch cut. The contribution of the pole is given by

$$(J'_s)_p = \frac{1}{(2\pi)^2 V} \int_0^1 dx \int_0^\infty dp_\perp p_\perp^2 \exp\left[-l^s \sqrt{p_\perp^2 + m^2 L^2}\right] \times \frac{\mathcal{F}_1(-m^2)\sqrt{V} + \mathcal{F}_2(-m^2)\mathcal{G}_s(i\sqrt{p_\perp^2 + m^2\sqrt{V}})\sqrt{V}}{\sqrt{p_\perp^2 + m^2\sqrt{V}}} \tag{5.52}$$

with $l^s = L^s/V^{1/4}$. The contribution of the branch cut is given by

$$(J'_s)_c = \frac{1}{(2\pi)^4} \int_0^1 dx \int d^3p_\perp \int_{i\sqrt{p_\perp^2 + m^2/x(1-x)}}^{i\infty} dp_0 \exp\left[iL^s p_0\right] \times \frac{\operatorname{Disc}\mathcal{F}_1(p^2) + \operatorname{Disc}\mathcal{F}_2(p^2)\mathcal{G}_s(p_0 V^{1/4})}{p^2 + m^2}\,, \tag{5.53}$$

where

$$\begin{aligned} \operatorname{Disc}\mathcal{F}_1(p^2) &= \lim_{\varepsilon\to 0}\left[\mathcal{F}_1(p_\perp^2 + (p_0+\varepsilon)^2) - \mathcal{F}_1(p_\perp^2 + (p_0-\varepsilon)^2)\right] \\ &= 2\pi i(m^2 + x(1-x)p^2)\,, \\ \operatorname{Disc}\mathcal{F}_2(p^2) &= \lim_{\varepsilon\to 0}\left[\mathcal{F}_2(p_\perp^2 + (p_0+\varepsilon)^2) - \mathcal{F}_2(p_\perp^2 + (p_0-\varepsilon)^2)\right] \\ &= 4\pi i x^2\,. \end{aligned} \tag{5.54}$$

Therefore

$$(J'_s)_c = \frac{2}{(2\pi)^2 V} \int_0^1 dx \int_0^\infty dp_\perp p_\perp^2 \int_{\sqrt{p_\perp^2 + m^2\sqrt{V}/x(1-x)}}^\infty dy \exp\left[-l^s y\right] \times \frac{m^2\sqrt{V} + x(1-x)(p_\perp^2 - y^2) + 2x^2\mathcal{G}_s(iy)\sqrt{V}}{y^2 - p_\perp^2 - m^2\sqrt{V}} \tag{5.55}$$

with $p_0 = iy$ and thus $dp_0 = idy$. In Sec. 5.4 we calculate $(P_6^{1C})_{\text{finite}}$ numerically at scale $V^{-1/4}$, i.e., we replace $\mathcal{F}_1$ and $\mathcal{F}_2$ by

$$\begin{aligned} \mathcal{F}_1(p^2) &= (m^2 + x(1-x)p^2)\log(m^2\sqrt{V} + x(1-x)p^2\sqrt{V})\,, \\ \mathcal{F}_2(p^2) &= 2x^2[1 + \log(m^2\sqrt{V} + x(1-x)p^2\sqrt{V})]\,. \end{aligned} \tag{5.56}$$

The term P_6^{1D}

The term P_6^{1D} is equal to the term P_6^{1C}. This can be seen by shifting the integration variables $p_\mu \to p_\mu - k_\mu$ and using the invariance of the integral under $k_\mu \to -k_\mu$.

The term P_6^{1E}

The term P_6^{1E} is finite and can be calculated numerically. We rewrite P_6^{1E} analog to P_6^{1B2} as

$$\begin{aligned} P_6^{1E} = &-\frac{1}{(8\pi)^2} \sum_{0\neq r\neq s\neq 0} \int_0^\infty dxdydz \, \frac{1}{(xy+xz+yz)^3} \\ &\times \left[2(x+y) - \frac{({L_0'}^2/\sqrt{V})(-2s_0 y + 2r_0(x+y))^2\pi}{(yz+xy+xz)} \right] \\ &\times \exp\left[-\sum_j \frac{({L_j'}^2/\sqrt{V})(-2r_j s_j y + r_j^2(x+y) + s_j^2(y+z))\pi}{(yz+xy+xz)} \right] \\ &\times \exp\left[-(x+y+z)\frac{m^2\sqrt{V}}{4\pi} \right] . \end{aligned} \tag{5.57}$$

This expression is suitable for a numerical evaluation of P_6^{1E} if we perform the integral over x, y and z in spherical coordinates.

The complete diagram

We combine all contributions to P_6 and find that the complete diagram at scale $V^{-1/4}$ is given by

$$\begin{aligned} (P_6)_{\text{UV}} &= \frac{1}{3}\lambda - \frac{10}{3}\lambda P_1 \,, \\ (P_6)_{\text{finite}} &= -\frac{1}{m^2\sqrt{V}} L_0'(\partial_{L_0'})\beta_1 - \frac{\beta_1}{2m^2\sqrt{V}} - \frac{\log(m^2\sqrt{V})}{(4\pi)^2} P_1 - (\partial_{L_0'})(L_0'\beta_2) \\ &\quad - \frac{1}{2(4\pi)^2} + 2(P_6^{1C})_{\text{finite}} - \frac{1}{(4\pi)^2} P_1 + P_6^{1B2} + P_6^{1E} \,. \end{aligned} \tag{5.58}$$

5.4 Two quark flavors in an asymmetric box

In the following we discuss the finite-volume corrections to Σ and F and the coefficients of the non-universal terms at NNLO in the ε expansion. We explicitly consider the case of $N_f = 2$ and an asymmetric box with geometry

$$\begin{aligned} &(a) \qquad L_0' = 2L \,, \qquad L_1' = L_2' = L_3' = L \,, \\ &(b) \qquad L_3' = 2L \,, \qquad L_0' = L_1' = L_2' = L \,. \end{aligned} \tag{5.59}$$

This case is relevant for the numerical discussion of chapter 6. The three-flavor coupling constants $L_1, \ldots, L_5$ can be related to the two-flavor coupling constants l_1, l_2, and l_4 by

$$l_1 = 4L_1 + 2L_3 \,, \qquad l_2 = 4L_2 \,, \qquad l_4 = 8L_4 + 4L_5 \,, \tag{5.60}$$

see, e.g., Eqs. (3.15) and (3.16) of Ref. [63]. Therefore

$$\frac{\Sigma_{\text{eff}}}{\Sigma} = 1 - \frac{3P_2}{2F^2\sqrt{V}} - \frac{3P_2^2}{8F^4V} + \frac{3P_4}{F^4V} + \frac{3l_4}{F^4V}, \tag{5.61}$$

and

$$\frac{F_{\text{eff}}^2}{F^2} = 1 - \frac{4P_2}{F^2\sqrt{V}} - \frac{4P_3}{F^2\sqrt{V}} + \frac{8P_2P_3 + 8P_3^2 + 4P_2^2}{F^4V} + \frac{8P_4 + 16P_5 + 4P_6}{F^4V} + \frac{1}{F^4V}\left[12l_1 + 4l_2\right] + \frac{P_1}{F^4V}\left[8l_1 + 16l_2\right]. \tag{5.62}$$

In Ref. [64] the scale dependence of the coupling constants l_i with $i = 1, \ldots, 7$ is separated as

$$l_i = l_i^r + \gamma_i \lambda\,, \tag{5.63}$$

where

$$\gamma_1 = \frac{1}{3}\,, \qquad \gamma_2 = \frac{2}{3}\,, \qquad \gamma_4 = 2\,. \tag{5.64}$$

It is straightforward to check that the divergences in Eqs. (5.61) and (5.62) cancel with this set of γ_1, γ_2, and γ_4. The renormalized coupling constants l_i^r can be related to scale-independent constants $\bar{l}_i$ by

$$l_i^r = \frac{\gamma_i}{2(4\pi)^2}\left[\bar{l}_i + \log(m_\pi^2/\mu^2)\right], \tag{5.65}$$

where m_π is the mass of the pion and

$$\bar{l}_1 = -2.3 \pm 3.7\,, \qquad \bar{l}_2 = 6.0 \pm 1.3\,, \qquad \bar{l}_4 = 4.3 \pm 0.9\,, \tag{5.66}$$

see Ref. [64]. We perform the calculation at scale $V^{-1/4}$ so that

$$l_i^r = \frac{\gamma_i}{2(4\pi)^2}\left[\bar{l}_i + \log(m_\pi^2\sqrt{V})\right] \approx \frac{\gamma_i}{2(4\pi)^2}\bar{l}_i \tag{5.67}$$

since $m_\pi^2\sqrt{V} \approx 1$ in the ε expansion (see Sec. 2.4). Note that the finite-volume corrections to Σ and F are independent of the scale.

We calculate the renormalized two-loop propagator P_6^r at scale $V^{-1/4}$ numerically and obtain

$$(a) \quad P_6^r = 0.016(2)\,, \qquad\qquad (b) \quad P_6^r = -0.028(2) \tag{5.68}$$

for geometries (a) and (b), see Figs. 5.2 and 5.3. The finite-volume corrections to Σ for $F = 90$ MeV and $L = 1.71$ fm at NLO and NNLO are given by

$$\frac{\Sigma_{\text{eff}}^{\text{NLO}}}{\Sigma} = 1.1454\,, \qquad\qquad \frac{\Sigma_{\text{eff}}^{\text{NNLO}}}{\Sigma} = 1.20(2)\,, \tag{5.69}$$

where the error is due to the uncertainty in $\bar{l}_4$. Note that Σ_{eff} is independent of the choice of geometry (a) or (b). The finite-volume corrections to F for $F = 90$ MeV and $L = 1.71$ fm at NLO and NNLO are given by

$$\begin{aligned} (a) \quad & \frac{F_{\text{eff}}^{\text{NLO}}}{F} = 1.3192\,, && \frac{F_{\text{eff}}^{\text{NNLO}}}{F} = 1.26(2)\,, \\ (b) \quad & \frac{F_{\text{eff}}^{\text{NLO}}}{F} = 1.06816\,, && \frac{F_{\text{eff}}^{\text{NNLO}}}{F} = 1.07(4)\,, \end{aligned} \tag{5.70}$$

for geometries (a) and (b), where the error is due to the uncertainty in $\bar{l}_1$, $\bar{l}_2$, and P_6^r. Therefore we confirm the picture obtained in Sec. 4.5 at NLO that the finite-volume corrections to F can be largely

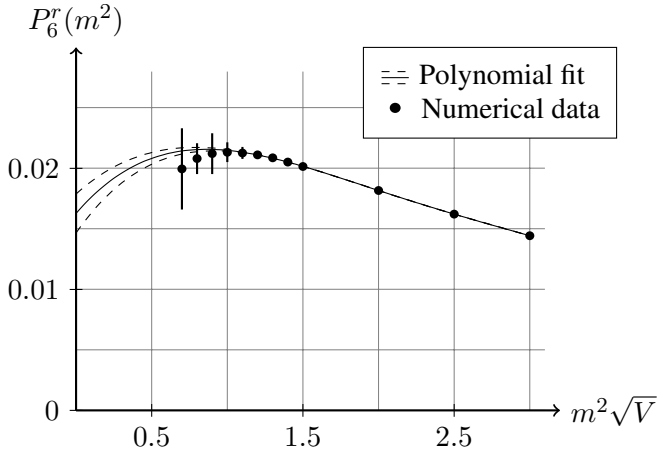


Figure 5.2: Extrapolation of $P_6^r = \lim_{m\to 0} P_6^r(m^2)$ for geometry (a) at scale $V^{-1/4}$. We fit a polynomial of order four. The dashed lines enclose the one-sigma error band.

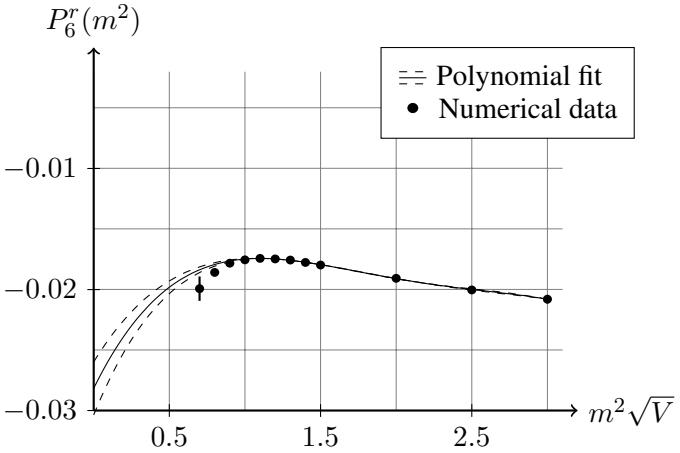


Figure 5.3: Extrapolation of $P_6^r = \lim_{m\to 0} P_6^r(m^2)$ for geometry (b) at scale $V^{-1/4}$. We fit a polynomial of order four. The dashed lines enclose the one-sigma error band.

reduced by an asymmetric geometry with one large spatial dimension instead of one large temporal dimension.

The coefficients $\Upsilon_2, \ldots, \Upsilon_5$, whose corresponding non-universal terms do not depend on the chemical potential, are independent of the choice of geometry (a) or (b). This is expected since only the chemical potential has a preferred direction and breaks the permutation symmetry of all four dimensions. The coefficients $\Upsilon_6, \ldots, \Upsilon_{10}$ are affected by the choice of geometry (a) or (b) through the following combinations of propagators,

$$P_4 + 2P_5\,, \qquad P_4 + 4P_5\,, \qquad P_5\,. \tag{5.71}$$

We give their values

$$\begin{aligned} &(a) \quad P_4 + 2P_5 = -0.023\,, && P_4 + 4P_5 = -0.033\,, && P_5 = -0.005\,, \\ &(b) \quad P_4 + 2P_5 = -0.003\,, && P_4 + 4P_5 = 0.007\,, && P_5 = 0.005 \end{aligned} \tag{5.72}$$

at scale $V^{-1/4}$ for geometry (a) and (b). Note that the contribution of the propagators is reduced significantly for the combinations $P_4 + 2P_5$ and $P_4 + 4P_5$ in geometry (b). In chapter 6 we show

numerically that the non-universal effects are indeed smaller for geometry (b). The coefficient Υ_1 does not have any physical effect.

Chapter 6

Results from lattice QCD

In this chapter we use numerical data for the spectrum of the Dirac operator in order to determine the low-energy constants Σ and F. We employ the dynamical two-flavor configurations of JLQCD [32, 65] on a $16^3 \times 32$ lattice with lattice spacing $a = 0.107(3)$ fm and quark mass $am = 0.002$. The quark fields and gluon fields have periodic boundary conditions in all four dimensions. In order to access the low-energy constant F we allow for valence quarks with nonzero imaginary chemical potential $i\mu$. The simulations are performed in two geometries

$$\begin{aligned} (a) \qquad & L_0 = 32a\,, \qquad L_1 = L_2 = L_3 = 16a\,, \\ (b) \qquad & L_3 = 32a\,, \qquad L_0 = L_1 = L_2 = 16a\,. \end{aligned} \tag{6.1}$$

In Sec. 6.1 we determine Σ by a fit to the distribution of the lowest Dirac eigenvalue without chemical potential. In Sec. 6.2 we determine F by a fit to the eigenvalue shift due to a nonzero chemical potential. For a detailed explanation of both eigenvalue correlation functions we refer to Sec. 3.4 of this thesis.

In Ref. [66] a similar method to obtain the low-energy constants F and Σ was used in an exploratory, qualitative study. In the following we obtain quantitative results for Σ and F. A publication containing the results of this chapter is in preparation [67].

6.1 The low-energy constant Σ

In this section we fit the distribution of the lowest Dirac eigenvalue to the analytic formula of RMT, see Sec. 3.4. The result of the fit is given by

$$a^3\Sigma_{\text{eff}} = 0.00208(2)\,, \tag{6.2}$$

or in physical units

$$\Sigma_{\text{eff}} = (235(6)(1)\ \text{MeV})^3\,, \tag{6.3}$$

where the errors are due to the uncertainty in a (left) and due to statistics (right). Note that the error in a dominates the error in Σ_{eff}. Since Σ_{eff} is independent of the choice of geometry (a) or (b), see chapter 5, we only perform the fit in one geometry.

The best fit, displayed in Fig. 6.1, has a $\chi^2/\text{dof} = 2.9$ which is uncomfortably large. The systematic errors in the shape of the lowest eigenvalue distribution due to non-universal terms in the finite-volume effective Lagrangian are thus quite large. Nevertheless, Σ_{eff} is not sensitive to the shape of the distribution but merely to the overall scale. Therefore we can assume that the fit gives a reasonable result.

We include the NNLO finite-volume corrections of Sec. 5.4 and find

$$\Sigma = \frac{\Sigma_{\text{eff}}}{1.20(2)} = (221(6)(1)(1)\ \text{MeV})^3\,, \tag{6.4}$$

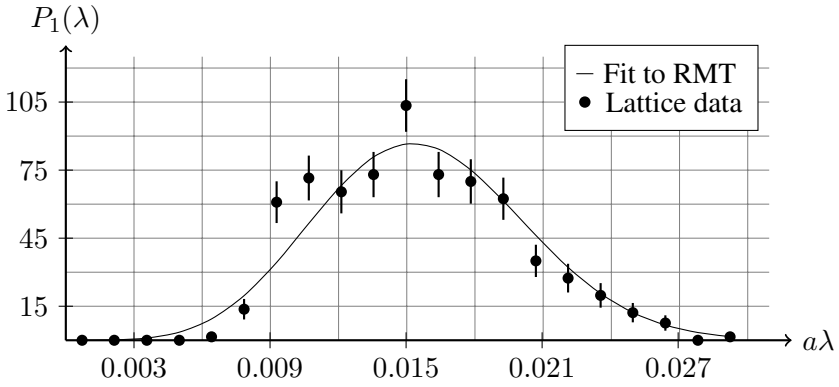


Figure 6.1: Fit to lowest eigenvalue distribution $P_1(\lambda)$ in geometry (b) with $\chi^2/\text{dof} = 2.9$. The best fit is given by $a^3\Sigma_{\text{eff}} = 0.00208(2)$.

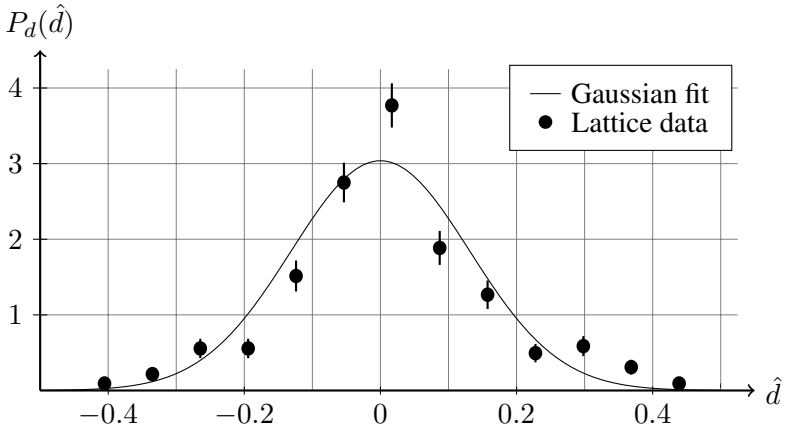


Figure 6.2: Gaussian fit to distribution $P_d(\hat{d})$ for $a\mu = 0.01$ in geometry (a) with $\chi^2/\text{dof} = 4.2$.

where the rightmost error is due to the uncertainty in the finite-volume corrections. Therefore

$$m\Sigma V = 0.452(4)(7)\,, \tag{6.5}$$

where the errors are due to statistics (left) and due to the uncertainty in the finite-volume corrections (right). We conclude that the ε expansion is indeed applicable for our choice of V and m, see Sec. 2.4.

6.2 The low-energy constant F

In this section we perform a fit to the eigenvalue shift P_d due to a nonzero imaginary chemical potential $i\mu$, see Sec. 3.4, in order to determine F_{eff}. Note that F_{eff} and some coefficients of the non-universal terms depend on the choice of geometry (a) or (b). In Sec. 5.4 we found that in geometry (a) there are larger finite-volume corrections and we can expect a larger contribution from non-universal terms. This is indeed confirmed by the fits in Figs. 6.2 and 6.3. In the case of geometry (a) we have a $\chi^2/\text{dof} = 4.2$, while $\chi^2/\text{dof} = 0.91$ in the case of geometry (b). Due to this large deviation from a Gaussian shape in case (a) we conclude that in this case a Gaussian fit is not applicable.[1] Nevertheless, we perform the fit in both geometries below. The result for $a\mu = 0.01$ in

[1] This problem could be solved by a calculation of P_d including the non-universal terms of Eq. (5.13). This is, however, beyond the scope of this thesis.

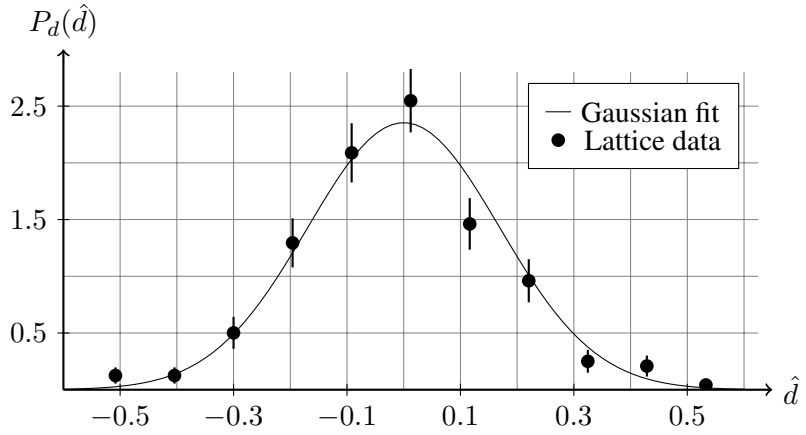


Figure 6.3: Gaussian fit to distribution $P_d(\hat{d})$ for $a\mu = 0.01$ in geometry (b) with $\chi^2/\text{dof} = 0.91$.

geometries (a) and (b) is given by

$$\begin{aligned} (a) \quad & F_{\text{eff}} = 67(5)(2)(1)\ \text{MeV}\,, \\ (b) \quad & F_{\text{eff}} = 86(4)(2)(1)\ \text{MeV}\,, \end{aligned} \tag{6.6}$$

where the errors are due to statistics (left), the uncertainty in a (center), and the error in Σ (right). We include the NNLO finite-volume corrections of Sec. 5.4 and find

$$\begin{aligned} (a) \quad & F = 53(4)(2)(1)(1)\ \text{MeV}\,, \\ (b) \quad & F = 80(4)(2)(1)(3)\ \text{MeV}\,, \end{aligned} \tag{6.7}$$

where the rightmost error is due to the uncertainty in the finite-volume corrections. Note that the results of geometries (a) and (b) are not compatible with each other. Indeed, the strong contribution of non-universal terms in geometry (a) has a significant effect on the result of the fit for F_{eff}, and thus we discard the result of geometry (a). Our final result for F,

$$F = 80(4)(2)(1)(3)\ \text{MeV}\,, \tag{6.8}$$

agrees within the errors with the result of

$$F = 87(6)\ \text{MeV} \tag{6.9}$$

obtained in a study of meson correlators on the same lattice configurations [68].

Note that it is justified to apply the theory of chapter 5 since

$$\mu^2 F^2 V = 0.025 \tag{6.10}$$

for $a\mu = 0.01$, and therefore higher orders in the chemical potential can be neglected.

Part III

Schematic models of QCD

Chapter 7

The Dirac spectrum at nonzero temperature and topology

In chapters 3-6 of this thesis we observed that in the limit of small quark masses m in a finite volume V with

$$mV\Sigma = \mathcal{O}(1) \tag{7.1}$$

QCD is effectively described by the chiral unitary ensemble of random matrix theory. In this limit RMT can be used to obtain exact results for quantities such as spectral correlation functions of Dirac eigenvalues. Random matrix models can, however, also be used as schematic models that qualitatively describe certain features of QCD. In this chapter we extend the work of Refs. [69, 70, 71] and calculate the quenched spectral density in a schematic random matrix model for, both, nonzero temperature and nonzero topology.

For a review of schematic random matrix models we refer to Ref. [37].

7.1 A schematic random matrix model

We use the random matrix model of Ref. [72] which is defined by the matrix Dirac operator

$$D = \begin{pmatrix} 0 & iW + i\mu \ \mathbb{1}_{N,N+\nu} \\ iW^\dagger + i\mu \ \mathbb{1}_{N+\nu,N} & 0 \end{pmatrix}, \tag{7.2}$$

where W is a complex $N \times (N+\nu)$ matrix, $\mu \in \mathbb{R}$, $\mathbb{1}_{N,N+\nu}$ is the identity matrix with N rows and $N+\nu$ columns, and ν is identified with the topological charge of the theory. This strongly resembles the random matrix model defined in Sec 3.2, where we multiplied the parameter μ with a second random matrix instead of the identity matrix. We can identify $i\mu$ with an imaginary chemical potential as in Sec. 3.2. Since the effect of the first Matsubara frequency is equal to an imaginary chemical potential, see Ref. [72], we can interpret μ also as temperature.

7.2 The partition function

In order to calculate the quenched spectrum we consider the partition function for $N_f = 0$ and $N_v = 1$,

$$Z = \int d[W] \frac{\det(D+m)}{\det(D+m')} \exp\left[-N\Sigma^2 \operatorname{Tr}(W^\dagger W)\right], \tag{7.3}$$

where m is the mass of the fermionic valence quark, m' is the mass of the bosonic valence quark, and the integral is over the real and imaginary part of the elements of the complex matrix W. We set

$\Sigma = 1$ and reinstate it later by

$$m \to \Sigma m\,, \qquad \mu \to \Sigma \mu\,. \tag{7.4}$$

We express the bosonic determinant as an integral over the real and imaginary part of complex N-dimensional vectors φ_l and $(N+\nu)$-dimensional vectors φ_r and write the fermionic determinant as an integral over vectors of anticommuting variables $\psi_l, \bar{\psi}_l, \psi_r, \bar{\psi}_r$ of dimension N and $N+\nu$. The result is given by

$$\begin{aligned} Z = \int d[\bar{\psi}\psi] d[\bar{\varphi}\varphi] \exp\big[& -m(\bar{\psi}_l\psi_l + \bar{\psi}_r\psi_r) - i\mu(\bar{\psi}_l\psi_r + \bar{\psi}_r\psi_l) \\ & - m'(\bar{\varphi}_l\varphi_l + \bar{\varphi}_r\varphi_r) - i\mu(\bar{\varphi}_l\varphi_r + \bar{\varphi}_r\varphi_l)\big] \\ \times \prod_{i=1}^{N}\prod_{j=1}^{N+\nu} \int d[W_{ij}] \exp\big[& -i\bar{\psi}_l^i W_{ij}\psi_r^j - i\bar{\psi}_r^j W_{ij}^*\psi_l^i - i\bar{\varphi}_l^i W_{ij}\varphi_r^j \\ & - i\bar{\varphi}_r^j W_{ij}^*\varphi_l^i - N W_{ij}^* W_{ij}\big], \end{aligned} \tag{7.5}$$

where φ_l^i is the i-th component of vector φ_l, $\bar{\varphi}_l^i = (\varphi_l^i)^\dagger$ for $i = 1, \ldots, N$, and $\bar{\varphi}_r^j = (\varphi_r^j)^\dagger$ for $j = 1, \ldots, N+\nu$. The scalar products of N-dimensional vectors v with $(N+\nu)$-dimensional vectors w are defined as

$$v^\dagger w = v^\dagger (\mathbb{1}_{N,N+\nu}\, w)\,. \tag{7.6}$$

The mass m' shall have a positive real part, so that the bosonic integrals converge. We integrate over the random matrix W and find

$$\begin{aligned} I &= \prod_{i,j} \int d[W_{ij}] \exp\big[-i\bar{\psi}_l^i W_{ij}\psi_r^j - i\bar{\psi}_r^j W_{ij}^*\psi_l^i - i\bar{\varphi}_l^i W_{ij}\varphi_r^j - i\bar{\varphi}_r^j W_{ij}^*\varphi_l^i - N W_{ij}^* W_{ij}\big] \\ &= \exp\left[\frac{1}{N}[a_1 a_2 - b_1 b_2 + \alpha_1\alpha_2 - \beta_1\beta_2]\right], \end{aligned} \tag{7.7}$$

where we ignore irrelevant overall constants, and

$$\begin{aligned} a_1 &= \sum_j \bar{\psi}_r^j \psi_r^j\,, & a_2 &= \sum_i \bar{\psi}_l^i \psi_l^i\,, & \alpha_1 &= \sum_j \bar{\varphi}_r^j \psi_r^j\,, \\ \alpha_2 &= \sum_i \bar{\psi}_l^i \varphi_l^i\,, & \beta_1 &= \sum_j \bar{\psi}_r^j \varphi_r^j\,, & \beta_2 &= \sum_i \bar{\varphi}_l^i \psi_l^i\,, \\ b_1 &= \sum_j \bar{\varphi}_r^j \varphi_r^j\,, & b_2 &= \sum_i \bar{\varphi}_l^i \varphi_l^i\,. \end{aligned} \tag{7.8}$$

7.3 Compact Hubbard-Stratonovich transformation

The four-point interactions can be reduced to quadratic terms by a Hubbard-Stratonovich transformation. There is a compact and a non-compact version of this transformation, and we shall see below that the well-known compact version fails for the theory defined by Eq. (7.3).

In both versions fermionic variables α_1 and α_2 are transformed as

$$\begin{aligned} \exp\left[\frac{1}{N}[\alpha_1\alpha_2]\right] &= \int d\sigma d\sigma^* \exp\left[-N\left(\sigma + \frac{1}{N}\alpha_1\right)\left(\sigma^* + \frac{1}{N}\alpha_2\right) + \frac{1}{N}\alpha_1\alpha_2\right] \\ &= \int d\sigma d\sigma^* \exp\left[-N\sigma\sigma^* - \sigma\alpha_2 - \alpha_1\sigma^*\right], \end{aligned} \tag{7.9}$$

where we introduce an integral over Grassmann variables σ and σ^*. In the compact version the bosonic variables a_1 and a_2 are transformed as

$$\begin{aligned}\exp\left[\frac{1}{N}[a_1 a_2]\right] &= \int ds ds^* \exp\left[-N\left(s+\frac{1}{N}a_1\right)\left(s^*+\frac{1}{N}a_2\right)+\frac{1}{N}a_1 a_2\right] \\ &= \int ds ds^* \exp\left[-N s s^* - s a_2 - a_1 s^*\right], \end{aligned} \tag{7.10}$$

where we introduce an integral over the real and imaginary part of a complex number s. We apply the compact transformation to Eq. (7.7) and find

$$\begin{aligned} Z = \int d[\bar\psi\psi] d[\bar\varphi\varphi]\ \exp\big[&-m(\bar\psi_l\psi_l+\bar\psi_r\psi_r) - i\mu(\bar\psi_l\psi_r+\bar\psi_r\psi_l) \\ &- m'(\bar\varphi_l\varphi_l+\bar\varphi_r\varphi_r) - i\mu(\bar\varphi_l\varphi_r+\bar\varphi_r\varphi_l)\big] \\ \times \int ds_1 ds_1^* ds_2 ds_2^* d\sigma_1 d\sigma_1^* d\sigma_2 d\sigma_2^*\ &\exp\big[-N\left[s_1 s_1^* + s_2 s_2^* + \sigma_1\sigma_1^* + \sigma_2\sigma_2^*\right]\big] \\ \times \exp\big[&-s_1\bar\psi_l\psi_l - \bar\psi_r\psi_r s_1^* - i s_2\bar\varphi_l\varphi_l - i\bar\varphi_r\varphi_r s_2^* - \sigma_1\bar\psi_l\varphi_l \\ &- \bar\varphi_r\psi_r\sigma_1^* - i\sigma_2\bar\varphi_l\psi_l - i\bar\psi_r\varphi_r\sigma_2^*\big]. \end{aligned} \tag{7.11}$$

Next we would like to integrate over the fields φ and ψ. However, the interchange of the integral over φ with the integral over s_2 does not leave Z invariant since the integrals over φ do not converge uniformly in s_2. Therefore we discard the compact Hubbard-Stratonovich transformation.

7.4 Non-compact Hubbard-Stratonovich transformation

In the non-compact version of the Hubbard-Stratonovich transformation [70] the bosonic variables a and b are transformed as

$$\exp\left[-a^2+b^2\right] = \frac{i}{\pi}\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dr\ r\ \exp\big[-r^2 - 2iar\cosh s - 2ibr\sinh s\big], \tag{7.12}$$

where a and $\mathrm{Re}(a^2-b^2)$ are restricted to $\mathbb{R}^+$. In our case we want to transform

$$\exp\left[-\frac{1}{N}b_1 b_2\right] = \exp\left[\left(\frac{1}{\sqrt{4N}}b_1 - \frac{1}{\sqrt{4N}}b_2\right)^2 - \left(\frac{1}{\sqrt{4N}}b_1 + \frac{1}{\sqrt{4N}}b_2\right)^2\right], \tag{7.13}$$

where $b_1, b_2 \in \mathbb{R}^+$ (up to a region of measure zero), and therefore the non-compact transformation can be applied. We find

$$\begin{aligned}\exp\left[-\frac{1}{N}b_1 b_2\right] = \frac{iN}{\pi}\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dr\ r\ \exp[&-Nr^2 - i(b_1+b_2)r\cosh s \\ &- i(b_1-b_2)r\sinh s]. \end{aligned} \tag{7.14}$$

Note that the integrals over φ_l and φ_r only converge if we introduce an infinitesimal shift of the integration contour of r that does not affect the Hubbard-Stratonovich transformation. This leads to

$$\begin{aligned}\exp\left[-\frac{1}{N}b_1 b_2\right] &= \frac{iN}{\pi}\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dr\ r\ \exp[-Nr^2 - i(b_1+b_2)(r-i\varepsilon)\cosh s \\ &\qquad - i(b_1-b_2)(r-i\varepsilon)\sinh s] \\ &= \frac{iN}{\pi}\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dr\ r\ \exp[-Nr^2 - ib_1(r-i\varepsilon)e^s - ib_2(r-i\varepsilon)e^{-s}]. \end{aligned} \tag{7.15}$$

Note the analogy to the compact Hubbard-Stratonovich transformation of Eq. (7.10)

$$\exp\left[-\frac{1}{N}b_1 b_2\right] \propto \int_0^{2\pi} d\varphi \int_0^{\infty} dr\, r\, \exp\left[-Nr^2 - ib_1 re^{i\varphi} - ib_2 re^{-i\varphi}\right]. \tag{7.16}$$

We apply the non-compact transformation to the partition function and find

$$\begin{aligned} Z = \int d[\bar\psi\psi] d[\bar\varphi\varphi] d\sigma_1 d\sigma_1^* d\sigma_2 d\sigma_2^* \int_0^{2\pi} d\varphi_1 \int_0^{\infty} dr_1\, r_1 \int_{-\infty}^{\infty} d\varphi_2 \int_{-\infty}^{\infty} dr_2\, r_2 \\ \times \exp\big[-N(m^2 - m'^2 + r_1^2 + r_2^2 + \sigma_1\sigma_1^* + \sigma_2\sigma_2^*) + 2Nm\, r_1\cos(\varphi_1) \\ - i2Nm'(r_2 - i\varepsilon)\cosh(\varphi_2) - i\mu(\bar\psi_l\psi_r + \bar\psi_r\psi_l) \\ - i\mu(\bar\varphi_l\varphi_r + \bar\varphi_r\varphi_l) - \left(\bar\psi_l\psi_l\right) r_1 e^{i\varphi_1} - \left(\bar\psi_r\psi_r\right) r_1 e^{-i\varphi_1} \\ - i\left(\bar\varphi_l\varphi_l\right)(r_2 - i\varepsilon)e^{\varphi_2} - i\left(\bar\varphi_r\varphi_r\right)(r_2 - i\varepsilon)e^{-\varphi_2} - \sigma_1(\bar\psi_l\varphi_l) \\ - (\bar\varphi_r\psi_r)\sigma_1^* - i\sigma_2(\bar\varphi_l\psi_l) - i(\bar\psi_r\varphi_r)\sigma_2^*\big]. \end{aligned} \tag{7.17}$$

Next we interchange the integral over the fields φ with the integral over r_2, so that

$$\begin{aligned} Z = \int d[\sigma] \int_0^{2\pi} d\varphi_1 \int_0^{\infty} dr_1\, r_1 \int_{-\infty}^{\infty} d\varphi_2 \int_{-\infty}^{\infty} dr_2\, r_2 \\ \times \exp\big[-N(m^2 - m'^2 + r_1^2 + r_2^2 + \sigma_1\sigma_1^* + \sigma_2\sigma_2^*) + 2Nm\, r_1\cos(\varphi_1) \\ - i2Nm'(r_2 - i\varepsilon)\cosh(\varphi_2)\big] \\ \times \mathrm{Sdet}\begin{pmatrix} r_1 e^{i\varphi_1} & i\mu & -\sigma_1 & 0 \\ i\mu & r_1 e^{-i\varphi_1} & 0 & i\sigma_2^* \\ i\sigma_2 & 0 & i(r_2 - i\varepsilon)e^{\varphi_2} & i\mu \\ 0 & -\sigma_1^* & i\mu & i(r_2 - i\varepsilon)e^{-\varphi_2} \end{pmatrix}^N \\ \times \mathrm{Sdet}\begin{pmatrix} r_1 e^{i\varphi_1} & -\sigma_1 \\ i\sigma_2 & i(r_2 - i\varepsilon)e^{\varphi_2} \end{pmatrix}^{\nu}, \end{aligned} \tag{7.18}$$

where $d[\sigma] = d\sigma_1 d\sigma_1^* d\sigma_2 d\sigma_2^*$, and we only considered $\nu \geq 0$, without loss of generality. For convenience we rescale the Grassmann variables

$$\begin{aligned} \sigma_1 &\to -\sigma_1 e^{i\varphi_1}, & \sigma_1^* &\to -\sigma_1^* e^{-i\varphi_1}, \\ \sigma_2 &\to -i\sigma_2 e^{\varphi_2}, & \sigma_2^* &\to -i\sigma_2^* e^{-\varphi_2} \end{aligned} \tag{7.19}$$

and use the identity [7]

$$\mathrm{Sdet}\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \frac{\det(A - BD^{-1}C)}{\det(D)} \tag{7.20}$$

to factor the angular dependence of the determinants. The result is given by

$$\begin{aligned}
Z = &\int d[\sigma] \int_0^\infty dr_1\, r_1 \int_{-\infty}^\infty dr_2\, r_2 \\
&\times \exp\left[-N(m^2 - m'^2 + r_1^2 + r_2^2 + \sigma_1\sigma_1^* - \sigma_2\sigma_2^*)\right] \\
&\times \mathrm{Sdet} \begin{pmatrix} r_1 & i\mu & \sigma_1 & 0 \\ i\mu & r_1 & 0 & \sigma_2^* \\ \sigma_2 & 0 & i(r_2 - i\varepsilon) & i\mu \\ 0 & \sigma_1^* & i\mu & i(r_2 - i\varepsilon) \end{pmatrix}^N \mathrm{Sdet} \begin{pmatrix} r_1 & \sigma_1 \\ \sigma_2 & i(r_2 - i\varepsilon) \end{pmatrix}^\nu \\
&\times \int_0^{2\pi} d\varphi_1 \int_{-\infty}^\infty d\varphi_2 \exp\big[2Nm\, r_1 \cos(\varphi_1) + i\varphi_1\nu \\
&\qquad\qquad - i2Nm'(r_2 - i\varepsilon)\cosh(\varphi_2) - \varphi_2\nu\big]\,. \qquad (7.21)
\end{aligned}$$

We use the integral representations of the I and K Bessel functions [73],

$$\begin{aligned}
I_\nu(\sqrt{ab}) &= \frac{(-1)^\nu}{2\pi} \left(\frac{a}{b}\right)^{\frac{\nu}{2}} \int_0^{2\pi} d\varphi\, \exp\left(-\frac{a}{2}e^{i\varphi} - \frac{b}{2}e^{-i\varphi} + i\nu\varphi\right), \\
K_\nu(\sqrt{ab}) &= \frac{1}{2}\left(\frac{a}{b}\right)^{\frac{\nu}{2}} \int_{-\infty}^\infty d\varphi\, \exp\left(-\frac{a}{2}e^{\varphi} - \frac{b}{2}e^{-\varphi} + \nu\varphi\right) \\
&= \frac{1}{2}\left(\frac{b}{a}\right)^{\frac{\nu}{2}} \int_{-\infty}^\infty d\varphi\, \exp\left(-\frac{a}{2}e^{\varphi} - \frac{b}{2}e^{-\varphi} - \nu\varphi\right), \qquad (7.22)
\end{aligned}$$

where the integral representation of K only converges for $\mathrm{Re}(a), \mathrm{Re}(b) > 0$, and find

$$\begin{aligned}
Z = &\int d[\sigma] \int_0^\infty dr_1\, r_1 \int_{-\infty}^\infty dr_2\, r_2 \\
&\times \exp\left[-N(m^2 - m'^2 + r_1^2 + r_2^2 + \sigma_1\sigma_1^* - \sigma_2\sigma_2^*)\right] \\
&\times \mathrm{Sdet} \begin{pmatrix} r_1 & i\mu & \sigma_1 & 0 \\ i\mu & r_1 & 0 & \sigma_2^* \\ \sigma_2 & 0 & i(r_2 - i\varepsilon) & i\mu \\ 0 & \sigma_1^* & i\mu & i(r_2 - i\varepsilon) \end{pmatrix}^N \mathrm{Sdet} \begin{pmatrix} r_1 & \sigma_1 \\ \sigma_2 & i(r_2 - i\varepsilon) \end{pmatrix}^\nu \\
&\times I_\nu(2Nm\, r_1) K_\nu(i2Nm'\,(r_2 - i\varepsilon))\,. \qquad (7.23)
\end{aligned}$$

Next we use Eq. (7.20) and integrate out the Grassmann numbers σ to obtain

$$\begin{aligned}
Z = &\int_0^\infty dr_1\, r_1 \int_{-\infty}^\infty dr_2\, r_2\, \exp\left[-N(m^2 - m'^2 + r_1^2 + r_2^2)\right] \\
&\times R_\nu^N(r_1, r_2 - i\varepsilon, \mu) \left(\frac{\mu^2 + r_1^2}{\mu^2 - (r_2 - i\varepsilon)^2}\right)^N \left(\frac{r_1}{ir_2 + \varepsilon}\right)^\nu \\
&\times I_\nu(2Nm\, r_1)\, K_\nu(i2Nm'\,(r_2 - i\varepsilon))\,, \qquad (7.24)
\end{aligned}$$

where

$$\begin{aligned}
R_\nu^N(r_1, r_2, \mu) = &\frac{r_1^2 r_2^2}{(\mu^2 + r_1^2)^2(\mu^2 - r_2^2)^2} + \left(1 - \frac{\mu^2}{(\mu^2 + r_1^2)(\mu^2 - r_2^2)}\right)^2 \\
&+ \frac{1}{N}\left[\frac{\mu^2(r_1^2 + r_2^2) - \nu(\mu^2 + r_1^2)(\mu^2 - r_2^2)}{(\mu^2 + r_1^2)^2(\mu^2 - r_2^2)^2}\right]. \qquad (7.25)
\end{aligned}$$

In order to access the eigenvalue spectrum we need to calculate the resolvent

$$G(m) = \frac{1}{Z(m,m)} \left(\partial_m Z(m,m')\right)_{m'=m} . \tag{7.26}$$

For $m = m'$ the mass-dependence of Z drops out, and therefore we calculate

$$G(m) \propto \left(\partial_m Z(m,m')\right)_{m'=m} \tag{7.27}$$

and re-introduce the correct normalization in the end. We use

$$\begin{aligned}\partial_m \left[\exp(-Nm^2) I_\nu(2Nm\, r_1)\right] &= N \exp(-Nm^2) \\ &\times \left[-2m I_\nu(2Nm\, r_1) + r_1 (I_{\nu-1}(2Nm\, r_1) + I_{\nu+1}(2Nm\, r_1))\right]\end{aligned} \tag{7.28}$$

and find

$$\begin{aligned}G \propto \int_0^\infty dr_1\, r_1 \int_{-\infty}^\infty dr_2\, r_2\, \exp\left(-N(r_1^2+r_2^2)\right) R_\nu^N(r_1, r_2 - i\varepsilon, \mu) \\ \times \left(\frac{\mu^2 + r_1^2}{\mu^2 - (r_2 - i\varepsilon)^2}\right)^N \left(\frac{r_1}{i r_2 + \varepsilon}\right)^\nu K_\nu(i2Nm\,(r_2 - i\varepsilon)) \\ \times \left[-2m I_\nu(2Nm\, r_1) + r_1 (I_{\nu-1}(2Nm\, r_1) + I_{\nu+1}(2Nm\, r_1))\right] .\end{aligned} \tag{7.29}$$

7.5 The limit of large matrices

In the large-N limit we can perform a saddle-point approximation of the integrals. The saddle points are determined by

$$r_1 = \frac{r_1}{\mu^2 + r_1^2} , \qquad\qquad r_2 = \frac{r_2}{\mu^2 - r_2^2} , \tag{7.30}$$

where we set $\varepsilon = 0$ for now. The dominating contributions arise from the nonzero saddle points

$$\tilde{r}_1 = \Sigma(\mu) , \qquad\qquad \tilde{r}_2 = \pm i \Sigma(\mu) \tag{7.31}$$

with

$$\Sigma(\mu) = \sqrt{1 - \mu^2} . \tag{7.32}$$

The pole and saddle-point structure of the r_2 integral is shown in Fig. 7.1. We deform the integration contour of r_2 such that it includes the saddle point at

$$\tilde{r}_2 = -i\Sigma . \tag{7.33}$$

Note that

$$R_\nu^N(\tilde{r}_1, \tilde{r}_2, \mu) = \tilde{r}_1^2 \tilde{r}_2^2 + (1-\mu^2)^2 + \frac{1}{N}\left[\mu^2(\tilde{r}_1^2 + \tilde{r}_2^2) - \nu\right] = -\frac{\nu}{N} , \tag{7.34}$$

and thus the factor R_ν^N vanishes for $N \to \infty$. Therefore we need to include all terms up to order $1/N$. We expand about the saddle point

$$r_1 = \tilde{r}_1 + \delta r_1, \qquad r_2 = \tilde{r}_2 + \delta r_2 \tag{7.35}$$

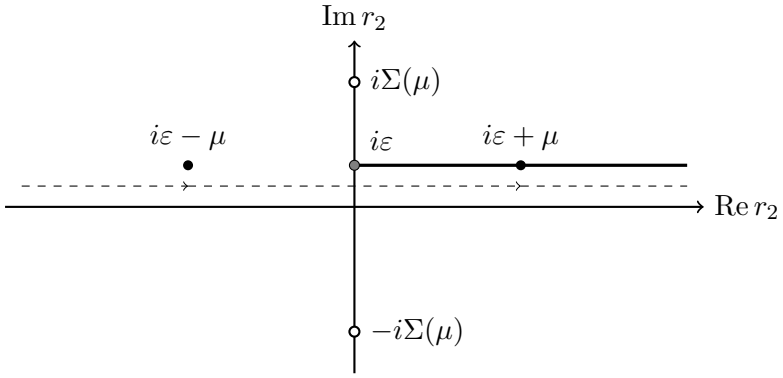


Figure 7.1: The complex plane of r_2 with $m \in i\mathbb{R}^+$.

and find

$$\begin{aligned} R_\nu^N &= 2\Sigma^3(\delta r_1 + i\delta r_2) + \Sigma^2(-3+8\mu^2)({\delta r_1}^2 - {\delta r_2}^2) \\ &\quad - 4i\Sigma^2(1-2\mu^2)\delta r_1\delta r_2 - \frac{\nu}{N}\,. \end{aligned} \tag{7.36}$$

Since $R_\nu^N = \mathcal{O}(1/\sqrt{N})$, we only need to expand the other contributions to leading order in $1/\sqrt{N}$. We find

$$\begin{aligned} S &= r_1^{2+\nu}(ir_2)^{1-\nu}(I_{\nu-1}(\hat{m}\,r_1) + I_{\nu+1}(\hat{m}\,r_1))K_\nu(i\hat{m}\,r_2) \\ &= \Sigma^3\big[(I_{\nu-1}+I_{\nu+1})K_\nu + \hat{m}(I'_{\nu-1}+I'_{\nu+1})K_\nu\delta r_1 \\ &\qquad + i\hat{m}(I_{\nu-1}+I_{\nu+1})K'_\nu\delta r_2\big] \\ &\quad + \big[\Sigma^2(2+\nu)\delta r_1 + \Sigma^2(1-\nu)i\delta r_2\big]\,(I_{\nu-1}+I_{\nu+1})K_\nu\,, \end{aligned} \tag{7.37}$$

where $\hat{m} = 2Nm$. The exponential becomes

$$\begin{aligned} L &= \exp[-N(r_1^2+r_2^2) + N\log[\mu^2+r_1^2] - N\log[\mu^2-r_2^2]] \\ &= \exp[-2N\Sigma^2({\delta r_1}^2 + {\delta r_2}^2))\left[1 + \frac{N\Sigma}{3}(2-8\mu^2)({\delta r_1}^3 + i{\delta r_2}^3)\right]. \end{aligned} \tag{7.38}$$

We combine L and R to

$$\begin{aligned} RL\exp(2N\Sigma^2({\delta r_1}^2+{\delta r_2}^2)) &= 2\Sigma^3(\delta r_1 + i\delta r_2) \\ &\quad + \Sigma^2(-3+8\mu^2)({\delta r_1}^2 - {\delta r_2}^2) - 4i\Sigma^2(1-2\mu^2)\delta r_1\delta r_2 - \frac{\nu}{N} \\ &\quad + \frac{2N\Sigma^4}{3}(2-8\mu^2)({\delta r_1}^3 + i{\delta r_2}^3)(\delta r_1 + i\delta r_2)\,. \end{aligned} \tag{7.39}$$

Next we include the contribution of S and keep only even terms in δr_1 and δr_2. This results in

$$\begin{aligned} SRL\exp(2N\Sigma^2({\delta r_1}^2+{\delta r_2}^2)) &= 2\Sigma^6\hat{m}(I'_{\nu-1}+I'_{\nu+1})K_\nu{\delta r_1}^2 \\ &\quad - 2\Sigma^6\hat{m}(I_{\nu-1}+I_{\nu+1})K'_\nu{\delta r_2}^2 + 2\Sigma^5(2+\nu)(I_{\nu-1}+I_{\nu+1})K_\nu{\delta r_1}^2 \\ &\quad - 2\Sigma^5(1-\nu)(I_{\nu-1}+I_{\nu+1})K_\nu{\delta r_2}^2 - \frac{\nu}{N}\Sigma^3(I_{\nu-1}+I_{\nu+1})K_\nu \\ &\quad + \Sigma^5(-3+8\mu^2)(I_{\nu-1}+I_{\nu+1})K_\nu({\delta r_1}^2 - {\delta r_2}^2) \\ &\quad + \frac{2N\Sigma^7}{3}(2-8\mu^2)(I_{\nu-1}+I_{\nu+1})K_\nu({\delta r_1}^4 - {\delta r_2}^4)\,. \end{aligned} \tag{7.40}$$

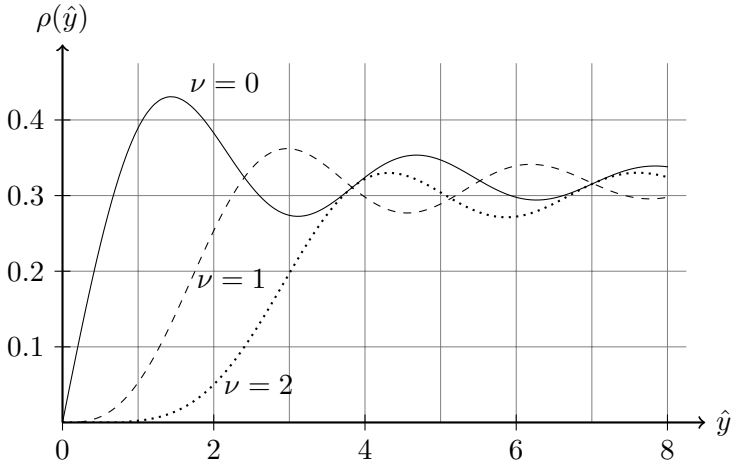


Figure 7.2: Microscopic spectral density for nonzero topology, $\Sigma = 1$, and $N_f = 0$.

Note that the integral over ${\delta r_1}^n$ is equal to the integral over ${\delta r_2}^n$ for $n = 2, 4$ and that

$$\int d(\delta r_1) \exp(-2N\Sigma^2 {\delta r_1}^2) = \sqrt{\frac{\pi}{2N\Sigma^2}}\,. \tag{7.41}$$

Therefore the terms proportional to ${\delta r_1}^2$ and ${\delta r_2}^2$ are suppressed by a factor of $1/4N\Sigma^2$, and we find

$$\begin{aligned} G &\propto \left[\Sigma\hat{m}(I'_{\nu-1} + I'_{\nu+1})K_\nu - \Sigma\hat{m}(I_{\nu-1} + I_{\nu+1})K'_\nu + (I_{\nu-1} + I_{\nu+1})K_\nu\right] \\ &= \frac{2}{\Sigma\hat{m}}(\nu^2 + \Sigma^2\hat{m}^2)I_\nu K_\nu + \frac{1}{2}\Sigma\hat{m}(I_{\nu-1} + I_{\nu+1})(K_{\nu+1} + K_{\nu-1})\,. \end{aligned} \tag{7.42}$$

For imaginary mass $\hat{m} = i\hat{y}$ this results in

$$\begin{aligned} G \propto \Bigg[&\frac{2}{\Sigma i\hat{y}}(\nu^2 - \Sigma^2\hat{y}^2) i^\nu J_\nu(\Sigma\hat{y})K_\nu(i\Sigma\hat{y}) + \frac{1}{2}\Sigma i\hat{y}\left[-i^{\nu+1}J_{\nu-1}(\Sigma\hat{y})K_{\nu+1}(i\Sigma\hat{y})\right. \\ &+ i^{\nu-1}J_{\nu-1}(\Sigma\hat{y})K_{\nu-1}(i\Sigma\hat{y}) + i^{\nu+1}J_{\nu+1}(\Sigma\hat{y})K_{\nu+1}(i\Sigma\hat{y}) \\ &\left.- i^{\nu-1}J_{\nu+1}(\Sigma\hat{y})K_{\nu-1}(i\Sigma\hat{y})\right]\Bigg]. \end{aligned} \tag{7.43}$$

We use the identity [73]

$$\mathrm{Im}\left[i^\nu K_\nu(iz)\right] = -\frac{\pi}{2}J_\nu(z)\,, \tag{7.44}$$

where J_ν are Bessel functions of the first kind, and calculate

$$\mathrm{Re}(G(y)) \propto 2\Sigma\hat{y}\left[J_\nu(\Sigma\hat{y})^2 - J_{\nu-1}(\Sigma\hat{y})J_{\nu+1}(\Sigma\hat{y})\right]. \tag{7.45}$$

We correct for the neglected overall constant and find

$$\rho(\hat{y}) = \frac{1}{2N\Sigma\pi}\,\mathrm{Re}(G(\hat{y})) = \frac{1}{2}\Sigma\hat{y}\left[J_\nu(\Sigma\hat{y})^2 - J_{\nu-1}(\Sigma\hat{y})J_{\nu+1}(\Sigma\hat{y})\right], \tag{7.46}$$

which is shown in Fig. 7.2 for $\mu = 0$. This is equal to the universal results of Refs. [72, 69, 70, 71] for $\mu = 0, \nu \neq 0$ and $\mu \neq 0, \nu = 0$.

Note that the correction due to nonzero temperature is merely a change of the chiral condensate from Σ to $\Sigma\sqrt{1-\mu^2}$. Also note that an infinitesimal positive real part of the mass $\hat{m}$ does not affect the analysis of this chapter and was therefore not included explicitly.

Chapter 8

The axial anomaly at nonzero temperature

In this chapter we discuss the effect of topology in schematic random matrix models at nonzero temperature (or imaginary chemical potential) in more detail. We point out and clarify a number of subtleties and non-universal effects that can arise when the effects of topology become important in such schematic random matrix models. In particular, we shall see that nontrivial normalization factors can occur which will be related to non-universal properties of the Dirac spectrum. These normalization factors significantly affect the distribution of topology in the corresponding schematic random matrix model and are therefore related to the axial anomaly.

The results of this chapter are published in Ref. [74].

8.1 Topology and the microscopic domain of QCD

Let us first consider QCD at zero temperature with N_f quark flavors, which for simplicity we take to be of equal mass m. The QCD partition function, $Z^{\rm QCD}$, can be considered at fixed θ-angle or at fixed topological charge ν. In the former case, the θ-angle can be introduced according to (see, e.g., [35, 37])

$$m_R \to m\, e^{i\theta/N_f}\,, \quad m_L \to m\, e^{-i\theta/N_f}\,, \tag{8.1}$$

where m_R (m_L) is the mass that couples right-handed (left-handed) quarks with anti-quarks of opposite chirality. We assume m to be real and positive.

If the number of right-handed and left-handed modes differs by ν, the product of the fermion determinants results in an overall factor $e^{i\nu\theta}$, and we have

$$Z^{\rm QCD}(m,\theta) = \sum_{\nu=-\infty}^{\infty} e^{i\nu\theta} Z_\nu^{\rm QCD}(m)\,. \tag{8.2}$$

This relation can be inverted to give the QCD partition function at fixed ν,

$$Z_\nu^{\rm QCD}(m) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{-i\nu\theta} Z^{\rm QCD}(m,\theta)\,, \tag{8.3}$$

which corresponds to a path integral restricted to gauge fields of topological charge ν.

It is generally assumed that the gauge field measure does not depend on the topological charge. When topological excitations can be considered as independent events, the central limit theorem dictates that the distribution of topological charge is given by

$$\mathcal{P}_\nu = \frac{1}{\sqrt{2\pi V\chi}} e^{-\nu^2/2V\chi}\,, \tag{8.4}$$

where V is the space-time volume and χ is the topological susceptibility at $\theta = 0$. In the quenched theory (or, equivalently, for heavy quarks), $\chi = \chi_q$ is a mass-independent constant, whereas for light

quarks, the topological charge is screened, resulting in a topological susceptibility at $\theta = 0$ given by [75, 76]

$$\chi = m\Sigma\,, \tag{8.5}$$

where Σ is the absolute value of the chiral condensate for $m = 0$ and $\theta = 0$.

In the microscopic domain of QCD, where the Compton wavelength of the pion is much larger than the size of the box, the mass- and θ-dependence of the QCD partition function is given by a random matrix theory (RMT) with the same global symmetries as those of QCD. Contrary to QCD, random matrix partition functions are defined in terms of integrals over the matrix elements of the Dirac operator at *fixed* topological charge rather than integrals over gauge fields at fixed θ-angle, which contain the sum over topological charges. In this chapter we study random matrix theories that are deformed by an imaginary chemical potential or temperature. The deformation parameter will be denoted by u.

Given a random matrix partition function at fixed ν, the partition function at fixed θ is defined by

$$Z^{\rm RMT}(m,\theta) = \sum_{\nu=-\infty}^{\infty} e^{i\nu\theta}\mathcal{P}_\nu\mathcal{N}_\nu Z_\nu^{\rm RMT}(m)\,, \tag{8.6}$$

where we separated a potentially nontrivial normalization factor $\mathcal{N}_\nu$ and a weight factor $\mathcal{P}_\nu$ from $Z_\nu^{\rm RMT}(m)$. The factor $\mathcal{P}_\nu$ corresponds to the quenched distribution of topological charge given in Eq. (8.4) (with $\chi = \chi_q$). Other ν-dependent normalization factors that may arise in random matrix models of the QCD partition function are included in the factor $\mathcal{N}_\nu$. One of our objectives is to discuss the significance of these two factors. We shall see in Sec. 8.3 that, contrary to QCD or chiral random matrix theories at $u = 0$ [36, 77], $\mathcal{N}_\nu$ can become a nontrivial function of the deformation parameter. On the other hand, as will be shown in Sec. 8.3, for light quarks it makes no difference whether or not $\mathcal{P}_\nu$ is included in the sum over ν [77].

A related question we would like to address in this chapter is which part of the Dirac spectrum is sensitive to the topological charge. The answer to this question could depend on the parameters of QCD or the chiral random matrix model, and we shall see below that this is actually the case. It also depends on the value of the quark mass, for which we distinguish the following scales, see Sec. 2.4: (i) The microscopic scale [36, 78] where $mV\Sigma$ is kept fixed in the thermodynamic limit. This corresponds to the ε-regime of chiral perturbation theory [29]. (ii) The chiral scale where $m\sqrt{V}$is kept fixed in the thermodynamic limit. This corresponds to the p-regime [28] of chiral perturbation theory. (iii) The macroscopic domain with $m \approx \Lambda_{\rm QCD}$. In the microscopic domain, the mass dependence of the QCD partition function is given by chiral random matrix theory. Actually, this domain extends beyond the microscopic domain all the way to the chiral scale. Therefore, it is appropriate to borrow the name "ergodic domain" from the theory of disordered systems [79] to distinguish the domain $m \ll 1/\Lambda_{\rm QCD}\sqrt{V}$ from the microscopic scaling domain. Note that we will sometimes consider the limit where $mV\Sigma$ approaches infinity with the understanding that the thermodynamic limit is taken first so that m is still in the microscopic domain.

The issues that will be addressed in this chapter are already manifest for one quark flavor, and for simplicity we will only discuss this case. The one-flavor QCD partition function, given by the average fermion determinant, is a function of the quark mass and of the θ-angle or the topological charge ν. If the eigenvalues of the (anti-Hermitian) Dirac operator at fixed ν are denoted by $i\lambda_k^\nu$, the QCD partition function at fixed ν can be expressed as

$$Z_\nu(m) = \left\langle \prod_k (i\lambda_k^\nu + m) \right\rangle, \tag{8.7}$$

where the average is over gauge fields with fixed ν.

We know that in the microscopic domain (and in fact in the ergodic domain) the mass dependence of the one-flavor QCD partition function in the sector of topological charge ν is given by [29, 35]

$$Z_\nu(m) \propto I_\nu(mV\Sigma)\,. \tag{8.8}$$

For large values of the argument the modified Bessel function I_ν becomes insensitive to its index ν, and thus Eq. (8.8) implies that the average fermion determinant does not depend on the topological charge when $mV\Sigma \gg 1$. In terms of Dirac eigenvalues one way to realize this is when only eigenvalues below this mass scale are affected by topology (see Eq. (8.7)). However, more exotic scenarios are also possible. It could be that eigenvalues beyond the microscopic domain are sensitive to the topological charge. If m is in the microscopic domain, this might result in a ν-dependent overall factor $\mathcal{N}_\nu$ that could depend on the deformation parameter u and restores the ν-independence of Z_ν for $mV\Sigma \gg 1$. To find out whether this scenario is realized, it makes sense to introduce the notion of the *topological domain of the Dirac spectrum*, which we define to be the part of the Dirac spectrum that is sensitive to the topological charge.

In QCD we have $\mathcal{N}_\nu = 1$ and, from Eqs. (8.2) and (8.8), the universal θ-dependence of the partition function is given by

$$Z^{\rm QCD}(m,\theta) \propto e^{mV\Sigma\cos\theta}\,. \tag{8.9}$$

It is plausible that the standard scenario discussed after Eq. (8.8) applies in this case, i.e., the topological domain of the Dirac spectrum does not extend beyond the microscopic domain. Exotic scenarios such as the one discussed above could occur in certain lattice formulations of QCD, and it would be interesting to test this directly. We shall further comment on this point in Sec. 8.7.

The ergodic domain of QCD is given by random matrix theory, but since the average fermion determinant is sensitive to *all* eigenvalues, it could be that deformations of the random matrix model result in a topological domain that extends beyond the microscopic domain. In this chapter we will see that this may happen in random matrix models at nonzero temperature/imaginary chemical potential.

The θ-dependence of random matrix theories at nonzero temperature was discussed before in the literature [80]. In that work the temperature was introduced such that it only affects the eigenmodes corresponding to nonzero Dirac eigenvalues. This resulted in the same θ-dependence as in the zero-temperature random matrix model [36]. Among others it was shown that the $O(m^2)$ term in the chiral Ward identity does not contribute in the chiral limit. This is not always the case. It was recently shown in the framework of chiral perturbation theory that in the superfluid phase of QCD at nonzero chemical potentials the $O(m^2)$ term cannot be neglected [81, 82]. In this chapter we will see that the $O(m^2)$ term in the chiral Ward identity contributes to the topological susceptibility for random matrix partition functions at nonzero temperature/imaginary chemical potential if the u-dependent normalization factor $\mathcal{N}_\nu$ is not included.

8.2 Chiral random matrix models

Definition of the random matrix model

The random matrix model for $N_f = 1$ in the sector of topological charge ν is defined by [36]

$$Z_\nu(m) = \mathcal{C}_{N,\nu} \int d[W]\,\det(D+m)\,e^{-\frac{1}{2}N\Sigma^2\,{\rm Tr}\,W^\dagger W} \tag{8.10}$$

with the random matrix Dirac operator defined by

$$D = \begin{pmatrix} 0 & iW \\ iW^\dagger & 0 \end{pmatrix}. \tag{8.11}$$

The integral is over the real and imaginary parts of the elements of the random matrix W, which has dimension $p \times q$. The Dirac operator (8.11) has $|p-q|$ exact zero modes. For this reason we interpret

$$\nu = p - q \tag{8.12}$$

as the topological charge. The total number of modes

$$N = p + q \tag{8.13}$$

will be interpreted as the volume. This corresponds to the choice of mode density

$$\frac{N}{V} = 1\,. \tag{8.14}$$

The normalization factor $\mathcal{C}_{N,\nu}$ is chosen such that the quenched partition function is normalized to unity, i.e.,

$$\mathcal{C}_{N,\nu} = \left(\frac{N\Sigma^2}{2\pi}\right)^{\frac{1}{4}(N^2-\nu^2)}. \tag{8.15}$$

We will consider this random matrix model in the presence of an imaginary chemical potential iu. Using the chiral representation of the γ-matrices, the u-deformed Dirac operator is given by [72, 83, 84, 85, 86]

$$D(u) = \begin{pmatrix} 0 & iW + iu\ \mathbb{1}_{p\times q} \\ iW^\dagger + iu\ \mathbb{1}_{q\times p} & 0 \end{pmatrix}, \tag{8.16}$$

where $(\mathbb{1}_{p\times q})_{k\ell} = \delta_{k\ell}$. Alternatively, u can be interpreted as a schematic temperature as was done in [72, 83, 84, 85]. The argument goes as follows. The temperature enters in the Dirac operator through the matrix elements corresponding to ∂_0, with eigenvalues that are given by the Matsubara frequencies. We include only the temperature dependence given by the lowest two Matsubara frequencies by adding the $p \times q$ temperature matrix $i\mathcal{T}$ to iW and $iW^\dagger$ in Eq. (8.11), where

$$\mathcal{T}_{kk} = \begin{cases} u & \text{for } k \le \min\{p,q\}/2\,, \\ -u & \text{for } k > \min\{p,q\}/2\,, \end{cases} \tag{8.17}$$

and $\mathcal{T}_{k\ell} = 0$ for $k \neq \ell$. Using the invariance of the integration measure under unitary transformations $W \to UWV^{-1}$ with $U \in \mathrm{U}(p)$ and $V \in \mathrm{U}(q)$, the temperature matrix can be transformed into a diagonal matrix with all diagonal matrix elements equal to u, so that the Dirac operator is given by Eq. (8.16).

In the following, we shall refer to the model defined by Eq. (8.16) as "model A".

Other random matrix models

Equation (8.16) is not the only way to introduce a nonzero temperature. Another possibility [80] is to first partition the N modes into $N_0 = p + q$ "zero" modes and a fixed number N_1 of "nonzero" modes, with $|\nu| = |p-q|$ actual zero modes of the Dirac operator. An $N_1 \times N_1$ temperature matrix

is then added to the "nonzero"-mode component of the Dirac operator, while the "zero"-mode matrix elements remain temperature independent. In terms of the Dirac operator (8.16) this means that we add to an $(N_1/2+p)\times(N_1/2+q)$ random matrix W a diagonal matrix with $N_1/2$ elements equal to iu and $\min\{p,q\}$ elements equal to zero. (This is technically equivalent to the model considered in Ref. [83, 84], although the physics background is different.) In the following, we shall refer to this model as "model B".

A third possibility is to add to W a random matrix with matrix elements that are proportional to u. This model was introduced in Ref. [40] for imaginary u (i.e., real chemical potential) to describe the microscopic domain of QCD at nonzero baryon chemical potential. For real u, this results in a model that differs from the original model (8.11) simply by a rescaling of the parameter Σ according to $\Sigma\to\Sigma/\sqrt{1+u^2}$. This model will be referred to as "model C". Note that this model does not have a chiral phase transition. A less trivial model is obtained by introducing two or more different imaginary chemical potentials [34], but we will not discuss this possibility in this chapter.

8.3 Normalization factors

In this section we solve the random matrix models that were introduced in the previous section. We will find that the universal θ-dependence is not recovered for model A at $u\neq 0$ unless additional normalization factors are included.

Solution of model A

In this subsection we solve the random matrix model A given by Eq. (8.10) with Dirac operator (8.16). The procedure is standard (see chapter 7 and Refs. [36, 72]). We start by writing the determinant as a Grassmann integral,

$$\det(D(u)+m)=\int d[\bar\psi\psi]\,\exp\left[\begin{pmatrix}\bar\psi_L\\ \bar\psi_R\end{pmatrix}^T(D(u)+m)\begin{pmatrix}\psi_R\\ \psi_L\end{pmatrix}\right], \tag{8.18}$$

and perform the Gaussian average over the random matrix elements. After a Hubbard-Stratonovich transformation and integration over the Grassmann variables we obtain the following σ-model,

$$Z_\nu^A(m)=\int d\sigma d\sigma^*\left(1+u^2|\sigma+m|^{-2}\right)^n(\sigma+m)^p(\sigma^*+m)^q\,e^{-\frac{1}{2}N\Sigma^2\sigma\sigma^*}, \tag{8.19}$$

where $n=\min\{p,q\}$. Notice that the ν-dependent normalization constant introduced in Eq. (8.10) has canceled.

After changing variables $\sigma\to\sigma-m$ and $\sigma^*\to\sigma^*-m$ in Eq. (8.19) and then expressing the integral over (σ,σ^*) in polar coordinates (r,φ), the angular integral results in a modified Bessel function, and the partition function is given by the remaining integral over r,

$$Z_\nu^A(m)=2\pi\int_0^\infty dr\,I_\nu(mN\Sigma^2r)r^{|\nu|+1}(r^2+u^2)^{(N-|\nu|)/2}e^{-\frac{1}{2}N\Sigma^2(r^2+m^2)}. \tag{8.20}$$

For large N, this partition function can be evaluated by a saddle-point approximation. For m in the ergodic domain, the saddle point in the broken phase is at $\bar r^2=1/\Sigma^2-u^2$. To leading order in $1/N$ the partition function is given by

$$Z_\nu^{A,\text{as}}(m)\propto I_\nu\big(mN\Sigma^A(u)\big)\tau^{|\nu|}, \tag{8.21}$$

where irrelevant prefactors have been ignored and

$$\Sigma^A(u) = \Sigma\tau \quad \text{with} \quad \tau(u) = \sqrt{1-\Sigma^2 u^2}\,. \tag{8.22}$$

A second-order phase transition to the chirally symmetric phase occurs at $u_c = 1/\Sigma$ [72].

The θ-dependence of the partition function is obtained after performing the sum over ν according to Eq. (8.6). As will be explained in detail in the next subsection, for light quarks the sum is not affected by the distribution function $\mathcal{P}_\nu$ [77]. We will therefore set $\mathcal{P}_\nu = 1$.

Let us first consider the case $u = 0$ and take $\mathcal{N}_\nu = 1$. Using the identity for Bessel functions given by [73, Eq. (9.6.33)]

$$\sum_{\nu=-\infty}^{\infty} I_\nu(x)\, t^\nu = e^{\frac{1}{2}x(t+1/t)}\,, \tag{8.23}$$

we find the universal result [35, 77]

$$Z^A(m,\theta)\big|_{u=0} \propto e^{mN\Sigma\cos\theta}\,. \tag{8.24}$$

This shows that we do not need nontrivial normalization factors at $u = 0$.

Now consider the case $u \neq 0$. Because of the factor $\tau^{|\nu|}$, in this case Eq. (8.21) depends on ν for $mN\Sigma^A(u) \gg 1$. This is a non-universal result and would also lead to a non-universal θ-dependence of Z^A after summing over ν. However, these problems can be fixed by introducing a u-dependent normalization factor

$$\mathcal{N}_\nu = \tau^{-|\nu|}\,. \tag{8.25}$$

Then with the replacement $\Sigma \to \Sigma^A(u)$ the sum over ν is the same as for $u = 0$. Again the sum is not affected by the distribution function $\mathcal{P}_\nu$, and we find the universal result

$$Z^A(m,\theta) \propto e^{mN\Sigma^A(u)\cos\theta}\,. \tag{8.26}$$

In QCD an imaginary chemical potential is equivalent to a constant vector field and can be gauged into the temporal boundary conditions of the fermion fields. This is not the case in random matrix theory, and therefore it should not come as a surprise that we need a ν-dependent normalization factor to recover the correct θ-dependence. In agreement with universality properties of Dirac spectra at fixed ν [69, 70, 71, 34] this normalization factor does not depend on the quark mass.

When u approaches $u_c = 1/\Sigma$, higher-order terms in the saddle-point approximation of Eq. (8.20) become important, and the integral has to be performed exactly. We will not further elaborate on this and only discuss the parameter domain where the leading-order saddle-point approximation is appropriate.

We will discuss further properties of model A in later sections but first turn to a discussion of the necessity of $\mathcal{P}_\nu$ and to a comparison with models B and C, where no u-dependent normalization factors will be needed.

On the necessity of $\mathcal{P}_\nu$

For large $|\nu|$ at fixed x the modified Bessel function can be approximated by (see Eq. (9.3.1) of [73])

$$I_\nu(x) \propto \frac{(x/2)^{|\nu|}}{|\nu|!}\,. \tag{8.27}$$

Therefore, if m is in the microscopic domain, the sum over ν in Eq. (8.6) is convergent without the Gaussian factor (8.4).

The sum over ν can be performed, up to exponentially suppressed contributions, using the approximation [35]

$$I_\nu(x) \propto \frac{1}{\sqrt{2\pi x}}\, e^{x-\nu^2/2x}\,, \tag{8.28}$$

which follows from the uniform large-order expansion of the modified Bessel function and is valid for $1 \ll |\nu| \ll x$ [73, Eq. (9.7.7)]. It makes no difference whether or not we include the factor $\mathcal{P}_\nu$ in Eq. (8.6) since

$$e^{-\frac{\nu^2}{2N}\left(\frac{1}{m\Sigma(u)}+\frac{1}{\chi_q}\right)} \propto e^{-\frac{\nu^2}{2mN\Sigma(u)}} \tag{8.29}$$

for m in the ergodic domain. The topological susceptibility at $\theta = 0$ is therefore given by Eq. (8.5). From the approximation (8.28) we also see that all topological sectors with $\nu^2 \ll mN\Sigma(u)$ contribute equally to the partition function.

It was argued by Damgaard [77] that the factor $\mathcal{P}_\nu$ should be absent in the sum over ν in Eq. (8.6), although he also pointed out that the quenched limit could not be taken properly in this case. Our point of view is that the presence of $\mathcal{P}_\nu$ is immaterial for m in the microscopic domain, but that $\mathcal{P}_\nu$ becomes important at length scales below the η' mass where it is believed to determine the local topological susceptibility and leads to the Witten-Veneziano formula for the η' mass [87, 88, 89, 90]. Beyond this scale the topological susceptibility at $\theta = 0$ is given by Eq. (8.5).

Comparison with models B and C

For fixed topological charge ν the partition function of model B is given by

$$Z^B_\nu(m) = \int d\sigma d\sigma^* (|\sigma+m|^2+u^2)^{N_1/2} (\sigma+m)^p (\sigma^*+m)^q e^{-\frac{1}{2}N\Sigma^2\sigma\sigma^*}\,, \tag{8.30}$$

or, after introducing polar coordinates,

$$Z^B_\nu(m) = 2\pi \int_0^\infty dr\; I_\nu(mN\Sigma^2 r) r^{N_0+1} \left(r^2+u^2\right)^{N_1/2} e^{-\frac{1}{2}N\Sigma^2(r^2+m^2)}\,. \tag{8.31}$$

Note that this partition function becomes independent of ν for large $mN\Sigma$. Since the correct θ-dependence is obtained at $u = 0$ this model does not require additional normalization factors. The sum over ν with $\mathcal{P}_\nu = 1$ results in

$$Z^B(m,\theta) = 2\pi \int_0^\infty dr\; e^{mN\Sigma^2 r\cos\theta} r^{N_0+1} \left(r^2+u^2\right)^{N_1/2} e^{-\frac{1}{2}N\Sigma^2(r^2+m^2)}\,. \tag{8.32}$$

Using a saddle-point approximation for large N, we find the universal θ-dependence

$$Z^B(m,\theta) \propto e^{mN\Sigma^B(u)\cos\theta}\,, \tag{8.33}$$

where [83, 84]

$$\frac{\Sigma^B(u)}{\Sigma} = \left[\frac{1-\Sigma^2u^2+\sqrt{(1+\Sigma^2u^2)^2-4\Sigma^2u^2N_1/N}}{2}\right]^{1/2}. \tag{8.34}$$

The partition function of model C at deformation parameter u is equivalent to Eq. (8.19) at $u = 0$ with $\Sigma \to \Sigma^C(u) = \Sigma/\sqrt{1+u^2}$, and we thus have the universal result

$$Z^C(m,\theta) \propto e^{mN\Sigma^C(u)\cos\theta}. \tag{8.35}$$

Hence we see that in order to obtain the universal θ-dependence of the partition function neither model B nor model C requires normalization factors $\mathcal{N}_\nu$ that depend on the deformation parameter u. However, let us emphasize again that the appearance of the $\mathcal{N}_\nu$ is a generic feature in RMT. In the remainder of this chapter we identify mechanisms that are responsible for this behavior.

8.4 Chiral condensate and topology

The case $N_f = 1$ we address in this chapter is special since there is no $\mathrm{SU}(N_f) \times \mathrm{SU}(N_f)$ symmetry that could be spontaneously broken. Nevertheless, there could still be a chiral condensate, which can be calculated in the usual way,

$$|\left\langle\bar\psi\psi\right\rangle| = \frac{1}{V}\partial_m \log Z(m,\theta)\,. \tag{8.36}$$

The parameter Σ introduced earlier is defined to be equal to $|\left\langle\bar\psi\psi\right\rangle|$ at $\theta = 0$ for $m \to 0$ and $V \to \infty$. The functions $\Sigma(u)$ computed in Secs. 8.3 and 8.3 correspond to the u-dependent chiral condensate in the same limits. These limits can be taken in different orders [91], either

$$\Sigma^{(1)} = \lim_{V\to\infty}\lim_{m\to 0}\frac{1}{V}\partial_m \log Z(m,\theta=0) \tag{8.37}$$

or in the reverse order,

$$\Sigma^{(2)} = \lim_{m\to 0}\lim_{V\to\infty}\frac{1}{V}\partial_m \log Z(m,\theta=0)\,. \tag{8.38}$$

In Eq. (8.37), a nonzero chiral condensate implies the breaking of the $\mathrm{U}_A(1)$ symmetry by instantons or the axial anomaly [92], whereas in Eq. (8.38) a nonzero chiral condensate implies "spontaneous symmetry breaking" in the following sense. At *fixed* topology the QCD partition function has a $\mathrm{U}_A(1)$ symmetry (in fact a covariance except at $\nu = 0$ where we have a symmetry). A nonzero chiral condensate spontaneously breaks this $\mathrm{U}_A(1)$ symmetry at fixed topology.

From the universal expression (8.9) for the one-flavor partition function it is clear that the order of limits should not matter. We will now see that for model A this is only the case if the normalization factors $\mathcal{N}_\nu$ are included. Because in this section we only consider model A we omit the superscript A. Using Eq. (8.6) and the mass dependence of $Z_\nu(m)$ given by Eq. (8.21), we find that $\Sigma^{(1)}$ of model A is given by

$$\Sigma^{(1)} = \lim_{N\to\infty}\lim_{m\to 0}\frac{\partial_m[\mathcal{N}_1 Z_1(m) + \mathcal{N}_{-1}Z_{-1}(m)]}{N\mathcal{N}_0 Z_0(m)}\,, \tag{8.39}$$

where the factor $\mathcal{P}_\nu$ has dropped out of numerator and denominator since it is essentially constant for $\nu \ll \sqrt{N}$. Using the result (8.21), we obtain

$$\Sigma^{(1)}(u) = (\mathcal{N}_1/\mathcal{N}_0)\Sigma\tau^2 = (\mathcal{N}_1/\mathcal{N}_0)\Sigma(1-\Sigma^2u^2)\,. \tag{8.40}$$

Next we calculate the chiral condensate using the reverse order of limits. Based on the discussion in Sec. 8.3 we find that for $|\nu| \ll \sqrt{mN\Sigma}$ the condensate for fixed ν does not depend on ν. Its value is therefore equal to the value in the $\nu = 0$ sector. This was calculated in Ref. [72], resulting in

$$\Sigma^{(2)}(u) = \Sigma\tau = \Sigma\sqrt{1 - \Sigma^2 u^2}\,. \tag{8.41}$$

We thus see that the two condensates are only equal if the normalization factor $\mathcal{N}_1/\mathcal{N}_0 = 1/\sqrt{1 - \Sigma^2 u^2}$ from Eq. (8.25) is included. Therefore we have a nice consistency check of Eq. (8.25).

So far, we have assumed that we can choose p and q to have arbitrary $\nu = p - q$. Let us now fix the total number of states N. In this case the Dirac operator with ν zero modes has nonzero off-diagonal blocks of dimension $(N + \nu)/2 \times (N - \nu)/2$, see Eqs. (8.12) and (8.13). This implies that the parity of the topology is the same as the parity of N. In the following we assume that N, and therefore also ν, is even. Equation (8.9) shows that the chiral condensate can be extracted from

$$(\Sigma^{(1)})^2 = \lim_{N\to\infty} \lim_{m\to 0} \frac{1}{N^2} \frac{\partial_m^2 Z(m, \theta = 0)}{Z(m, \theta = 0)}\,. \tag{8.42}$$

For $m \to 0$, the numerator receives contributions from $\nu = 0$ and $\nu = \pm 2$, while only the $\nu = 0$ sector contributes to the denominator. For the $\nu = 0$ contribution we find [35]

$$(\Sigma^{(1)})^2_{\nu=0} = \lim_{N\to\infty} \lim_{m\to 0} \frac{1}{N^2} \frac{\partial_m^2 Z_0(m)}{Z_0(m)} = \lim_{N\to\infty} \frac{2}{N^2} \left\langle \sum_{k=1}^{N/2} \frac{1}{(\lambda_k^{\nu=0})^2} \right\rangle_{N_f=1}\,, \tag{8.43}$$

where the average includes the fermion determinant. The r.h.s. of Eq. (8.43) is dominated by the smallest eigenvalues. Note that this contribution is independent of the normalization of the partition function. The contributions of $\nu = \pm 2$ to the condensate are the same and can be written in terms of the Dirac eigenvalues as

$$(\Sigma^{(1)})^2_{\nu=\pm 2} = \lim_{N\to\infty} \frac{2}{N^2} \frac{\mathcal{N}_2}{\mathcal{N}_0} \frac{\left\langle \prod_{k=1}^{N/2-1} (\lambda_k^{\nu=2})^2 \right\rangle}{\left\langle \prod_{k=1}^{N/2} (\lambda_k^{\nu=0})^2 \right\rangle}\,, \tag{8.44}$$

where averages without subscript are with respect to the quenched partition function. This is essentially the ratio of the fermion determinants in the sectors $\nu = 2$ and $\nu = 0$. In the random matrix model A the expressions (8.43) and (8.44) evaluate to

$$(\Sigma^{(1)})^2_{\nu=0} = \frac{1}{2}\Sigma^2\tau^2\,, \qquad\qquad (\Sigma^{(1)})^2_{\nu=\pm 2} = \frac{1}{4}\Sigma^2\tau^4 \frac{\mathcal{N}_2}{\mathcal{N}_0}\,, \tag{8.45}$$

so that the correct result for the chiral condensate is obtained with the normalization factors from Eq. (8.25).

The question we wish to address in the sections below is why model A requires the u-dependent normalization factors (8.25). We will relate this question to the properties of the Dirac eigenvalues. As we have already discussed in Sec. 8.1, the requirement that $Z_\nu(m)$ be independent of ν for $mV\Sigma \gg 1$ can explain why a normalization factor $\mathcal{N}_\nu \neq 1$ is needed if the topological domain of the Dirac spectrum extends beyond the microscopic domain. Equation (8.44) shows that the consistency relation $\Sigma^{(1)} = \Sigma^{(2)}$ should also be related to the properties of the Dirac eigenvalues, to which we turn now.

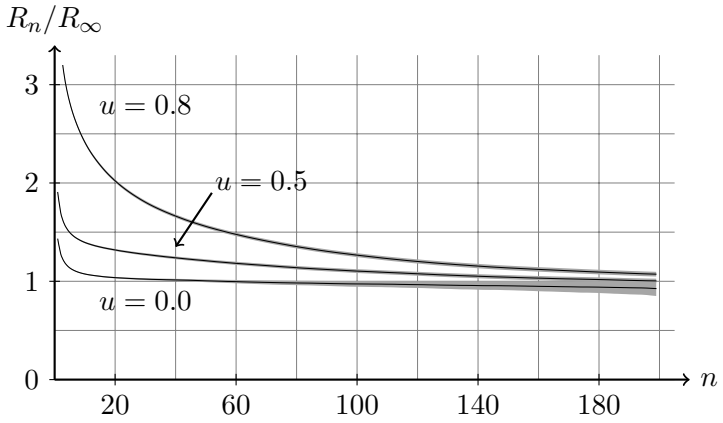


Figure 8.1: Convergence of the ratio R_n of determinants for $\nu = 2$ and $\nu = 0$ as a function of the number n of eigenvalues included for an ensemble of 10^6 400×400 matrices. Results are shown for $u = 0.0$, $u = 0.5$, and $u = 0.8$. The shaded areas correspond to the statistical errors.

8.5 Eigenvalue fluctuations and microscopic universality

In the numerical calculation of this section we keep N fixed as discussed at the end of the previous section. Motivated by Eq. (8.44), we consider the ratio R_n of the products of eigenvalues for $\nu = 2$ and $\nu = 0$ as a function of the number of eigenvalues included in the product,

$$R_n = \frac{1}{N^2} \frac{\left\langle \prod_{k=1}^{n-1} (\lambda_k^{\nu=2})^2 \right\rangle}{\left\langle \prod_{k=1}^{n} (\lambda_k^{\nu=0})^2 \right\rangle} . \tag{8.46}$$

For $n = N/2$ all eigenvalues are included in the product, and for model A the value of this ratio follows from Eqs. (8.44) and (8.45),

$$R_\infty = \lim_{N\to\infty} R_{N/2} = \frac{1}{8}\Sigma^2\tau^4 . \tag{8.47}$$

We have evaluated the ratio R_n numerically for model A, using an ensemble of 10^6 random matrices (8.16) of dimension $N = 400$ distributed according to the Gaussian factor in Eq. (8.10). The mass has been set to zero. In Fig. 8.1 we plot the ratio R_n/R_∞ versus n for $u = 0$, $u = 0.5$, and $u = 0.8$. We observe that for $u = 0$ the ratio of determinants saturates in the ergodic domain ($n \lesssim \sqrt{N} = 20$). This is not the case for $u = 0.5$ and $u = 0.8$, where *all* eigenvalues contribute to the ratio of the two determinants.

This is further illustrated in Fig. 8.2, where we plot the ratio

$$\Delta\lambda_n = \frac{\left\langle \lambda_n^{\nu=2} \right\rangle - \left\langle \lambda_{n+1}^{\nu=0} \right\rangle}{\left\langle \lambda_n^{\nu=0} \right\rangle - \left\langle \lambda_{n+1}^{\nu=0} \right\rangle} \tag{8.48}$$

versus n. The motivation for constructing this particular ratio is as follows. The microscopic eigenvalues are expected to behave universally after rescaling with the chiral condensate and the volume. The universal result for the spectral density of microscopic eigenvalues in the quenched case and in the topological sector ν is [93]

$$\rho_s(\xi) = \frac{\xi}{2}\left[J_\nu(\xi)^2 - J_{\nu+1}(\xi) J_{\nu-1}(\xi) \right] , \tag{8.49}$$

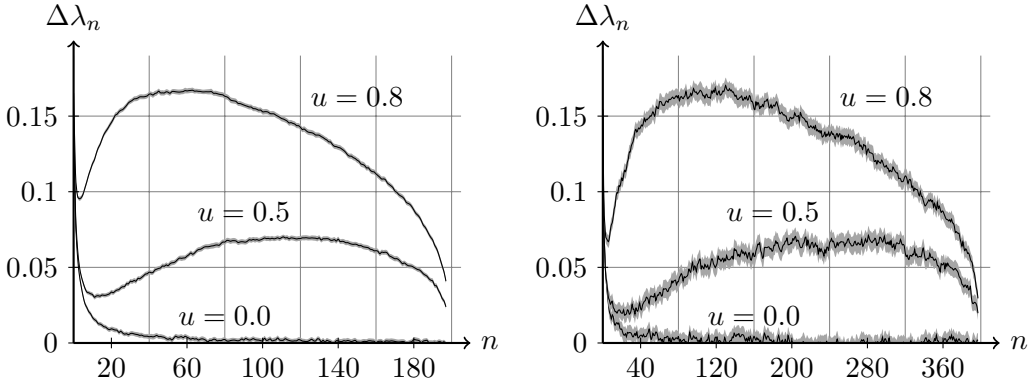


Figure 8.2: Topological shift $\Delta\lambda_n$ of the eigenvalues for an ensemble of 10^6 400×400 matrices (left) and an ensemble of 10^5 800×800 matrices (right). The shaded areas correspond to the statistical errors.

where J_ν is a Bessel function and $\xi = \lambda N\Sigma$. Its large-ξ behavior is given by

$$\rho_s(\xi) = \frac{1}{\pi} - \frac{\cos(\nu\pi - 2\xi)}{2\pi\xi} \tag{8.50}$$

so that for $\lambda_n N\Sigma \gg 1$ we have $\left\langle \lambda_n^{\nu=2} \right\rangle \approx \left\langle \lambda_{n+1}^{\nu=0} \right\rangle$ and therefore $\Delta\lambda_n \to 0$. This is indeed what we find in Fig. 8.2 for $u = 0$. Notice that Eq. (8.49) has been obtained by taking the microscopic limit and is only valid for eigenvalues well below the chiral scale. For $u = 0$ we find that $\Delta\lambda_n = 0$ also beyond the microscopic domain and conclude that in this case the topological domain does not extend beyond the microscopic domain. For $u \neq 0$, however, the situation is completely different. All eigenvalues are in the topological domain and only the first few eigenvalues show universal behavior. Comparing the results for $N = 400$ and $N = 800$ in Fig. 8.2, we observe that the universal domain, i.e., the domain where the eigenvalue ratio $\Delta\lambda_n$ does not depend on u, increases with N proportional to $\sqrt{N}$. This is in agreement with microscopic universality for $u < u_c = 1/\Sigma$, which states that the distribution of low-lying eigenvalues is universal after rescaling them by the chiral condensate. If we consider the Dirac spectrum around x, the correction terms to this universal behavior are of the order Nx^2. This implies that the number of eigenvalues with universal fluctuations around $\lambda = 0$ scales with $\sqrt{N}$.

Based on Fig. 8.2, a plausible explanation for the behavior of the ratio of the determinants seen in Fig. 8.1 can be given in terms of the u-dependence of the average position of the eigenvalues. For this reason we plot in Fig. 8.3 the same ratios as in Fig. 8.1, but normalized with respect to the average positions of the eigenvalues. The ratio $\tilde{R}_n$ defined by

$$\tilde{R}_n = \frac{\left\langle \prod_{k=1}^{n-1} \left(\lambda_k^{\nu=2} / \left\langle \lambda_k^{\nu=2} \right\rangle\right)^2 \right\rangle}{\left\langle \prod_{k=1}^{n} \left(\lambda_k^{\nu=0} / \left\langle \lambda_k^{\nu=0} \right\rangle\right)^2 \right\rangle} \tag{8.51}$$

is shown for $u = 0.0$, $u = 0.5$, and $u = 0.8$.

We conclude that the u-dependence of the ratio of the determinants is almost exclusively due to the effect of u on the average position of the eigenvalues.

In the theory of disordered systems, a frequently used measure to test the breakdown of universality is the number variance [79]. This is the variance of the number of levels in an interval containing $\bar{n}$ eigenvalues on average. In Fig. 8.4 we display the number variance Σ^2 versus the average number

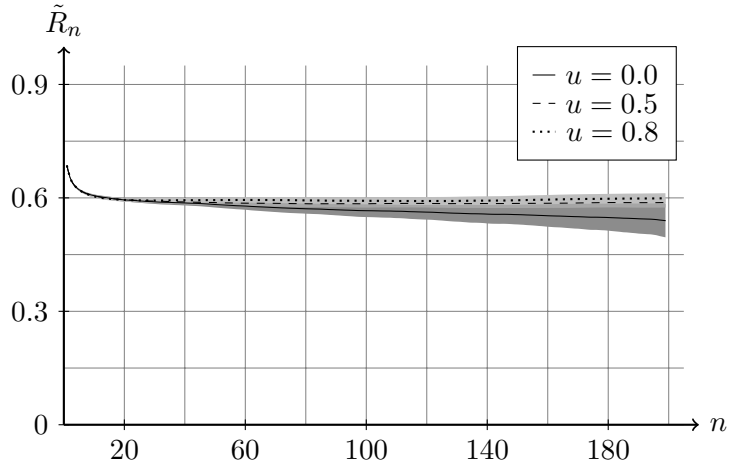


Figure 8.3: Convergence of the ratio $\tilde{R}_n$ of determinants for $\nu = 2$ and $\nu = 0$ as a function of the number n of eigenvalues included. Results are for an ensemble of 10^6 400×400 matrices. The shaded areas correspond to the statistical errors.

$\bar{n}$ of eigenvalues in an interval starting at zero. The curves for $u = 0.0$ and $u = 0.5$ coincide for $\bar{n} \leq 15$, while the deviations between $u = 0.0$ and $u = 0.8$ are already significant for $\bar{n} \geq 5$. This is in agreement with the discussion of Fig. 8.2.

In Fig. 8.5 we show the behavior of the Dirac eigenvalues in model B. We observe that in this model the topological domain does not extend beyond the microscopic domain even for $u \neq 0$. This is also the case for model C, which at $u \neq 0$ is equivalent to model A at $u = 0$ after rescaling the chiral condensate $\Sigma \to \Sigma^C(u)$. The results for model C are therefore identical to the $u = 0$ results in Figs. 8.1–8.4. We thus have a further piece of evidence that nontrivial normalization factors $\mathcal{N}_\nu$ only appear if the topological domain extends beyond the microscopic domain.

8.6 Topological and pseudoscalar susceptibility

As mentioned in Sec. 8.1, the θ-dependence of the QCD partition function is obtained by introducing left-handed and right-handed quark masses according to $z = me^{i\theta}$ and $z^* = me^{-i\theta}$, respectively, see Eq. (8.1). Denoting the l.h.s. of Eq. (8.2) by $Z(z, z^*)$, with the superscript QCD omitted for simplicity, the topological susceptibility at arbitrary θ-angle is given by

$$\begin{aligned}\chi_t &= \frac{1}{V}\left(\langle\nu^2\rangle - \langle\nu\rangle^2\right) = -\frac{1}{V}\partial_\theta^2 \log Z(z, z^*) \\ &= \frac{1}{V}\left(z\partial_z + z^*\partial_{z^*}\right)\log Z(z, z^*) \\ &\quad + \frac{1}{V}\left[z^2\partial_z^2 + z^{*2}\partial_{z^*}^2 - 2zz^*\partial_z\partial_{z^*}\right]\log Z(z, z^*)\,.\end{aligned} \tag{8.52}$$

Because $m\partial_m = z\partial_z + z^*\partial_{z^*}$, the first term on the r.h.s. of this equation is equal to $m|\langle\bar{\psi}\psi\rangle|$, see Eq. (8.36). The second term on the r.h.s. of Eq. (8.52) is equal to m^2 times the pseudoscalar susceptibility given by

$$m^2\chi_{\rm PS} = V\left\langle(z\bar{\psi}_L\psi_R - z^*\bar{\psi}_R\psi_L)^2\right\rangle_{N_f=1} - V\left\langle z\bar{\psi}_L\psi_R - z^*\bar{\psi}_R\psi_L\right\rangle^2_{N_f=1}\,. \tag{8.53}$$

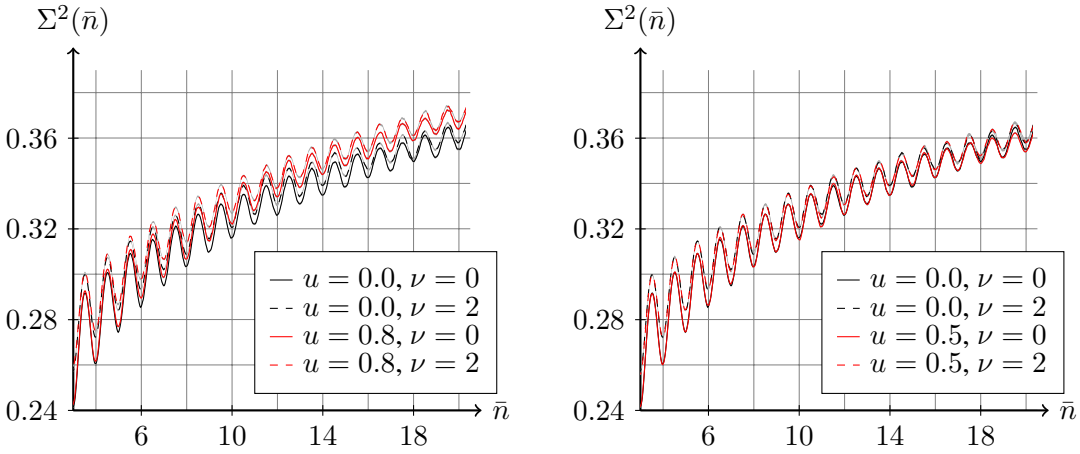


Figure 8.4: Number variance versus the average number $\bar{n}$ of levels in the interval $[0, n]$ for an ensemble of 10^6 400×400 matrices. The curves for $u = 0.0$ and $u = 0.5$ only start to deviate from each other at $\bar{n} \geq 15$.

Thus Eq. (8.52) becomes

$$\chi_t = m|\left\langle\bar{\psi}\psi\right\rangle| + m^2\chi_{\text{PS}}\,. \tag{8.54}$$

This is the well-known chiral Ward identity relating χ_t to the chiral condensate and the pseudoscalar susceptibility [75, 76]. Note that $|\left\langle\bar{\psi}\psi\right\rangle| = \Sigma\cos\theta + O(m)$.

The random matrix partition function $Z^A(m,\theta)$ with m in the ergodic domain can be calculated explicitly from Eq. (8.6), setting $\mathcal{P}_\nu = 1$ according to the discussion in Sec. 8.3. We will set $\mathcal{N}_\nu = \tau^{-|\nu|(1-\varepsilon)}$, where setting ε to 0 or 1 allows us to switch between including or not including $\mathcal{N}_\nu$.

We first replace the Bessel function I_ν in Eq. (8.20) by the integral representation

$$I_\nu(x) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{i\nu\varphi + x\cos\varphi}\,, \tag{8.55}$$

sum the resulting geometric series in ν, and perform a saddle-point approximation of the radial integral including next-to-leading order corrections in m to find

$$\begin{aligned} Z^A(m,\theta) \propto \int_0^{2\pi} d\varphi\, \frac{1-\tau^{2\varepsilon}}{1-2\tau^\varepsilon\cos\varphi+\tau^{2\varepsilon}} \exp\left[mN\Sigma\tau\cos(\varphi-\theta)\right] \\ \times \exp\left[\frac{1}{4\tau^2}Nm^2\Sigma^2\cos^2(\varphi-\theta)\right]. \end{aligned} \tag{8.56}$$

Note that

$$\lim_{u\to 0}\frac{1-\tau^{2\varepsilon}}{2\pi(1-2\tau^\varepsilon\cos\varphi+\tau^{2\varepsilon})} = \delta(\varphi) \tag{8.57}$$

but also

$$\lim_{\varepsilon\to 0}\frac{1-\tau^{2\varepsilon}}{2\pi(1-2\tau^\varepsilon\cos\varphi+\tau^{2\varepsilon})} = \delta(\varphi)\,. \tag{8.58}$$

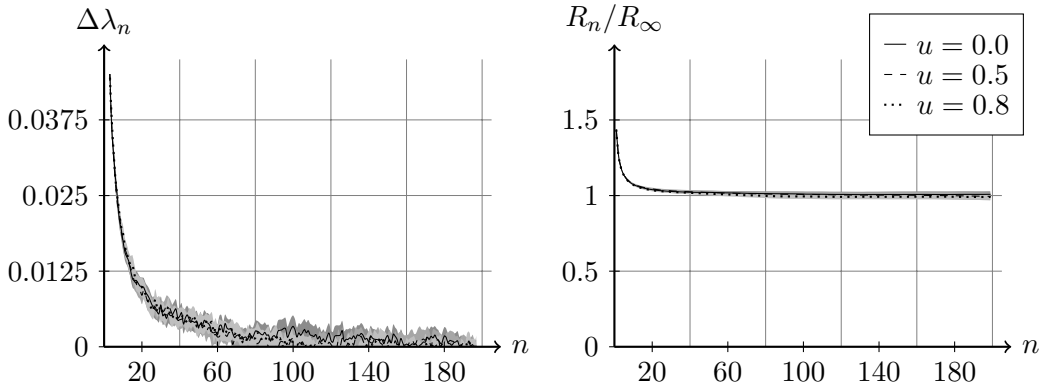


Figure 8.5: Topological shift $\Delta\lambda_n$ and the ratio R_n/R_∞ for an ensemble of 10^6 400×400 matrices with $N_1/N = 0.75$ for model B [80].

Therefore for $\varepsilon \to 0$ or $u \to 0$ we find

$$Z^A(m,\theta) \propto \exp\left[mN\Sigma\tau\cos\theta + \frac{1}{4\tau^2}Nm^2\Sigma^2\cos^2\theta\right] \tag{8.59}$$

and thus by Eq. (8.52)

$$\chi_t^A(u) = m\Sigma^A(u)\cos\theta + O(m^2)\,, \tag{8.60}$$

which is consistent with results obtained by Crewther [75, 76]. We conclude that for $u = 0$ or if we include the normalization factor (8.25) the contribution of the pseudoscalar susceptibility vanishes in the chiral limit.

The situation is different, however, if we do not include the $\mathcal{N}_\nu$. For $mN\Sigma \gg 1$ the contribution of the pseudoscalar susceptibility to the topological susceptibility becomes comparable to that of the chiral condensate but with opposite sign and thus leads to a significant suppression of the topological susceptibility (see Fig. 8.6). Because the saddle-point approximation breaks down close to $u = 1$ we do not plot the curves of Fig. 8.6 in this region. For $mN\Sigma \ll 1$ the exponent in Eq. (8.56) can be be expanded, and after evaluating the integral analytically we find

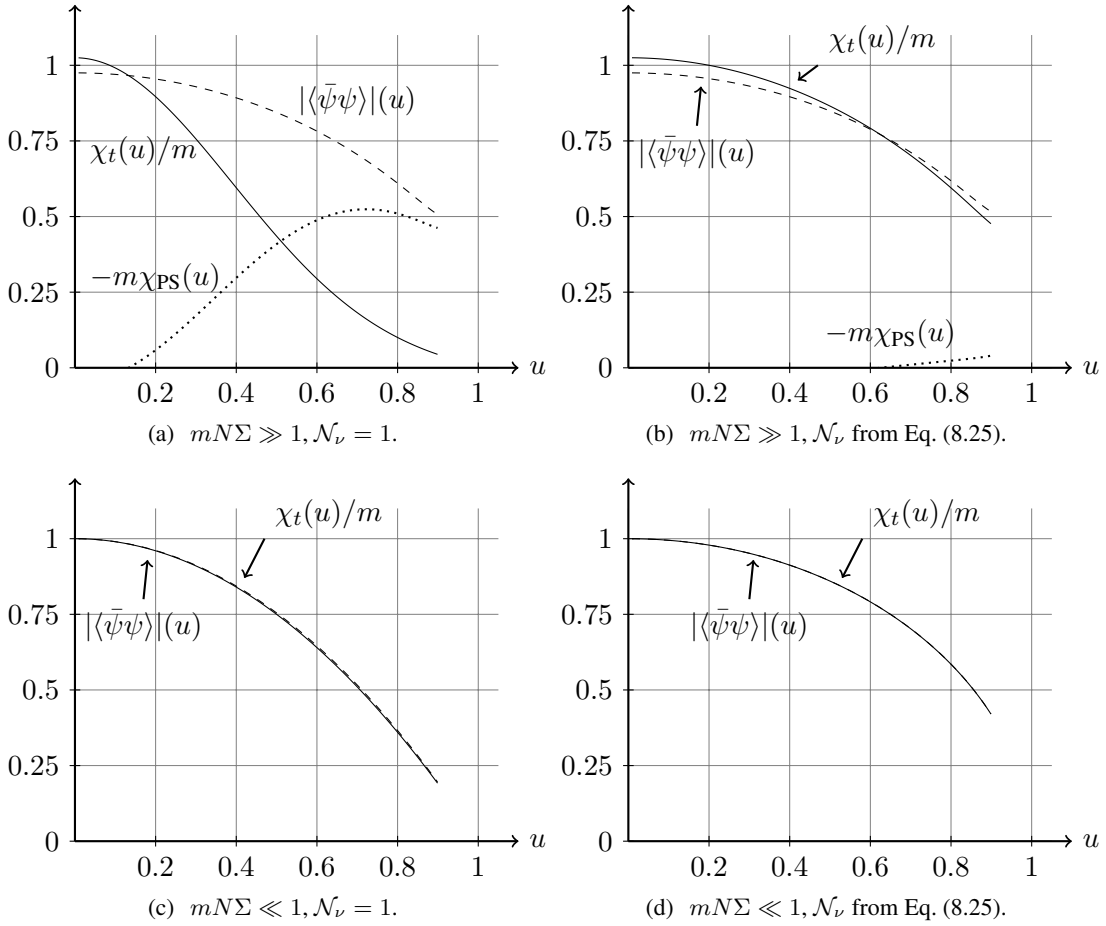
$$Z^A(m,\theta) \propto 1 + mN\Sigma\tau^{1+\varepsilon}\cos\theta\,. \tag{8.61}$$

This result agrees with Fig. 8.6 and shows that in this limit the contribution of the pseudoscalar susceptibility at $u \neq 0$ is small also without $\mathcal{N}_\nu$.

Metlitski and Zhitnitsky have recently found another situation in which the $O(m^2)$ term in Eq. (8.54) becomes important, i.e., the superfluid phase of QCD with two or three colors [81, 82]. Of course, if we include the $\mathcal{N}_\nu$ in model A (as we should) we do not see this effect. Nevertheless, our observation may potentially be of importance, see Sec. 8.7.

For models B and C no normalization factors $\mathcal{N}_\nu$ are needed to ensure a vanishing contribution of the pseudoscalar susceptibility.

The vanishing of the contribution of the pseudoscalar susceptibility also imposes constraints on the ν-dependence of pseudoscalar correlators and can be used as a check of results that were recently derived for the ε-domain [23, 51].



(a) $mN\Sigma \gg 1, \mathcal{N}_\nu = 1$. (b) $mN\Sigma \gg 1, \mathcal{N}_\nu$ from Eq. (8.25).

(c) $mN\Sigma \ll 1, \mathcal{N}_\nu = 1$. (d) $mN\Sigma \ll 1, \mathcal{N}_\nu$ from Eq. (8.25).

Figure 8.6: Contributions to χ_t^A for $N = 10^3$ and $m = 5 \cdot 10^{-2}$ (top) and $m = 5 \cdot 10^{-5}$ (bottom) with or without the normalization factor $\mathcal{N}_\nu$. We set $\theta = 0$ and $\Sigma = 1$. The curves were obtained by numerical evaluation of Eq. (8.56) in connection with Eq. (8.52).

8.7 The topological domain and lattice QCD

It is well known that random matrix models for QCD at *zero* imaginary chemical potential (or temperature) u have the correct θ-dependence. In this chapter we have shown that this is not automatically the case for $u \neq 0$. We obtain the correct θ-dependence only after introducing ν-dependent normalization factors $\mathcal{N}_\nu$ in the sum over topologies.

To explain this we have introduced the topological domain of the Dirac spectrum, which is defined as the part of the Dirac spectrum that is sensitive to the topological charge. We have shown that for $u = 0$ the topological domain coincides with the microscopic domain. This is also the case at $u \neq 0$ for models for which no ν-dependent normalization factors are needed to obtain the correct θ-dependence. However, for the model we analyzed that requires nontrivial normalization factors, the complete Dirac spectrum is inside the topological domain. This results in a partition function that gives universal behavior for small Dirac eigenvalues, but has bulk spectral correlations that depend both on u and on the topological charge. In the thermodynamic limit this leads to an additional u-dependent factor in the partition function at fixed topological charge which results in an incorrect θ-dependence of the partition function. To obtain a partition function with the usual behavior in

the chiral limit, one has to introduce additional ν-dependent normalization factors in the sum over topologies.

Our observations are of potential importance for lattice QCD at nonzero imaginary chemical potential or temperature. Depending on, e.g., the fermion formulation or the algorithm used, it could be that nontrivial normalization factors are needed in the sum over topological sectors, and these could even persist in the continuum limit. To find out whether such normalization factors might be necessary, it would be interesting to determine the topological domain as a function of the deformation parameters. This is feasible with current lattice technology. To be consistent with the general properties of QCD, the topological domain should not extend beyond the microscopic domain. Future work will tell us if this interesting picture prevails.

Part IV

Epilogue

Chapter 9

Conclusions and outlook

The low-energy limit of QCD at sufficiently small quark masses in a finite volume can be viewed as a finite-volume expansion about a zero-dimensional theory that is uniquely determined by its universality class. Since QCD is in the same universality class as the chiral unitary ensemble of RMT, we can use predictions of RMT to describe the properties of QCD in this limit. The dimensionless quantities of RMT can be mapped to dimensionful quantities of QCD using the two leading-order low-energy constants Σ and F.

These constants can be determined from fits to Dirac eigenvalue correlation functions obtained from lattice QCD simulations in the ε regime. The low-energy constant Σ can be extracted from the position of the lowest Dirac eigenvalue, and the low-energy constant F can be extracted from the shift of Dirac eigenvalues due to the presence of a nonzero imaginary chemical potential. The relevant eigenvalue correlation functions can be calculated efficiently in lattice QCD since the Dirac operator remains anti-Hermitian for nonzero imaginary chemical potential. Furthermore, it is sufficient to introduce nonzero imaginary chemical potential only for valence quarks, and therefore also existing lattice QCD configurations that were generated at zero chemical potential can be used to extract the low-energy constant F in this way.

In order to correct for the effect of the finite simulation volume we have calculated the partially quenched low-energy effective theory with imaginary chemical potential at NNLO in the ε expansion. While at NLO the predictions of RMT still hold with Σ and F replaced by effective low-energy constants Σ_{eff} and F_{eff}, at NNLO also non-universal terms arise. We have discussed how to minimize these non-universal terms and the finite-volume corrections to Σ and F by a suitable choice of lattice geometry. It was shown that at simulation volumes of approximately $(2\text{ fm})^4$ and at $F = 90$ MeV an optimal result can be obtained by using an asymmetric lattice with one spatial dimension that is twice the size of the other dimensions. Since many lattice configurations are generated on a similar geometry, where the large spatial dimension is exchanged with the temporal dimension, one can minimize the effects of the finite simulation volume by a suitable rotation of the lattice. We performed such a rotation on dynamical two-flavor lattice configurations of the JLQCD collaboration and extracted Σ and F with good precision.

In future work we will use the exact form of the non-universal terms derived in chapter 5 to calculate analytic expressions for Dirac eigenvalue correlation functions at NNLO in the ε expansion. In this way we can reduce the systematic error of the fits and construct eigenvalue correlation functions that allow for an extraction of further low-energy constants.

In the second part of this thesis we discussed the role of topology in schematic random matrix models. Such models can be used to obtain a schematic description of the chiral phase transition of QCD. We have classified different schematic random matrix models according to the topological domain of their respective Dirac spectra. The topological domain was defined as the part of the eigenvalue spectrum that is sensitive to the topological charge. We have shown that additional normalization factors need to be included in the sum over topological sectors to remedy an unphysical suppression of topological fluctuations if the topological domain of the Dirac eigenvalues extends beyond the

microscopic domain

Recently, there has been progress in the formulation of schematic random matrix models at nonzero temperature and topology. In Ref. [94] a model was proposed that properly incorporates the dependence of the chiral phase transition on the number of quark flavors and allows for finite topological fluctuations. The model of Ref. [94] at fixed topological charge is equivalent to the model of Ref. [80]. Therefore the topological domain of its Dirac eigenvalues does not extend beyond the microscopic domain. This is in accordance with our results.

Appendix A

One-loop propagators at finite volume

In this chapter we discuss one-loop propagators at finite volume with periodic boundary conditions in dimensional regularization. These propagators were calculated originally in Refs. [30, 57]. The propagator of a scalar field with mass m at finite volume V is given by

$$G(x) = \frac{1}{V} \sum_k \frac{e^{ikx}}{k^2 + m^2}\,, \tag{A.1}$$

where the sum is over all finite-volume momenta k. A related quantity of interest is the massless propagator

$$\bar{G}(x) = \frac{1}{V} \sum_{k \neq 0} \frac{e^{ikx}}{k^2}\,, \tag{A.2}$$

where the sum is over all nonzero finite-volume momenta k. Since the constant mode is subtracted, $\bar{G}$ has no infrared singularity. All one-loop combinations of G and $\bar{G}$ can be related to

$$G_r = \frac{\Gamma(r)}{V} \sum_k \frac{1}{(k^2 + m^2)^r} \tag{A.3}$$

and

$$\bar{G}_r = \frac{\Gamma(r)}{V} \sum_{k \neq 0} \frac{1}{(k^2)^r}\,. \tag{A.4}$$

In the following we first calculate G_r at spacetime dimension $d = 1$ and extract the spectrum of the harmonic oscillator from G_0 as an exercise. Then we calculate G_r at arbitrary spacetime dimension d, and finally we relate $\bar{G}_r$ to G_r and give explicit formulas and numbers for common spacetime geometries.

A.1 Poisson's sum over momenta

In this section we use Poisson's summation formula

$$\sum_{n=-\infty}^{\infty} e^{2\pi i n \varphi} = \sum_{n=-\infty}^{\infty} \delta(\varphi - n) \tag{A.5}$$

to obtain a convenient expression for the sum over finite-volume momenta k. The d-dimensional generalization of Eq. (A.5) is given by

$$\sum_{\vec{n} \in \mathbb{Z}^d} e^{2\pi i \vec{n} \cdot \vec{\varphi}} = \sum_{\vec{n} \in \mathbb{Z}^d} \delta^{(d)}(\vec{\varphi} - \vec{n})\,, \tag{A.6}$$

and therefore the integral over φ with a test function $f(\vec{\varphi})$ results in

$$\sum_{\vec{n}\in\mathbb{Z}^d} f(\vec{n}) = \sum_{\vec{n}\in\mathbb{Z}^d} \int d^d\varphi \, e^{2\pi i \vec{n}\cdot\vec{\varphi}} f(\vec{\varphi}) \,, \tag{A.7}$$

where $\vec{n}$ and $\vec{\varphi}$ are d-dimensional vectors. The sum over finite-volume momenta $\vec{k}$ with components

$$\vec{k}_i = \frac{2\pi n_i}{L_i} \,, \tag{A.8}$$

where $i = 1, \ldots, d$, and L_i is the extent of the spacetime volume in dimension i, can thus be written as

$$\begin{aligned} \sum_{\vec{k}} g(\vec{k}) &= \sum_{\vec{n}\in\mathbb{Z}^d} g(2\pi n_i/L_i) = \sum_{\vec{n}\in\mathbb{Z}^d} \int d^d\varphi \, e^{2\pi i \vec{n}\cdot\vec{\varphi}} g(2\pi\varphi_i/L_i) \\ &= V \sum_{\vec{n}\in\mathbb{Z}^d} \int \frac{d^dk}{(2\pi)^d} \, e^{i\sum_{j=1}^d (L_j n_j) k_j} g(\vec{k}) \end{aligned} \tag{A.9}$$

with $V = L_1 \cdots L_d$. In the following we drop the vector notation.

A.2 The spectrum of the harmonic oscillator

The partition function of the one-dimensional harmonic oscillator with potential

$$V_{\text{HO}}(x) = \frac{1}{2} m^2 x^2 \tag{A.10}$$

is given by

$$\begin{aligned} Z &= \oint d[x] \exp\left[-\frac{1}{2} \int_0^\beta d\tau \left([\partial_\tau x(\tau)][\partial_\tau x(\tau)] + m^2 x(\tau)^2 \right) \right] \\ &= \oint d[x] \exp\left[-\frac{1}{2} \int_0^\beta d\tau \, x(-\partial_\tau^2 + m^2) x \right] = \det(D)^{-1/2} \,, \end{aligned} \tag{A.11}$$

where β is the inverse temperature of the system, and the first integral is over all paths $x(\tau)$ with periodic boundary conditions $x(0) = x(\beta)$. The operator D is given by

$$D = -\partial_\tau^2 + m^2 \,, \tag{A.12}$$

and the corresponding determinant can be written in momentum space as

$$\det(D) = \prod_p (p^2 + m^2) \,, \tag{A.13}$$

where the product is over all finite-volume momenta p. In the following we regularize this formal expression in the dimensional regularization scheme. Note that

$$\ln Z = \ln \sum_n e^{-\beta E_n} = -\frac{1}{2} \sum_p \ln(p^2 + m^2) \,, \tag{A.14}$$

where E_n are the energy eigenvalues of the one-dimensional harmonic oscillator with $n = 0, 1, \ldots$, which can be related to G_r for small r by

$$\begin{aligned} G_r &= \frac{1}{Vr} \sum_p [1 + r(\Gamma'(1) - \log(p^2 + m^2))] + \mathcal{O}(r) \\ &= -\frac{1}{V} \sum_p \log(p^2 + m^2) + \text{power divergence in } p + \mathcal{O}(r) \,. \end{aligned} \tag{A.15}$$

In dimensional regularization power divergences are *defined* to vanish and therefore

$$\ln Z = \frac{\beta}{2} G_0 \tag{A.16}$$

with $d = 1$ and $V = \beta$.

Infinite-volume propagator

The ground-state energy of the harmonic oscillator can be extracted from the large-β limit of G_0. In general this corresponds to the large-V limit of G_r, which we determine next. We find

$$\begin{aligned} G_r^\infty &= \frac{\Gamma(r)}{V} \sum_p \frac{1}{(p^2 + m^2)^r} = \frac{\Gamma(r)}{(2\pi)^d} \int d^d p \left(p^2 + m^2\right)^{-r} \\ &= \frac{2\Gamma(r)}{2^d \pi^{d/2} \Gamma(d/2)} \int_0^\infty dp\, p^{d-1} \left(p^2 + m^2\right)^{-r} \\ &= \frac{2\Gamma(r)}{2^d \pi^{d/2} \Gamma(d/2) m^{2r}} \int_0^\infty dp\, p^{d-1} \left(\frac{p^2}{m^2} + 1\right)^{-r} \\ &= \frac{\Gamma(r)}{2^d \pi^{d/2} \Gamma(d/2) m^{2r-d}} \int_0^\infty dt\, t^{d/2-1} (t+1)^{-r} \,. \end{aligned} \tag{A.17}$$

The integral represents the beta function [73]

$$B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int_0^\infty dt\, t^{x-1} (1+t)^{-x-y} \tag{A.18}$$

for $\operatorname{Re} x > 0$ and $\operatorname{Re} y > 0$ with $x = d/2$ and $y = r - d/2$ in Eq. (A.17). For general d and r we analytically continue the gamma functions. Therefore

$$G_r^\infty = \frac{1}{(4\pi)^{d/2}} \Gamma(r - d/2) m^{d-2r} \,. \tag{A.19}$$

The ground-state energy of the harmonic oscillator can thus be obtained from

$$\ln Z = \frac{\beta}{2} G_0 = -\beta \frac{1}{2} m \stackrel{!}{=} -\beta E_0 \tag{A.20}$$

with $\Gamma(-1/2) = -2\sqrt{\pi}$ and $\beta E_0 \gg 1$. Therefore

$$E_0 = \frac{m}{2} \tag{A.21}$$

which is the expected result for the one-dimensional harmonic oscillator defined by Eq. (A.10).

Finite-volume propagator

The complete spectrum of the harmonic oscillator can only be obtained by a discussion of G_r in a finite volume. We calculate

$$\begin{aligned} G_r &= \Gamma(r) \left[\sum_{n\in\mathbb{Z}^d} \int \frac{d^dp}{(2\pi)^d} \, (p^2+m^2)^{-r} \exp\left[i \sum_j L_j n_j p_j \right] \right] \\ &= G_r^\infty + \Gamma(r) \left[\sum_{n\neq 0} \int \frac{d^dp}{(2\pi)^d} \, (p^2+m^2)^{-r} \exp\left[i \sum_j L_j n_j p_j \right] \right], \end{aligned} \tag{A.22}$$

where we used Eq. (A.9). This representation of G_r separates the finite volume corrections in a very clear way from the infinite volume result. We write

$$G_r - G_r^\infty = g_r \tag{A.23}$$

with

$$g_r = \sum_{n\neq 0} \frac{\Gamma(r)}{(2\pi)^d} \int d^dp \, (p^2+m^2)^{-r} \exp\left[i \sum_j L_j n_j p_j \right]. \tag{A.24}$$

The higher energy levels of the harmonic oscillator are thus determined by

$$\log Z = \frac{\beta}{2} G_0 = \frac{\beta}{2} G_0^\infty + \frac{\beta}{2} g_0 = -\beta E_0 + \frac{\beta}{2} g_0 \,. \tag{A.25}$$

The contribution of the first two terms $n = \pm 1$ to g_0 is given by

$$\begin{aligned} g_0^{(1)} &= \lim_{r\to 0} \sum_{n=\pm 1} \frac{\Gamma(r)}{2\pi} \int dp \, (p^2+m^2)^{-r} \exp\left[i\beta n p \right] \\ &= \lim_{r\to 0} \frac{\Gamma(r)}{\pi} \operatorname{Re} \int dp \, (p^2+m^2)^{-r} \exp\left[i\beta p \right] \qquad \text{(A.26)} \\ &= \operatorname{Re} \lim_{r\to 0} \frac{2}{\sqrt{\pi}} \left(\frac{2m}{\beta} \right)^{1/2-r} K_{r-1/2}(\beta m) = \frac{2}{\beta} \exp\left[-\beta m \right], \qquad \text{(A.27)} \end{aligned}$$

where K_ν are modified Bessel functions of the second kind [73]. We obtain the contribution of higher terms $g_0^{(n)}$ in the sum over n from $g_0^{(1)}$ by replacing $\beta \to n\beta$, and therefore

$$g_0 = \sum_{n=1}^\infty g_0^{(n)} = \frac{2}{\beta} \sum_{n=1}^\infty \frac{1}{n} \left(\exp\left[-\beta m \right] \right)^n = -\frac{2}{\beta} \log\left(1 - \exp\left[-\beta m \right] \right). \tag{A.28}$$

The partition function of the one-dimensional harmonic oscillator is thus given by

$$\begin{aligned} Z &= e^{-\beta E_0} e^{-\log(1-\exp[-\beta m])} = \frac{\exp\left[-\beta E_0 \right]}{1 - \exp\left[-\beta m \right]} \\ &= \sum_{n=0}^\infty \exp\left[-\beta (nm + E_0) \right] = \sum_{n=0}^\infty \exp\left[-\beta E_n \right] \end{aligned} \tag{A.29}$$

with

$$E_n = E_0 + nm \,. \tag{A.30}$$

This is the expected result for the higher energy levels of the one-dimensional harmonic oscillator defined by Eq. (A.10).

A.3 Massive propagators at finite volume

In this section we study a systematic expansion of g_r for arbitrary spacetime dimension d in terms of m^2. We first calculate

$$\begin{aligned}
g_r &= \sum_{n\neq 0} \frac{\Gamma(r)}{(2\pi)^d} \int d^d p\, (p^2+m^2)^{-r} \exp\left[i \sum_j L_j n_j p_j \right] \\
&= \sum_{n\neq 0} \frac{\Gamma(r)}{2^d \pi^{d+r}} \int d^{2r}x \int d^d p\, \exp\left[i \sum_j L_j n_j p_j - \sum_{j=1}^{2r} x_j^2 (p^2+m^2) \right] \\
&= \sum_{n\neq 0} \frac{\Gamma(r) C_{2r}}{2^d \pi^{d+r}} \int_0^\infty dx \int d^d p\, x^{2r-1} \exp\left[i \sum_j L_j n_j p_j - x^2 (p^2+m^2) \right] \\
&= \sum_{n\neq 0} \frac{\Gamma(r) C_{2r}}{2^d \pi^{d+r}} \int_0^\infty dx \int d^d p\, x^{2r-1} \exp\left[-\sum_j \left(p_j x - \frac{i}{2x} L_j n_j \right)^2 - \sum_j \frac{L_j^2 n_j^2}{4x^2} - x^2 m^2 \right] \\
&= \sum_{n\neq 0} \frac{\Gamma(r) C_{2r}}{2^d \pi^{d/2+r}} \int_0^\infty dx\, x^{2r-1-d} \exp\left[-\sum_j \frac{L_j^2 n_j^2}{4x^2} - x^2 m^2 \right],
\end{aligned} \tag{A.31}$$

where C_n is the surface of an $(n-1)$-sphere,

$$C_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}\,. \tag{A.32}$$

We next substitute $\lambda = x^2$ with $d\lambda = 2x dx$ and find

$$\begin{aligned}
g_r &= \sum_{n\neq 0} \frac{\Gamma(r) C_{2r}}{2^{d+1} \pi^{d/2+r}} \int_0^\infty d\lambda\, \lambda^{r-1-d/2} \exp\left[-\sum_j \frac{L_j^2 n_j^2}{4\lambda} - \lambda m^2 \right] \\
&= \sum_{n\neq 0} \frac{1}{(4\pi)^{d/2}} \int_0^\infty d\lambda\, \lambda^{r-1-d/2} \exp\left[-\sum_j \frac{L_j^2 n_j^2}{4\lambda} - \lambda m^2 \right].
\end{aligned} \tag{A.33}$$

Note that g_r satisfies the recurrence relation

$$\frac{\partial g_r}{\partial (m^2)} = -g_{r+1}\,. \tag{A.34}$$

We define $L = [\prod_j L_j]^{1/d}$ and rewrite g_r with $\lambda = tL^2/4\pi$,

$$\begin{aligned}
g_r &= \frac{1}{(4\pi)^{d/2}} \int_0^\infty d\lambda\, \lambda^{r-1-d/2} \exp\left[-\lambda m^2\right] \sum_{n\neq 0} \exp\left[-\sum_j \frac{L_j^2 n_j^2}{4\lambda} \right] \\
&= \frac{1}{(4\pi)^r} L^{2r-d} \int_0^\infty dt\, t^{r-d/2-1} \exp\left[-\frac{m^2 L^2 t}{4\pi} \right] \sum_{n\neq 0} \exp\left[-\sum_j \frac{L_j^2 n_j^2 \pi}{t L^2} \right]
\end{aligned} \tag{A.35}$$

which can be written as

$$g_r = \frac{1}{(4\pi)^r} L^{2r-d} \int_0^\infty dt\, t^{r-d/2-1} \exp\left[-\frac{m^2 L^2 t}{4\pi}\right] \left[\prod_j S\left(\frac{L_j^2}{tL^2}\right) - 1\right] \tag{A.36}$$

with the Jacobi theta function

$$\vartheta(z;\tau) = \sum_{n=-\infty}^{\infty} \exp\left[\pi i n^2 \tau + 2\pi i n z\right] \tag{A.37}$$

and

$$S(x) = \vartheta(0; ix)\,. \tag{A.38}$$

The Jacobi theta function transforms under the modular group and thus has a $\tau \to 1/\tau$ covariance. We show this property for $S(x)$ using Poisson's summation formula given in Eq. (A.9),

$$\begin{aligned}
S(x) &= \sum_{n=-\infty}^{\infty} e^{-\pi n^2 x} = \sum_{n=-\infty}^{\infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ink} e^{-\pi (k/2\pi)^2 x} \\
&= \sum_{n=-\infty}^{\infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \exp\left[ink - \frac{k^2 x}{4\pi}\right] \\
&= \sum_{n=-\infty}^{\infty} \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \exp\left[-\left(\frac{k\sqrt{x}}{2\sqrt{\pi}} - \frac{in\sqrt{\pi}}{\sqrt{x}}\right)^2 - \frac{n^2\pi}{x}\right] \\
&= \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{x}} \exp\left[-\frac{n^2\pi}{x}\right] = \frac{1}{\sqrt{x}} S(1/x)\,.
\end{aligned} \tag{A.39}$$

Next we split the integration over t in $0 < t < 1$ and $1 < t$, i.e.,

$$\begin{aligned}
&g_r - \frac{1}{(4\pi)^r} L^{2r-d} \int_0^1 dt\, t^{r-d/2-1} \exp\left[-\frac{m^2 L^2 t}{4\pi}\right] \left[\prod_j S\left(\frac{L_j^2}{tL^2}\right) - 1\right] \\
&= \frac{1}{(4\pi)^r} L^{2r-d} \int_1^\infty dt\, t^{r-d/2-1} \exp\left[-\frac{m^2 L^2 t}{4\pi}\right] \left[\prod_j S\left(\frac{L_j^2}{tL^2}\right) - 1\right] \\
&= \frac{1}{(4\pi)^r} L^{2r-d} \int_1^\infty dt\, t^{r-1} \exp\left[-\frac{m^2 L^2 t}{4\pi}\right] \prod_j \frac{L}{L_j} S\left(\frac{tL^2}{L_j^2}\right) - \frac{1}{(4\pi)^r} L^{2r-d} b_{r-d/2} \\
&= \frac{1}{(4\pi)^r} L^{2r-d} \int_0^1 dt\, t^{-r-1} \exp\left[-\frac{m^2 L^2}{4\pi t}\right] \prod_j S\left(\frac{L^2}{tL_j^2}\right) - \frac{1}{(4\pi)^r} L^{2r-d} b_{r-d/2} \\
&= \frac{1}{(4\pi)^r} L^{2r-d} \int_0^1 dt\, t^{-r-1} \exp\left[-\frac{m^2 L^2}{4\pi t}\right] \left[\prod_j S\left(\frac{L^2}{tL_j^2}\right) - 1\right] \\
&\quad + \frac{1}{(4\pi)^r} L^{2r-d} b_r - \frac{1}{(4\pi)^r} L^{2r-d} b_{r-d/2}
\end{aligned} \tag{A.40}$$

with

$$b_s = \int_1^\infty dt\, t^{s-1} \exp\left[-\frac{m^2L^2t}{4\pi}\right] = \int_0^1 dt\, t^{-s-1} \exp\left[-\frac{m^2L^2}{4\pi t}\right]. \tag{A.41}$$

Therefore the finite-volume contribution g_r can be written as

$$g_r = \frac{1}{(4\pi)^r} L^{2r-d} \left[a_r + b_r - b_{r-d/2}\right], \tag{A.42}$$

where

$$\begin{aligned} a_r = &\int_0^1 dt\, t^{r-d/2-1} \exp\left[-\frac{m^2L^2t}{4\pi}\right] \left[\prod_j S\left(\frac{L_j^2}{tL^2}\right) - 1\right] \\ &+ \int_0^1 dt\, t^{-r-1} \exp\left[-\frac{m^2L^2}{4\pi t}\right] \left[\prod_j S\left(\frac{L^2}{tL_j^2}\right) - 1\right]. \end{aligned} \tag{A.43}$$

The function $a_r(m^2)$ is analytic in m^2 and can be expanded as

$$a_r = \sum_{n=0}^\infty \frac{1}{n!} \left(-\frac{m^2L^2}{4\pi}\right)^n \alpha_{r+n} \tag{A.44}$$

with

$$\begin{aligned} \alpha_s &= \int_0^1 dt\, t^{s-d/2-1} \left[\prod_j S\left(\frac{L_j^2}{tL^2}\right) - 1\right] + \int_0^1 dt\, t^{-s-1} \left[\prod_j S\left(\frac{L^2}{tL_j^2}\right) - 1\right] \\ &= \hat{\alpha}_{s-d/2}(L_j/L) + \hat{\alpha}_{-s}(L/L_j)\,, \end{aligned} \tag{A.45}$$

where

$$\hat{\alpha}_n(x_j) = \int_0^1 dt\, t^{n-1} \left[\prod_j S(x_j^2/t) - 1\right]. \tag{A.46}$$

Note that α_s only depends on the ratios L_i/L of the spacetime box and is therefore called a *shape coefficient*. The function $b_r(m^2)$ has a pole in m^2 which can be separated as

$$\begin{aligned} b_s &= \int_0^\infty dt\, t^{s-1} \exp\left[-\frac{m^2L^2t}{4\pi}\right] - \int_0^1 dt\, t^{s-1} \exp\left[-\frac{m^2L^2t}{4\pi}\right] \\ &= \left(\frac{4\pi}{m^2L^2}\right)^s \int_0^\infty dt\, t^{s-1} \exp\left[-t\right] - \sum_{n=0}^\infty \frac{1}{n!} \left(-\frac{m^2L^2}{4\pi}\right)^n \int_0^1 dt\, t^{n+s-1} \\ &= \left(\frac{4\pi}{m^2L^2}\right)^s \Gamma(s) - \sum_{n=0}^\infty \frac{1}{n!} \left(-\frac{m^2L^2}{4\pi}\right)^n \left[\frac{t^{n+s}}{n+s}\right]_0^1 \\ &= \left(\frac{4\pi}{m^2L^2}\right)^s \Gamma(s) - \sum_{n=0}^\infty \frac{1}{n!} \left(-\frac{m^2L^2}{4\pi}\right)^n \frac{1}{n+s}\,. \end{aligned} \tag{A.47}$$

At negative integer values of s poles in the gamma function cancel with poles in the analytic part. To make this cancellation explicit we first note that for positive integer N

$$\Gamma(-N+\varepsilon) = -\frac{1}{N-\varepsilon}\Gamma(-(N-1)+\varepsilon) = -\frac{1}{N}\Gamma(-(N-1)+\varepsilon)\left[1+\frac{\varepsilon}{N}+\mathcal{O}(\varepsilon^2)\right], \quad \text{(A.48)}$$

and therefore

$$\begin{aligned}\Gamma(-N+\varepsilon) &= \frac{(-1)^N}{N!}\Gamma(\varepsilon)\prod_{n=1}^{N}\left[1+\frac{\varepsilon}{n}+\mathcal{O}(\varepsilon^2)\right] \\ &= \frac{(-1)^N}{N!}\Gamma(\varepsilon)\left[1+\varepsilon\sum_{n=1}^{N}\frac{1}{n}+\mathcal{O}(\varepsilon^2)\right]. \end{aligned} \quad \text{(A.49)}$$

Furthermore note that

$$\varepsilon\Gamma(\varepsilon) = \Gamma(1+\varepsilon) = \Gamma(1)+\varepsilon\Gamma'(1)+\mathcal{O}(\varepsilon^2) = 1-\varepsilon\gamma+\mathcal{O}(\varepsilon^2) \quad \text{(A.50)}$$

with $\gamma = -\Gamma'(1)$, and thus

$$\Gamma(\varepsilon) = \frac{1}{\varepsilon}-\gamma+\mathcal{O}(\varepsilon)\,. \quad \text{(A.51)}$$

The gamma function close to a negative integer is therefore given by

$$\begin{aligned}\Gamma(-N+\varepsilon) &= \frac{(-1)^N}{N!}\left[\frac{1}{\varepsilon}-\gamma+\mathcal{O}(\varepsilon)\right]\left[1+\varepsilon\sum_{n=1}^{N}\frac{1}{n}+\mathcal{O}(\varepsilon^2)\right] \\ &= \frac{(-1)^N}{N!}\left[\frac{1}{\varepsilon}+\sum_{n=1}^{N}\frac{1}{n}-\gamma+\mathcal{O}(\varepsilon)\right]. \end{aligned} \quad \text{(A.52)}$$

We insert this expression into $b_{-N+\varepsilon}$ and calculate

$$\begin{aligned} b_{-N+\varepsilon} &= \left(\frac{m^2L^2}{4\pi}\right)^{N-\varepsilon}\Gamma(-N+\varepsilon)+\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{N-n-\varepsilon} \\ &= \left(\frac{m^2L^2}{4\pi}\right)^N\left(1-\varepsilon\log\left[\frac{m^2L^2}{4\pi}\right]\right)\frac{(-1)^N}{N!}\left[\frac{1}{\varepsilon}+\sum_{n=1}^{N}\frac{1}{n}-\gamma+\mathcal{O}(\varepsilon)\right] \\ &\quad +\sum_{n\neq N}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{N-n}-\frac{(-1)^N}{N!}\left(\frac{m^2L^2}{4\pi}\right)^N\frac{1}{\varepsilon}+\mathcal{O}(\varepsilon) \\ &= \frac{(-1)^N}{N!}\left(\frac{m^2L^2}{4\pi}\right)^N\left(\frac{1}{\varepsilon}-\log\left[\frac{m^2L^2}{4\pi}\right]+\sum_{n=1}^{N}\frac{1}{n}-\gamma\right) \\ &\quad +\sum_{n\neq N}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{N-n}-\frac{(-1)^N}{N!}\left(\frac{m^2L^2}{4\pi}\right)^N\frac{1}{\varepsilon}+\mathcal{O}(\varepsilon) \\ &= \frac{(-1)^{N+1}}{N!}\left(\frac{m^2L^2}{4\pi}\right)^N\left(\log\left[\frac{m^2L^2}{4\pi}\right]-\sum_{n=1}^{N}\frac{1}{n}+\gamma\right) \\ &\quad +\sum_{n\neq N}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{N-n}+\mathcal{O}(\varepsilon)\,. \end{aligned} \quad \text{(A.53)}$$

In four spacetime dimensions we find

$$\begin{aligned}
g_0 &= \frac{1}{V}\left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\alpha_n - \left(\log\left[\frac{m^2L^2}{4\pi}\right]+\gamma\right) - \sum_{n=1}^{\infty}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{n}\right. \\
&\quad \left. +\frac{1}{2}\left(\frac{m^2L^2}{4\pi}\right)^2\left(\log\left[\frac{m^2L^2}{4\pi}\right]-\frac{3}{2}+\gamma\right) - \sum_{n\neq 2}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{2-n}\right] \\
&= \frac{1}{V}\left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\alpha_n - 2\log\left[mL\right]+\log\left[4\pi\right]-\gamma\right. \\
&\quad +\left(\frac{m^2L^2}{4\pi}\right)^2\log\left[mL\right] - \frac{1}{2}\left(\frac{m^2L^2}{4\pi}\right)^2\log\left[4\pi\right] - \frac{1}{2}\left(\frac{m^2L^2}{4\pi}\right)^2\left(\frac{3}{2}-\gamma\right) \\
&\quad \left. -\sum_{n=1}^{\infty}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{n} - \sum_{n\neq 2}\frac{1}{n!}\left(-\frac{m^2L^2}{4\pi}\right)^n\frac{1}{2-n}\right] \\
&= \sum_{n=0}^{\infty}\frac{\beta_n}{n!}m^{2n}L^{2n-4} - \frac{2}{V}\log\left[mL\right] + \frac{m^4}{16\pi^2}\left(\log\left[mL\right]-\frac{3}{4}+\frac{\gamma}{2}-\frac{1}{2}\log[4\pi]+K\right)
\end{aligned} \tag{A.54}$$

with

$$\begin{aligned}
\beta_0 &= \alpha_0 + \log[4\pi] - \gamma - \frac{1}{2}\,, \\
\beta_2 &= \frac{1}{16\pi^2}\left(\alpha_2 - \frac{1}{2} - 2K\right), \\
\beta_n &= \frac{(-1)^n}{(4\pi)^n}\left(\alpha_n - \frac{1}{n} - \frac{1}{2-n}\right) = \frac{(-1)^n}{(4\pi)^n}\left(\alpha_n + \frac{2}{n(n-2)}\right),
\end{aligned} \tag{A.55}$$

where K is an arbitrary constant. In order to be consistent with Ref. [30] we choose

$$K = \frac{1}{2} - \frac{\gamma}{2} + \frac{1}{2}\log[4\pi]\,. \tag{A.56}$$

This leads to

$$g_0 = \sum_{n=0}^{\infty}\frac{\beta_n}{n!}m^{2n}L^{2n-4} - \frac{2}{V}\log\left[mL\right] + \frac{m^4}{16\pi^2}\left(\log\left[mL\right]-\frac{1}{4}\right) \tag{A.57}$$

and

$$\beta_2 = \frac{1}{16\pi^2}\left(\alpha_2 - \frac{3}{2} + \gamma - \log[4\pi]\right). \tag{A.58}$$

As we have already noted in Eq. (A.34), the finite-volume contributions g_r can be obtained from g_0 for all positive integer r by partial differentiation. Therefore

$$g_1 = -\frac{\partial g_0}{\partial(m^2)} = -\sum_{n=0}^{\infty}\frac{\beta_{n+1}}{n!}(m^2)^nL^{2n-2} + \frac{1}{Vm^2} - \frac{m^2}{8\pi^2}\left(\log\left[mL\right]-\frac{1}{4}\right) - \frac{m^2}{32\pi^2}\,. \tag{A.59}$$

A.4 Massless propagators at finite volume

The massless one-loop propagators $\bar{G}_r$ are related to the massive one-loop propagators G_r by

$$\bar{G}_r = \lim_{m\to 0}\left[G_r - \frac{\Gamma(r)}{Vm^{2r}}\right], \tag{A.60}$$

where the second term subtracts the infrared singularity of G_r at $m^2 = 0$. In the following we give explicit formulas for the relevant one-loop propagators of chapter 4. The finite-volume propagators of chapter 4 are related to $\bar{G}_1$ by

$$\bar{G}(0) = \bar{G}_1\,, \qquad \int d^4x \left(\partial_0 \bar{G}(x)\right)^2 = \frac{L_0}{2}\partial_{L_0}\bar{G}_1 + \frac{1}{2}\bar{G}_1\,. \tag{A.61}$$

We first calculate

$$\begin{aligned}
\bar{G}_1 &= \lim_{m\to 0}\left[G_1^\infty + g_1 - \frac{\Gamma(r)}{Vm^{2r}}\right] \\
&= \lim_{m\to 0}\left[\frac{1}{(4\pi)^2}\Gamma(1-d/2)m^2 - \sum_{n=0}^{\infty}\frac{\beta_{n+1}}{n!}(m^2)^n L^{2n-2} + \frac{1}{Vm^2}\right. \\
&\qquad \left. -\frac{m^2}{8\pi^2}\left(\log[mL] - \frac{1}{4}\right) - \frac{m^2}{32\pi^2} - \frac{1}{Vm^2}\right] \\
&= \lim_{m\to 0}\left[\frac{1}{(4\pi)^2}\Gamma(1-d/2)m^2 - \sum_{n=0}^{\infty}\frac{\beta_{n+1}}{n!}(m^2)^n L^{2n-2} - \frac{m^2}{8\pi^2}\left(\log[mL] - \frac{1}{4}\right) - \frac{m^2}{32\pi^2}\right] \\
&= -\beta_1 L^{-2}\,.
\end{aligned} \tag{A.62}$$

The variation of G_1 w.r.t. the temporal extent L_0 is given by

$$\partial_{L_0} G_1(m) = \partial_{L_0}\frac{1}{L_0L_1L_2L_3}\sum_{n_1,n_2,n_3=-\infty}^{\infty}\sum_{n_0=-\infty}^{\infty}\frac{1}{\sum_{j=0}^{4}(2\pi n_j/L_j)^2 + m^2}\,. \tag{A.63}$$

The sum over n_0 can be simplified by the identity

$$\begin{aligned}
\sum_{n=-\infty}^{\infty}\frac{g(2\pi n/L)}{(2\pi n/L)^2 + m^2} &= \frac{L}{2\pi}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, e^{iLnx}\frac{g(x)}{x^2+m^2} \\
&= \frac{L}{2\pi}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty} dx\, e^{iLnx}\frac{g(x)}{(x-im)(x+im)} \\
&= iL\sum_{n=0}^{\infty} e^{-Lnm}\frac{g(im)}{2im} + iL\sum_{n=-\infty}^{-1} e^{Lnm}\frac{g(-im)}{2im} \\
&= iL\sum_{n=0}^{\infty} e^{-Lnm}\frac{g(im)}{2im} + iL\sum_{n=1}^{\infty} e^{-Lnm}\frac{g(-im)}{2im} \\
&= \frac{L}{2m}\left[\frac{g(im)}{1-e^{-Lm}} + \frac{g(-im)\,e^{-Lm}}{1-e^{-Lm}}\right] = \frac{L}{2m}\left[\frac{g(im)}{1-e^{-Lm}} - \frac{g(-im)}{1-e^{Lm}}\right] \\
&= \frac{L}{2m}\left[\frac{g(im)\,e^{Lm/2}}{e^{Lm/2}-e^{-Lm/2}} - \frac{g(-im)\,e^{-Lm/2}}{e^{-Lm/2}-e^{Lm/2}}\right] \\
&= \frac{L}{4m\sinh[Lm/2]}\left[g(im)\,e^{Lm/2} + g(-im)\,e^{-Lm/2}\right],
\end{aligned} \tag{A.64}$$

where we used Eq. (A.9), and $g(x)$ is an arbitrary analytic function which is finite at $g(\pm i\infty)$. Therefore

$$\begin{aligned}\partial_{L_0} G_1(m) &= \partial_{L_0} \frac{1}{L_0 L_1 L_2 L_3} \sum_{\vec{n}} \frac{L_0 \cosh[L_0 m/2]}{2m \sinh[L_0 m/2]} = \frac{1}{L_1 L_2 L_3} \sum_{\vec{n}} \partial_{L_0} \frac{\cosh[L_0 m/2]}{2m \sinh[L_0 m/2]} \\ &= -\frac{L_0}{V} \sum_{\vec{n}} \frac{1}{4 \sinh[L_0 m/2]^2} \end{aligned} \tag{A.65}$$

with

$$m^2 = \sum_{j=1}^{3} (2\pi n_j / L_j)^2 + m^2 = q^2 + m^2 \,. \tag{A.66}$$

The variation of $\bar{G}_1$ w.r.t. the temporal extent L_0 is given by

$$\begin{aligned} L_0 \partial_{L_0} \bar{G}_1 &= \lim_{m\to 0} L_0 \partial_{L_0} \left[G_1(m) - V^{-1} m^{-2} \right] = \lim_{m\to 0} L_0 \left[\partial_{L_0} G_1(m) + L_0^{-1} V^{-1} m^{-2} \right] \\ &= \lim_{m\to 0} \left[V^{-1} m^{-2} - \frac{L_0^2}{V} \sum_{\vec{n}} \frac{1}{4 \sinh[L_0 \sqrt{q^2 + m^2}/2]^2} \right] \\ &= \lim_{m\to 0} \left[V^{-1} m^{-2} - \frac{L_0^2}{V} \frac{1}{4 \sinh[L_0 m/2]^2} \right] - \frac{L_0^2}{V} \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \\ &= \lim_{m\to 0} \left[V^{-1} m^{-2} - \frac{L_0^2}{V} \frac{1}{4[L_0 m/2 + (L_0 m/2)^3/6]^2} \right] - \frac{L_0^2}{V} \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \\ &= \lim_{m\to 0} \left[V^{-1} m^{-2} - \frac{L_0^2}{V} \frac{1}{L_0^2 m^2 + (L_0 m)^4/12} \right] - \frac{L_0^2}{V} \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \\ &= \lim_{m\to 0} V^{-1} m^{-2} \left[1 - \frac{1}{1 + (L_0 m)^2/12} \right] - \frac{L_0^2}{V} \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \\ &= \lim_{m\to 0} V^{-1} m^{-2} \left[1 - \left(1 - \frac{(L_0 m)^2}{12} + \mathcal{O}(m^4) \right) \right] - \frac{L_0^2}{V} \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \\ &= \lim_{m\to 0} V^{-1} \left[\frac{L_0^2}{12} + \mathcal{O}(m^2) \right] - \frac{L_0^2}{V} \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \\ &= \frac{L_0^2}{V} \left[\frac{1}{12} - \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \right] = \frac{L_0^2}{V} k_{00} \end{aligned} \tag{A.67}$$

with

$$k_{00} = \frac{1}{12} - \sum_{\vec{n}\neq\vec{0}} \frac{1}{4 \sinh[L_0 q/2]^2} \,. \tag{A.68}$$

The results of this section can be summarized by

$$\bar{G}(0) = -\frac{\beta_1}{\sqrt{V}} \tag{A.69}$$

L_0/L	1	2	3	4
β_1	0.1404610	0.0836011	−0.0419417	−0.215097
k_{00}	0.0702305	0.0833122	0.0833333	0.0833333

Table A.1: Coefficients for an asymmetric box with $L_1 = L_2 = L_3 = L$ and temporal dimension L_0.

L_3/L	1	2	3	4
β_1	0.1404610	0.0836011	−0.0419417	−0.215097
k_{00}	0.0702305	−0.0322630	−0.2984300	−0.731240

Table A.2: Coefficients for an asymmetric box with $L_0 = L_1 = L_2 = L$ and spatial dimension L_3. Note that β_1 is symmetric under the exchange of the temporal with a spatial dimension.

and

$$\int d^4x \left(\partial_0 \bar{G}(x)\right)^2 = -\frac{1}{2\sqrt{V}} \left[\beta_1 - \frac{L_0^2}{\sqrt{V}} k_{00}\right]. \tag{A.70}$$

In tables A.1 and A.2 we give numerical values for β_1 and k_{00} for common shapes.

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