Chiral Perturbation Theory for 2+1+1 Flavor of Wilson Quarks with Twisted Masses

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1. Introduction

Quantum Chromodynamics (QCD) is the theory of strong interaction. Its building blocks, the fermion fields representing quarks, and the gauge bosons referred to as gluons, are the appropriate degrees of freedom at high energy scales. This property is called asymptotic freedom. At low energies, on the other hand, quarks exclusively appear in bound states, so called hadrons. This is referred to as confinement. Asymptotic freedom in QCD was proven analytically, whereas the respective proof is lacking for confinement. However, non-perturbative studies strongly suggest confinement to be a feature of the theory. As both phenomena are observed in experiments, QCD is believed to be the appropriate theory of strong interaction and hence included in the Standard Model of particle physics.

Due to the running of the coupling in QCD, applicability of perturbative methods to obtain predictions from the theory is limited to high energy scales. At low energies, different strategies to explore the dynamics must be employed. Lattice QCD is, to date, the only known non-perturbative definition of QCD. Replacing the continuous space-time by a discrete Euclidean grid and restraining computations to finite volumes renders the theory finite and hence non-perturbatively well defined. The lattice formulation of QCD is particularly well suited for a treatment via Monte Carlo methods, allowing for computation of observables from first principles.

However, computational cost increases with decreasing lattice spacing and increasing volumes. Additionally, it is not yet possible to conduct calculations using the physical quark masses, as decreasing quark masses again drastically raise demands regarding the required computational effort. Therefore, extrapolations to the physical limit must be performed. An effective field theory provides a description of the way the continuum limit is approached.

The appropriate low energy effective field theory for QCD is Chiral Perturbation theory. The observed light hadrons such as pions and kaons are considered as adequate degrees of freedom at low energies. They are reinterpreted as Goldstone bosons of spontaneously broken symmetry chiral of massless QCD, allowing for a systematic expansion in their small momenta. That way, an effective field theory allowing for a meaningful perturbative treatment at low energies is constructed from QCD. Besides, the underlying spontaneously broken symmetry is explicitly broken by nonvanishing quark masses. However, as long as the respective masses are small compared to the energy scale of QCD, the explicit symmetry breaking can be treated as a perturbation. The pseudo Goldstone bosons then acquire a nonzero though still small mass. The low energy behavior is deduced from a simultaneous expansion in small boson momenta and quark masses, whereby an adequate power counting scheme has to be imposed. The associated Lagrangian can be constructed using symmetry arguments only, ensuring that the symmetry be explicitly broken in the same way in both the effective theory and the underlying physical theory it describes. Unknown constants referred to

as Low Energy Constants are introduced, that parametrize the effects of the dynamics of QCD involving higher energy degrees of freedom.
Chiral Perturbation Theory up to that point is the effective theory of continuum QCD. In order to incorporate lattice effects for Wilson fermions, its Symanzik effective theory is constructed, making all cutoff effects near the continuum limit explicit by means of an effective continuum theory. One thus obtains an expansion in powers of the lattice spacing, whose leading order action is just the QCD action. As the lattice constitutes another source of explicit breaking of the spontaneously broken chiral symmetry that was used to construct the continuum effective theory, terms occurring at higher orders in the Symanzik effective theory can be translated to their Chiral Perturbation Theory counterparts based again on their symmetry breaking pattern. The effective theory then incorporates all sources of explicit symmetry breaking and involves an expansion in small momenta of the hadrons, that are the dynamical degrees of freedom of the theory, the quark masses and the lattice spacing. An appropriate power counting is to be imposed in order to organize the expansion consistently. With some additional effort, the analysis can be extended to Lattice QCD with twisted mass Wilson fermions which is subject to current numerical studies.
As is evident from its construction principles the effective theory can not be employed to model the hadronic spectrum inferred from including arbitrarily heavy quarks. For the desired perturbative expansion to be meaningful, masses of the flavors included in the theory have to be well below the energy scale of QCD. This restricts computations in the framework of Chiral Perturbation Theory to hadrons built from up, down and strange quarks, hence pions, kaons and the η meson. All higher-energy hadronic degrees of freedom can be thought of as having been integrated out explicitly, thus contributing to the Low Energy Constants.
For the effective theory to be descriptive of numerical simulations as they are currently carried out, we start from the theory including mass degenerate up and down quarks, and non-degenerate strange and charm quarks, referred to as 2+1+1 flavor theory. Twisted masses are implemented in the light and the heavy sector separately in accordance with the setup of numerical studies. We subsequently remove the charm degrees of freedom at Lagrangian level, leading to a charmless effective theory. Without using any information from the full four flavor theory, we demonstrate this reduction to yield consistent results when compared to published results in the GSM regime. We then proceed to calculating pseudoscalar meson masses in the LCE regime, which is likely to be the appropriate power counting scheme to describe current numerical simulations. The masses we calculate obtain corrections connected to lattice effects that have not been recognized before. Particularly, we predict a different finite volume dependence of the meson masses due to the presence of neutral pion chiral logarithms. Expressions for decay constants also differ from continuum Chiral Perturbation Theory. Our findings presumably impact the analysis of current twisted mass simulations at an order of magnitude comparable to statistical and systematic uncertainties claimed in recent publications.

2. Continuum Chiral Perturbation Theory

A number of introductory works on Chiral Perturbation theory can be found in the literature [1, 2, 3]. In the following two chapters, the foundations of Chiral Perturbation Theory and its extension to describe lattice QCD with Wilson fermions are reviewed, guided by [4].

2.1. Spontaneously Broken Chiral Symmetry in Quantum Chromodynamics

The starting point for the development of Continuum Chiral Perturbation Theory is the fermionic part of the Lagrangian of Quantum Chromodynamics with N_f flavors,

$$\mathscr{L}_{\mathrm{QCD}} = \sum_{f=1}^{N_f} \bar{q}_f \not{D} q_f + \mathscr{L}_{\mathrm{massive}}, \tag{2.1}$$

where the covariant derivative is defined as

$$\not{D} = \gamma^\mu D_\mu, \quad D_\mu = \partial_\mu + \mathrm{i} g A_\mu^a T^a$$

to enforce invariance under local $\mathrm{SU}(3)_c$ transformations generated by the T^a acting in color space, and A_μ^a are the gauge fields of QCD. Introducing

$$P_{L,R} = \frac{1}{2}\left(1 \pm \gamma_5\right),$$

with Dirac matrices acting in spinor space and γ_5 defined as usual, one readily checks the projector properties

$$P_L + P_R = 1, \qquad P_L P_R = 0 = P_R P_L, \qquad P_{L,R}^2 = P_{L,R},$$

using the first of the following identities,

$$\gamma_5^2 = 1, \qquad \{\gamma_5, \gamma_\mu\} = 0,$$

that can be straightforwardly derived from the Clifford algebra. The left- and right-handed components of the quark fields are then obtained by action of the respective projectors,

$$q_{L,R} = P_{L,R} q, \qquad \bar{q}_{L,R} = \bar{q} P_{R,L}.$$

The massless part of the Lagrangian given in eq. (2.1) can be rewritten as

$$\mathscr{L}^0_{\mathrm{QCD}} = \bar{q}_L \not{D} q_L + \bar{q}_R \not{D} q_R,$$

where additionally the flavor indices are implicit, collecting the flavors in a vector

$$q_{L,R} = \begin{pmatrix} (q_1)_{L,R} \\ (q_2)_{L,R} \\ \vdots \\ \left(q_{N_f}\right)_{L,R} \end{pmatrix}.$$

The Dirac operator of course acts as the identity in flavor space. It is then apparent that the left-handed and right-handed components decouple in the massless limit, therefore often referred to as chiral limit, and $\mathscr{L}^0_{\mathrm{QCD}}$ exhibits a global symmetry

$$\underbrace{\mathrm{SU}(N_f)_L \times \mathrm{SU}(N_f)_R}_{\mathrm{G}} \times \mathrm{U}(1)_V \times \mathrm{U}(1)_A$$

with the so called chiral group G.[1] This symmetry corresponds to invariance of the massless part of the Lagrangian in (2.1) under the transformations

$$\begin{aligned} q_L &\xrightarrow{G} L q_L, \qquad & \bar{q}_L &\xrightarrow{G} \bar{q}_L L^\dagger \\ q_R &\xrightarrow{G} R q_R, \qquad & \bar{q}_R &\xrightarrow{G} \bar{q}_R R^\dagger. \end{aligned}$$

Additional symmetries include invariance under parity and charge conjugation.
The symmetry under the chiral group G is widely believed to be spontaneously broken down to the *diagonal* or *vector subgroup*

$$\mathrm{H} = \mathrm{SU}(N_f)_V = \mathrm{G}|_{L=R}.$$

This notion is supported by hadron phenomenology. The Goldstone theorem predicts the existence of a massless boson for any spontaneously broken symmetry. For the symmetry breaking pattern G $\to$ H, this corresponds to $N_f^2 - 1$ massless Goldstone bosons, as the spontaneously broken axial subgroup of G / H is itself isomorphic to $\mathrm{SU}(N_f)$. Hence, for any of the $N_f^2 - 1$ spontaneously broken generators of $\mathrm{SU}(N_f)$, there should be a massless Goldstone boson. As long as the explicit symmetry breaking by nonvanishing quark masses, that will be discussed later on, can be treated as a small perturbation, the Goldstone bosons should at most acquire a small mass compared to the rest of the hadronic spectrum. This mass difference is in fact observed for pions and kaons, that are thus taken to be the (pseudo) Goldstone bosons of a spontaneously broken $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$ symmetry, whose moderately small masses reflect the explicit symmetry breaking by nonzero quark masses.
Additional evidence comes from lattice computations. Though not directly accessible experimentally, the so-called quark condensate

$$\langle 0|\bar{q}q|0\rangle$$

[1] The additional $\mathrm{U}(1)_V$ symmetry leads to baryon number conservation, $\mathrm{U}(1)_A$ is an anomalous symmetry, that does not hold on the quantum level for the number of colors $N_c = 3$ realized in nature. Both symmetries will not be discussed any further.

can be measured in lattice computations. Realizing that left-handed and right-handed components couple in the quark condensate,

$$\langle 0|\bar{q}_L q_R + \bar{q}_R q_L|0\rangle \xrightarrow{G} \langle 0|\bar{q}_L L^\dagger R q_R + \bar{q}_R R^\dagger L q_L|0\rangle\,,$$

a nonvanishing quark condensate is a sufficient, though not necessary, condition for spontaneous breaking of the axial subgroup of G, while the vector subgroup H remains unbroken. Both, lattice computations of the quark condensate (see e.g. [5, 6] and references therein) and its extraction from QCD sum rules [7] strongly suggest a non-vanishing quark condensate, hence supporting the notion of spontaneous symmetry breaking.

2.2. Chiral Perturbation Theory as an Effective Theory

The observation that the coupling of Goldstone bosons is proportional to their momenta allows for a perturbative expansion of the low-energy behavior of observables. Results for soft-pion processes such as pion scattering in the framework of *current-algebra* were found to be equivalent to leading order results from what was called the *dynamical framework*, starting from a particular Lagrangian density [8, 9]. In modern language, current-algebra results correspond to the tree-level predictions of an effective field theory [10]. In this framework it is clear how higher order corrections can be studied systematically. The appropriate Lagrangian can be constructed from symmetry arguments alone, such that the resulting scattering matrix elements are just the most general expressions compatible with all the underlying symmetries. In combination with the requirement, that the resulting effective theory be an expansion in pion momenta, possible terms that can occur in the Lagrangian are limited to a manageable number. The according effective low-energy field theory is called *Chiral Perturbation Theory* (ChPT) [11], and was then extended to include the strange flavor [12].
We want to write down the most general Lagrangian respecting the desired underlying symmetries in a compact way. Therefore, the meson fields as relevant degrees of freedom are used to parametrize a matrix-valued field, that transforms linearly under G. The matrix-valued field is an element of the spontaneously broken part of the full chiral group, the coset G/H, which is in turn isomorphic to SU(N_f). A possible parametrization of the group elements $\Sigma(x)$ describing the fluctuations around the ground state of the theory is hence given by

$$\Sigma(x) = \exp\left(\frac{2\mathrm{i}}{f}\pi(x)\right), \tag{2.2}$$

where the physical meson fields enter as combinations of $\pi^a(x)$,

$$\pi(x) = \sum_{a=1}^{N_f^2-1} \pi^a(x) T^a, \tag{2.3}$$

with T^a denoting the generators of SU(N_f) for $a \in 1, 2, \ldots, N_f^2 - 1$. We use the normalization

$$\left\langle T^a T^b \right\rangle = \frac{1}{2}\delta_{ab}, \tag{2.4}$$

where $\langle \cdot \rangle$ denotes the trace over the respective $N_f \times N_f$-matrices in flavor space. In order to satisfy the normalization condition, we have

$$T^a = \begin{cases} \frac{1}{2}\sigma^a & \text{for SU(2)} \\ \frac{1}{2}\lambda^a & \text{for SU(3)} \end{cases} \tag{2.5}$$

with Pauli and Gell-Mann matrices σ^a and λ^a, respectively. Generalized Gell-Mann matrices to generate SU(N) can readily be constructed [13]. The physical fields of three flavor ChPT are incorporated in

$$\pi = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta_8 & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta_8 & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta_8 \end{pmatrix}.$$

In two flavor ChPT, π reduces to the upper left 2×2 matrix with η_8 omitted. The charged pions are thus linear combinations of π^1 and π^2, whereas the neutral pion is just π^3. η_8 is related to π^8, and the kaons are given by linear combinations of π^4, π^5, π^6 and π^7.
The inverse power of f in the exponential in eq. (2.2) is included for dimensional reasons. The benefit of working in the exponential parametrization is the particularly simple transformation behavior of Σ under action of the chiral group G,

$$\Sigma \xrightarrow{G} L\Sigma R^\dagger. \tag{2.6}$$

Other symmetries are the discrete symmetries parity (P) and charge conjugation (C), that act on Σ as

$$\Sigma \xrightarrow{P} \Sigma^\dagger, \qquad \Sigma \xrightarrow{C} \Sigma^{\mathrm{T}}. \tag{2.7}$$

The chiral Lagrangian is now constructed from the field Σ and its partial derivatives, amounting to the anticipated expansion in pion momenta. It must be an O(4) scalar[2], which restricts the number of derivatives to even integers, and a singlet under G, P and C. The term

$$\left\langle \Sigma\Sigma^\dagger \right\rangle$$

has the desired transformation property. But since $\Sigma \in \mathrm{SU}(N_f)$, it contributes only via a constant that is irrelevant for the equations of motion. The first nontrivial and in fact unique term involving two derivatives is given by

$$\mathscr{L}_{p^2} = \frac{f^2}{4} \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle. \tag{2.8}$$

The coefficient f of the term is one of the aforementioned Low Energy Constants (LECs). Although it is in principle determined by the parameters of Quantum Chromodynamics through the requirement that the effective theory has to reproduce the low-energy physics of the underlying theory, spelling out the explicit connection requires solving QCD exactly. In practice, the parameters of an effective theory can be

[2] Or SO(1,3), which corresponds to Lorentz invariance, in Minkowski space.

determined by matching appropriate correlation functions in both, the effective theory and the underlying theory. In the case of Chiral Perturbation Theory, the Low Energy Constants are obtained by comparison with non-perturbative results from lattice QCD. The particular parameter f is the pion decay constant in the chiral limit, as can be seen from evaluation of the pion-to-vacuum matrix element mediated by the axial vector of chiral symmetry[3].

Expanding the Lagrangian given in eq. (2.8) only up to two meson fields, one recovers the standard kinetic term of a scalar field theory,

$$\mathscr{L}_{p^2} = \frac{1}{2}\partial_\mu \pi^a(x)\partial_\mu \pi^a(x),$$

where the sum over a is implied. The correct normalization explains the seemingly somewhat arbitrary coefficient in the Lagrangian. At order $\mathcal{O}(p^4)$, there are two possible contributions. On the one hand, contributions come from a loop diagram built from interaction vertices of $\mathscr{L}_{p^2}$, once expanded to fourth order in the meson fields. On the other hand, two-pion vertices from the Lagrangian $\mathscr{L}_{p^4}$ have to be taken into account. The respective Lagrangian containing all terms that are compatible with the aforementioned symmetries and involve four derivatives is given by [12]

$$\mathscr{L}_{p^4} = -L_1 \left\langle \partial_\mu\Sigma\partial_\mu\Sigma^\dagger \right\rangle^2 - L_2 \left\langle \partial_\mu\Sigma\partial_\nu\Sigma^\dagger \right\rangle \left\langle \partial_\mu\Sigma\partial_\nu\Sigma^\dagger \right\rangle - L_3 \left\langle \left(\partial_\mu\Sigma\partial_\mu\Sigma^\dagger\right)^2 \right\rangle. \tag{2.9}$$

The new Low Energy Constants L_k are called Gasser-Leutwyler coefficients. As, however, the expansion of the Lagrangian in eq. (2.9) in terms of meson fields starts only at four fields, these terms will not contribute to masses and decay constants up to order $\mathcal{O}(p^4)$.

This language alludes to the organizing principle involved in the construction of the effective theory. Since it is supposed to describe the low-energy physics of QCD with vanishing coupling of mesons as their momenta tend to zero, the field theory is organized as a perturbative expansion in the external meson momenta. In the effective theory this is equivalent to an expansion in the number of derivatives. The dimensionless expansion parameter is the ratio

$$r = \frac{p^2}{\Lambda^2}.$$

When working out calculations to a fixed order $r^n \sim p^{2n}$ in the derivative expansion one thus has to take into account a finite number of terms involving at most $2n$ derivatives, rendering the nonrenormalizable effective theory predictive once the LECs are known.

2.3. Explicit Symmetry Breaking and Spurion Analysis

The spontaneously broken chiral symmetry of massless QCD is additionally broken explicitly by nonzero quark massses. The mass term in the QCD Lagrangian,

$$\mathscr{L}_{\text{massive}} = \bar{q}Mq,$$

[3] In the convention used throughout this work, $f \approx 93$ MeV.

with diagonal quark mass matrix

$$M = \mathrm{diag}(m_u, m_d, \dots), \tag{2.10}$$

shares the transformation behavior of the quark condensate under action of the chiral group G in the mass-degenerate case, in that it couples left- and right-handed components of the fermion fields, and thus explicitly breaks chiral symmetry. For sufficiently small quark masses compared to the energy scale Λ, the explicit symmetry breaking may be treated as a perturbation to the approximate chiral symmetry. The pseudo Goldstone bosons then acquire a nonzero, though small mass. In order to reproduce the explicit symmetry breaking in the effective theory, it has to be incorporated properly. The starting point for the so-called spurion analysis is the observation, that the massive QCD Lagrangian can be made invariant under action of the chiral group G, C and P, once a nontrivial transformation behavior of M is imposed,

$$M \xrightarrow{G} LMR^\dagger, \qquad M \xrightarrow{C} M^{\mathrm{T}}, \qquad M \xrightarrow{P} M^\dagger.$$

This unphysical, hence *spurious*, intermediate transformation behavior serves as a mnemonic in order to carry over the explicit symmetry breaking pattern to the effective theory correctly. After, again, all terms consistent with the desired symmetries built from Σ, $\partial_\mu\Sigma$, M and their Hermitian conjugates have been written down, the spurion M is reset to its physical value given in eq. (2.10). The sole term with one mass insertion is

$$\mathscr{L}_m = \frac{f^2}{4}\left\langle \chi^\dagger\Sigma + \Sigma^\dagger\chi \right\rangle, \tag{2.11}$$

where χ encompasses the new Low Energy Constant B,

$$\chi = 2BM,$$

that is connected to the quark condensate.
The effective theory then becomes a joint expansion in mass spurion insertions and small pion momenta, hence derivatives in the effective Lagrangian. Expanding eq. (2.11) in meson fields, the first nontrivial terms occur at quadratic order in meson fields and reproduce the mass term of a scalar field theory. This induces the standard power counting scheme of ChPT,

$$p^2 \sim m, \tag{2.12}$$

where the single m refers to the number of (quark) mass, thus mass spurion, insertions. Once this power counting scheme is adopted, the consistent (Euclidean) leading order continuum ChPT Lagrangian is given by

$$\begin{aligned} \mathscr{L}_2 &= \mathscr{L}_{p^2} + \mathscr{L}_m \\ &= \frac{f^2}{4}\left\langle \partial_\mu\Sigma\partial_\mu\Sigma^\dagger \right\rangle - \frac{f^2}{4}\left\langle \chi^\dagger\Sigma + \Sigma^\dagger\chi \right\rangle. \end{aligned} \tag{2.13}$$

Other power counting schemes can appear to be reasonable based on what one assumes to be the predominant trigger of spontaneous symmetry breaking [14], referred to as generalized ChPT. However, throughout this work the standard power counting scheme (2.12) is assumed. The orders of the expansion are then organized as follows:

$$\begin{array}{lcl} \text{LO} & : & p^2,\, m \\ \text{NLO} & : & p^4,\, p^2 m,\, m^2. \end{array}$$

The Lagrangian involving four derivatives has already been given in eq. (2.9). Adding all other invariants contributing at next to leading order, one ends up with the continuum ChPT Lagrangian [12]

$$\begin{aligned} \mathscr{L}_4 = &- L_1 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle^2 - L_2 \left\langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \right\rangle \left\langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \right\rangle - L_3 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \partial_\nu \Sigma \partial_\nu \Sigma^\dagger \right\rangle \\ &+ L_4 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle \left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle + L_5 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \left(\chi^\dagger \Sigma + \Sigma^\dagger \chi \right) \right\rangle \\ &- L_6 \left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle^2 - L_7 \left\langle \chi^\dagger \Sigma - \Sigma^\dagger \chi \right\rangle^2 - L_8 \left\langle \chi^\dagger \Sigma \chi^\dagger \Sigma + \Sigma^\dagger \chi \Sigma^\dagger \chi \right\rangle . \end{aligned} \tag{2.14}$$

Eq. (2.14) now incorporates all Gasser-Leutwyler coefficients encoding the lack of complete knowledge about QCD. They are determined as a byproduct when using formulae calculated from ChPT as fit functions for results obtained in lattice QCD.
The number of Low Energy Constants increases rapidly with the considered order in the joint expansion, and amounts to over 100 constants already at NNLO in the prescribed power counting scheme [15]. However, when computing physical observables in SU(2) ChPT, characteristic combinations of Low Energy Constants occur. The respective terms in the Lagrangian are hence not linearly independent. Redundant terms can be identified on Lagrangian level already, employing Cayley-Hamilton relations [16]. These very relations can not be exploited to simplify the Lagrangian given so far for $N_f = 4$, which is the case of primary interest throughout this work. The Lagrangian is therefore kept in its most general form given in eq. (2.14).
With the Lagrangian of ChPT up to NLO at hand, meson masses can readily be computed to that order. The respective results for $N_f = 2$ and $N_f = 3$ were worked out in the pioneering publications [11, 12].
In order to compute other quantities of interest, such as decay constants, the (vector and axial) currents and (scalar and pseudoscalar) densities have to be constructed as the most general expressions transforming accordingly under the various symmetries considered before. They can either be obtained by introducing external sources in the Lagrangian and taking sensible functional derivatives [11, 12], or by following the prescription of writing down the most general expression in terms of the building blocks given before [17].

3. Chiral Perturbation Theory for Lattice QCD

3.1. Symanzik Effective Theory

So far, the effective theory for QCD has been established. Once the LECs are known, ChPT predicts observables accessible in experiments. On the other hand, ChPT can be extended to describe cutoff effects encountered in lattice QCD. Lattice QCD is the formulation of QCD on a discrete Euclidean space-time grid, that naturally provides an ultraviolet-regulator through its momentum cutoff Λ_{UV} inversely proportional to the lattice spacing a. Present day simulations are performed at lattice spacings of about $a = 0.05 \ldots 0.1$ fm (see e.g. [18]), implying a momentum cutoff at $\Lambda_{UV} = 2 \ldots 4$ GeV. This cutoff is not too large compared to the QCD scale $\Lambda = 1$ GeV and will thus impact the results from continuum ChPT. The resulting effective theory then describes lattice QCD including cutoff effects, and particularly guides the extrapolation to the point of physical (light) pion masses not yet accessible in simulations.
Studying cutoff effects in lattice QCD via an expansion in

$$r_a = \frac{\Lambda}{\Lambda_{UV}} \sim a\Lambda$$

yields another effective field theory. The idea to make the lattice spacing dependence of lattice QCD explicit near the continuum culminates in *Symanzik's effective theory* [19].
Starting from a properly normalized formulation of lattice QCD, which means it has to reproduce QCD in the continuum limit, the effective action near the continuum is expressed as expansion in the lattice spacing a,

$$S_{\text{Sym}} = S_0 + aS_1 + a^2 S_2 + \ldots \quad . \tag{3.1}$$

According to the assumption, that the effective theory reduces to QCD in the continuum limit, S_0 is the usual QCD action. The other S_k are built of all local operators $O_i^{(k+4)}$ of the respective mass dimension k comprising the fermion and gauge fields and their derivatives, such that the product $a^k S_k$ has the desired dimension of an action,

$$S_k = \int \mathrm{d}^4x \sum_i \bar{c}_i^{(k+4)} O_i^{(k+4)},$$

and the operators O_i obey all the symmetries of the respective formulation of lattice QCD. The $\bar{c}_i^{(k+4)}$ are, again, unknown constants of the effective theory. Therefore, the form of the Symanzik effective action depends on the details of how the fermions are implemented, as different available discretizations compromise different symmetries

of continuum QCD. Apart from the apparent breaking of O(4) invariance, Wilson fermions as the sole formulation of lattice QCD covered in this work explicitly break chiral symmetry at $\mathcal{O}(a)$. The respective term thus appears in S_1 of the Symanzik effective action in eq. (3.1). Terms entering the Symanzik effective action were worked out and are thus available [20]. Their number can be reduced realizing that terms related by partial integration are redundant, since the action is defined only up to a constant anyway. Additionally, different expressions compatible with the preserved symmetries can be discarded if they are related by the equations of motion, as long as only on-shell quantities, such as masses, are considered.
At $\mathcal{O}(a)$, only the Pauli term remains [20],

$$S_1 = \int \mathrm{d}^4x\, \bar{c}_{\mathrm{sw}} \bar{q}(x) \mathrm{i}\sigma_{\mu\nu} G_{\mu\nu}(x) q(x),$$

where $G_{\mu\nu}(x)$ is the gauge field strength tensor and

$$\sigma_{\mu\nu} = \frac{\mathrm{i}}{2} \left[\gamma_\mu, \gamma_\nu\right]$$

leads to the aforementioned explicit chiral symmetry breaking. Decomposing the Pauli term into its chiral components,

$$S_1 = \int \mathrm{d}^4x\, \bar{c}_{\mathrm{sw}} \left\{\bar{q}_L(x) \mathrm{i}\sigma_{\mu\nu} G_{\mu\nu}(x) q_R(x) + \bar{q}_R(x) \mathrm{i}\sigma_{\mu\nu} G_{\mu\nu}(x) q_L(x)\right\}, \tag{3.2}$$

the explicit breaking of chiral symmetry becomes apparent.

3.2. Chiral Perturbation Theory for Wilson Fermions

Starting from the Symanzik effective theory, which is the effective continuum theory for lattice QCD, the corresponding ChPT can readily be constructed. Only the behavior of terms in the Symanzik effective action under chiral transformation enters its construction. The *Pauli term* in eq. (3.2) breaks chiral symmetry in a mass term-like fashion. In order to carry over the symmetry breaking pattern to ChPT correctly, the spurion analysis introduced before is employed. Assigning a nontrivial transformation behavior to the overall coefficient of the Pauli term via a spurion field $A = a\bar{c}_{\mathrm{sw}}$,

$$A \xrightarrow{G} LAR^\dagger, \qquad A \xrightarrow{C} A^{\mathrm{T}}, \qquad A \xrightarrow{P} A^\dagger, \tag{3.3}$$

invariance of the Pauli term under G, P and C is enforced. The effective action is then constructed in analogy to the treatment of explicit chiral symmetry breaking by the masses and encompasses all terms built from the building blocks Σ, its derivatives, M and A. Subsequently, the spurion field A is reset to its physical value,

$$A \to a\bar{c}_{\mathrm{sw}},$$

that acts as identity in flavor space, in contrast to the mass spurion at its physical value if quark masses are not degenerate. Considering only terms without derivatives, and limiting the number of A spurion field insertions to one, there is essentially one invariant [21],

$$\mathscr{L}_a = -\frac{f^2 W_0}{2}\left\langle A^\dagger\Sigma + \Sigma^\dagger A\right\rangle \to -\frac{f^2}{4}\rho\left\langle\Sigma + \Sigma^\dagger\right\rangle, \tag{3.4}$$

where

$$\rho = 2W_0 a$$

incorporates the new LEC W_0, which in a sense constitutes the counterpart of B encountered in the mass term. There are different conventions on whether or not to keep the coefficient $\bar{c}_{\mathrm{sw}}$ explicit, although it is always accompanied by unknown constants. Keeping $\bar{c}_{\mathrm{sw}}$ explicit is of no particular interest for the present work.
The only other possible term $\left\langle A^\dagger M + M^\dagger A\right\rangle$ amounts to a constant in the effective action and is thus discarded. Including terms with two derivatives or, according to the standard power counting scheme of continuum ChPT, equivalently one mass insertion, one finds [21]

$$\begin{aligned}\mathscr{L}_{p^2a} &= \rho W_4\left\langle\partial_\mu\Sigma\partial_\mu\Sigma^\dagger\right\rangle\left\langle\Sigma + \Sigma^\dagger\right\rangle + W_5\rho\left\langle\partial_\mu\Sigma\partial_\mu\Sigma^\dagger\left(\Sigma + \Sigma^\dagger\right)\right\rangle,\\ \mathscr{L}_{ma} &= -W_6\rho\left\langle\chi^\dagger\Sigma + \Sigma^\dagger\chi\right\rangle\left\langle\Sigma + \Sigma^\dagger\right\rangle - W_7\rho\left\langle\chi^\dagger\Sigma - \Sigma^\dagger\chi\right\rangle\left\langle\Sigma - \Sigma^\dagger\right\rangle\\ &\qquad - W_8\rho\left\langle\chi^\dagger\Sigma\Sigma + \Sigma^\dagger\Sigma^\dagger\chi\right\rangle.\end{aligned} \tag{3.5}$$

At order $\mathcal{O}(a^2)$, there are in principle two distinct sources of additional terms. First, terms involving two A spurion field insertions contribute. Additionally, new spurion fields are spawned to make terms occurring in S_2 invariant under the chiral group G, parity and charge conjugation. However, careful analysis of all bilinears and four-quark operators appearing in S_2 shows, that the total number of terms remains manageable and no spurion fields other than A and powers of it are needed [22]. The resulting Lagrangian reads

$$\mathscr{L}_{a^2} = -W_6'\rho^2\left\langle\Sigma + \Sigma^\dagger\right\rangle^2 - W_7'\rho^2\left\langle\Sigma - \Sigma^\dagger\right\rangle^2 - \rho^2 W_8'\left\langle\Sigma\Sigma + \Sigma^\dagger\Sigma^\dagger\right\rangle. \tag{3.6}$$

3.3. Power Counting Schemes for the Systematic Expansion

Chiral Perturbation Theory for Wilson fermions (WChPT) is hence a joint expansion in momenta, quark masses and the lattice spacing. For the expansion to be consistent to a given order, one has to impose an appropriate power counting scheme describing the relative impact of the three expansion parameters. The relative size dictates, which terms involving mass and lattice spurion insertions need be included in calculations accurate to a prescribed order. It has to be guided by the actual sizes of quark masses and the lattice spacing used in simulations. There are two relevant scenarios for present day simulations.
In the *Generically Small Masses* (GSM) regime [23], the explicit chiral symmetry breaking due to masses and the lattice are of comparable size. Symbolically, this

statement is expressed as[1]

$$p^2 \sim m \sim a.$$

In this power counting scheme, the expansion is organized as follows:

$$\begin{array}{lll} \text{LO} & : & p^2,\, m,\, a \\ \text{NLO} & : & p^4,\, p^2 m,\, p^2 a,\, m^2,\, ma,\, a^2. \end{array}$$

In this regime, all parts of the Lagrangian up to NLO have already been specified. In the leading order Lagrangian,

$$\mathscr{L}_{\text{LO}} = \frac{f^2}{4}\left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle - \frac{f^2}{4}\left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle - \frac{f^2}{4}\rho \left\langle \Sigma + \Sigma^\dagger \right\rangle,$$

the $\mathcal{O}(a)$ term can be absorbed by redefinition of χ [24],

$$\chi \to \chi' = \chi + \rho\, \mathbb{1}_{N_f}, \tag{3.7}$$

which amounts to an $\mathcal{O}(a)$ shift in the quark masses. Working out the redefinition (3.7), the LECs at order $\mathcal{O}(ma)$ and $\mathcal{O}(a^2)$ are altered. The Lagrangian up to NLO in the GSM regime in terms of χ', whereby the prime is dropped again right away, reads

$$\begin{aligned}
\mathscr{L}_2 =& \frac{f^2}{4}\left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle - \frac{f^2}{4}\left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle \\
\mathscr{L}_4 =& -L_1 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle^2 - L_2 \left\langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \right\rangle \left\langle \partial_\mu \Sigma \partial_\nu \Sigma^\dagger \right\rangle - L_3 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \partial_\nu \Sigma \partial_\nu \Sigma^\dagger \right\rangle \\
&+ L_4 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle \left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle + L_5 \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \left(\chi^\dagger \Sigma + \Sigma^\dagger \chi \right) \right\rangle \\
&- L_6 \left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle^2 - L_7 \left\langle \chi^\dagger \Sigma - \Sigma^\dagger \chi \right\rangle^2 - L_8 \left\langle \chi^\dagger \Sigma \chi^\dagger \Sigma + \Sigma^\dagger \chi \Sigma^\dagger \chi \right\rangle \\
\mathscr{L}_{p^2 a} =& \overline{W}_4 \rho \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right\rangle \left\langle \Sigma + \Sigma^\dagger \right\rangle + \overline{W}_5 \rho \left\langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \left(\Sigma + \Sigma^\dagger \right) \right\rangle \\
\mathscr{L}_{ma} =& -\overline{W}_6 \rho \left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle \left\langle \Sigma + \Sigma^\dagger \right\rangle - \overline{W}_7 \rho \left\langle \chi^\dagger \Sigma - \Sigma^\dagger \chi \right\rangle \left\langle \Sigma - \Sigma^\dagger \right\rangle \\
&- \overline{W}_8 \rho \left\langle \chi^\dagger \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \chi \right\rangle \\
\mathscr{L}_{a^2} =& -\overline{W}'_6 \rho^2 \left\langle \Sigma + \Sigma^\dagger \right\rangle^2 - \overline{W}'_7 \rho^2 \left\langle \Sigma - \Sigma^\dagger \right\rangle^2 - \overline{W}'_8 \rho^2 \left\langle \Sigma \Sigma + \Sigma^\dagger \Sigma^\dagger \right\rangle
\end{aligned} \tag{3.8}$$

with the respective redefined LECs

$$\begin{aligned}
\overline{W}_i &= \begin{cases} W_i - L_i & i = 4, 5 \\ W_i - 2L_i & i = 6, 7, 8 \end{cases} \\
\overline{W}'_i &= W'_i - W_i + L_i \qquad i = 6, 7, 8.
\end{aligned}$$

Decreasing the quark mass with the lattice spacing held fixed, eventually m will become comparable to a^2, which is the defining property of the *Large Cutoff Effects* (LCE) regime, also referred to as *Aoki regime* in the literature [23],

$$p^2 \sim m \sim a^2.$$

In this power counting scheme, one has

[1] In all the expansion ratios encountered before, appropriate powers of the QCD scale Λ have to be multiplied in order to make the expansion parameter dimensionless. The precise power can readily be inferred from the mass dimension and is thus not stated explicitly any more.

LO	:	p^2, m, a^2
NLO	:	p^2a, ma, a^3
NNLO	:	p^4, p^2m, p^2a^2, m^2, ma^2, a^4.

Recall that the leading order m already refers to $\mathcal{O}(a)$ shifted masses. All terms up to NNLO enter the calculation of pseudo Goldstone boson masses to one loop. The corresponding results in the GSM regime can be obtained from the result in the LCE regime, once appropriate terms are discarded. One can readily think of various other power counting schemes. However, the GSM regime and the LCE regime appear to be the relevant scenarios in practice. Having the respective WChPT Lagrangian at hand, meson masses to one-loop can now be computed. They are determined as the pole of the two-point correlation function. Correlation functions, in turn, are computed by saddle point expansion, such that the matrix-valued field Σ_p parametrizes fluctuations around the *vacuum state* or *ground state* Σ_0 of the theory,

$$\Sigma(x) = \Sigma_0^{\frac{1}{2}}\,\Sigma_p(x)\,\Sigma_0^{\frac{1}{2}}. \tag{3.9}$$

Put differently, the expansion around the ground state of the theory implies there are no terms linear in the fields $\pi^a(x)$ when inserting the parametrization of the *physical fields*

$$\Sigma_p(x) = \exp\left(\frac{2\mathrm{i}}{f}\pi^a(x)T^a\right),$$

and subsequently expanding in meson fields. The ground state is obtained from minimizing the potential energy. Since

$$\mathscr{L} = T - U,$$

the potential energy is given by all terms in the Lagrangian not containing derivatives, if the ground state is taken to be constant over spatial directions.

In continuum ChPT, the ground state is just the $\mathrm{SU}(N_f)$ identity to all orders of contributions to the potential energy [12]. In the LCE regime of WChPT with $\mathcal{O}(a^2)$ contributing at leading order, the ground state of the theory is a nontrivial element of $\mathrm{SU}(N_f)$, depending on the relative sizes of m and a and the signs of the LECs $\overline{W}_i$. The connection to the nontrivial phase structure of the theory was examined in the two flavor theory. The existence of the Aoki phase [25] is predicted by WChPT [26].

3.4. Twisted Mass Wilson Fermions

QCD with twisted masses differs from standard QCD by its mass term. Starting from the generalized expression for a mass matrix in two flavor QCD with degenerate masses[2],

$$M = m^{(q)} + \mathrm{i}\mu^{(q)}\gamma_5\sigma_3, \tag{3.10}$$

[2] We use the additional index to distinguish the bare parameters entering the QCD Lagrangian at quark level from their renormalized ChPT counterparts.

with the third Pauli matrix σ_3 acting in flavor space, it is not immediately clear that this is in fact a mass term. But it can be shown that, in the continuum, QCD with twisted masses is related to QCD with a standard mass term with mass $\sqrt{m_{(q)}^2 + \mu_{(q)}^2}$ by a field redefinition

$$\Psi \to \Psi' = \exp\left(\mathrm{i}\alpha\gamma_5\sigma_3/2\right)\Psi, \qquad \bar{\Psi} \to \bar{\Psi}' = \bar{\Psi}\exp\left(\mathrm{i}\alpha\gamma_5\sigma_3/2\right),$$

and hence merely by a change of variables [27]. This statement does however not hold for lattice QCD with Wilson fermions, where only either the mass term or the Wilson term can be untwisted. It was then proposed to regard the twisted mass formulation as an alternative regularization of QCD, instead of thinking of a nonvanishing $\mu^{(q)}$ as unphysical [27]. This proves useful since twisted mass terms with $\mu^{(q)} \neq 0$ impose a lower limit on the spectrum of the Dirac operator and thereby prevent *exceptional configurations* that otherwise pose a problem for numerical simulations. Additionally, tuning the *twist angle* α to a specific value referred to as *maximal twist*, one can achieve *automatic* $\mathcal{O}(a)$ *improvement* [28].

3.4.1. ChPT for 2 Wilson Quarks with Twisted Masses

Chiral Perturbation Theory for twisted mass lattice QCD with two mass-degenerate flavors of Wilson fermions ($N_f = 2$ tmWChPT) was studied to one loop in both, the GSM regime [29], and the LCE regime [30]. In the following, we briefly recall prominent features of the respective studies.
Since, in the massless case, all symmetry considerations so far remain valid, the incorporation of twisted masses in SU(2) ChPT with degenerate up and down quark masses solely alters the ChPT mass term, which then reads

$$\chi = 2BM_l = 2B\left(m + \mathrm{i}\mu\sigma_3\right). \tag{3.11}$$

The mass matrix can be re-expressed as

$$M_l = m'\left(\cos\phi\,\mathbb{1}_2 + \mathrm{i}\sin\phi\,\sigma_3\right) = m'\mathrm{e}^{\mathrm{i}\phi\sigma_3},$$

in terms of the twist angle ϕ and *radial mass* m',

$$\begin{aligned} \cot\phi &= \frac{m}{\mu}, \\ m' &= \sqrt{m^2 + \mu^2}. \end{aligned} \tag{3.12}$$

This reparametrization simply corresponds to using polar coordinates instead of Cartesian coordinates in the complex mass plane,

$$\begin{pmatrix} m \\ \mu \end{pmatrix} \longleftrightarrow \begin{pmatrix} m' \\ \phi \end{pmatrix}.$$

In this language, a twist is simply a rotation in the complex mass plane. This mass term singles out the σ_3 direction and leads to a so-called vacuum alignment to this very direction, as can be seen from expanding the ChPT mass term in meson fields, whereby a term linear in π^3 is spawned. The hence nontrivial ground state is now determined by minimizing the potential energy (density) for a homogeneous ground state,

$$V = -\mathscr{L}_m - \mathscr{L}_{ma} - \mathscr{L}_{a^2}. \tag{3.13}$$

The particular choice for the mass matrix suggests for the ground state to be of the form [24]

$$\Sigma_0 = \mathrm{e}^{\mathrm{i}\omega\sigma_3}, \tag{3.14}$$

where ω is referred to as vacuum angle, and minimizing the potential energy amounts to plugging the ansatz (3.14) into eq. (3.13) and minimizing with respect to ω. The condition

$$\frac{\partial V}{\partial \omega} \stackrel{!}{=} 0$$

is called *gap equation* and determines the vacuum angle by means of an implicit equation,

$$\omega = \omega(m, \mu, a) = \omega(m', \phi, a).$$

One finds

$$2B\mu\cos\omega = \sin\omega\left(2Bm + 16\frac{\rho^2}{f^2}\overline{W}'_{68}\cos\omega\right) + 8\frac{\rho}{f^2}\overline{W}_{68}\left(2Bm\sin 2\omega + 2B\mu\cos 2\omega\right), \tag{3.15}$$

where we have introduced the shorthand notations[3]

$$\begin{aligned} \overline{W}_{68} &= 2\overline{W}_6 + \overline{W}_8, \\ \overline{W}'_{68} &= 2\overline{W}'_6 + \overline{W}'_8. \end{aligned} \tag{3.16}$$

Eq. (3.15) matches the findings of [30], when $\overline{W}_{68}$ is set to zero, which amounts to minimizing the leading order potential in the LCE regime. The gap equation was studied extensively in the literature [31, 32]. On the other hand, working in the GSM regime the gap equation can be expressed in terms of the radial mass and the twist angle and subsequently be solved iteratively order by order to yield [29]

$$\omega = \phi - \frac{8}{f^2}\rho\sin\phi\left(\overline{W}_{68} + 2\overline{W}'_{68}\frac{\rho}{m'}\cos\phi\right).$$

One has to keep in mind that not all of the variables m, μ, a, ϕ and ω are independent, whenever encountering mixed expressions.
Once the ground state has been determined, the Lagrangian can be expanded in terms of meson fields around this vacuum state according to eq. (3.9). In kinetic terms, the vacuum does not enter explicitly,

$$\left\langle \partial_\mu\Sigma\partial_\mu\Sigma^\dagger\right\rangle = \left\langle \Sigma_0^{\frac{1}{2}}\partial_\mu\Sigma_p \underbrace{\Sigma_0^{\frac{1}{2}}\left(\Sigma_0^{\frac{1}{2}}\right)^\dagger}_{=\mathbb{1}}\partial_\mu\Sigma_p^\dagger\left(\Sigma_0^{\frac{1}{2}}\right)^\dagger\right\rangle = \left\langle \partial_\mu\Sigma_p\partial_\mu\Sigma_p^\dagger\right\rangle, \tag{3.17}$$

[3] Note that this definition differs from the respective definition in [29] by a factor of 2.

where cyclicity of the trace has been used. The ground state can be reshuffled to the mass matrix in mass terms,

$$\begin{aligned}\left\langle\chi^\dagger\Sigma+\Sigma^\dagger\chi\right\rangle &= \left\langle\chi^\dagger\Sigma_0^{\frac{1}{2}}\Sigma_p\Sigma_0^{\frac{1}{2}}+\left(\Sigma_0^{\frac{1}{2}}\right)^\dagger\Sigma_p^\dagger\left(\Sigma_0^{\frac{1}{2}}\right)^\dagger\chi\right\rangle\\ &= \left\langle\underbrace{\Sigma_0^{\frac{1}{2}}\chi^\dagger\Sigma_0^{\frac{1}{2}}}_{\chi_p^\dagger}\Sigma_p+\Sigma_p^\dagger\left(\Sigma_0^{\frac{1}{2}}\right)^\dagger\chi\left(\Sigma_0^{\frac{1}{2}}\right)^\dagger\right\rangle\\ &= \left\langle\chi_p^\dagger\Sigma_p+\Sigma_p^\dagger\chi_p\right\rangle,\end{aligned}\tag{3.18}$$

but enters explicitly in lattice terms[4]

$$\begin{aligned}\left\langle\Sigma+\Sigma^\dagger\right\rangle &= \left\langle\Sigma_0\Sigma_p+\Sigma_p^\dagger\Sigma_0^\dagger\right\rangle,\\ \left\langle\Sigma\Sigma+\Sigma^\dagger\Sigma^\dagger\right\rangle &= \left\langle\Sigma_0\Sigma_p\Sigma_0\Sigma_p+\Sigma_p^\dagger\Sigma_0^\dagger\Sigma_p^\dagger\Sigma_0^\dagger\right\rangle.\end{aligned}\tag{3.19}$$

The apparent flavor symmetry breaking by the twisted mass term manifests itself through the so-called *pion mass splitting* entering at $\mathcal{O}(a^2)$. The mass splitting can be understood, if for instance the expansion of the $\overline{W}_6'$ up to the leading terms in mesons fields is worked out,

$$\begin{aligned}&-\overline{W}_6'\rho^2\left\langle\Sigma_p\Sigma_0+\Sigma_0^\dagger\Sigma_p^\dagger\right\rangle^2\\ &\quad\sim -\overline{W}_6'\rho^2\left\langle\left(\mathbb{1}+\frac{2i}{f}\pi^aT^a+\dots\right)\left(\cos\omega+2\mathrm{i}\sin\omega T^3\right)+\text{h.c.}\right\rangle^2\\ &\quad\sim -\overline{W}_6'\rho^2\sin\omega\pi_3^2.\end{aligned}\tag{3.20}$$

The pion mass splitting appears as a direct consequence of twisted masses implemented along a determinate direction, leading to a nontrivial ground state parametrized by ω, and subsequently to a differing mass of the meson field associated with this very direction. In the untwisted case $\mu\to 0$, the vacuum angle tends to zero and flavor symmetry is restored. In practical applications, so-called maximal twist $\cos\omega=0$ is of interest, since then automatic $\mathcal{O}(a)$ improvement is achieved [28, 31]. The splitting becomes maximal in this setup. The order, at which the splitting contributes, is defined by the adopted power counting scheme.

In the *GSM regime*, the pion mass splitting enters at NLO. The hence degenerate tree level masses are given by

$$m_{\pi^\pm}^2=m_{\pi^0}^2=2B\left(m\cos\omega+\mu\sin\omega\right).$$

By comparison with continuum ChPT results indicating that the leading order mass is determined by the quark content of the respective meson, μ is essentially the degenerate up and down quark mass at maximal twist.

[4] In this loose vocabulary, *lattice terms* and *mass terms* refer to contributions to the Lagrangian stemming from A and M spurion field insertions respectively, hence terms describing effects related to explicit symmetry breaking by the lattice and nonzero masses.

The pion masses to one loop - denoted by capital letters - are given by [29]

$$M_{\pi^\pm}^2 = m_{\pi^\pm}^2 \left[1 + \frac{1}{32\pi^2 f^2} m_{\pi^\pm}^2 \log \frac{m_{\pi^\pm}^2}{\mu^2} - \frac{8}{f^2} m_{\pi^\pm}^2 \left(2L_4 + L_5 - 4L_6 - 2L_8\right)\right], \quad (3.21)$$

$$M_{\pi^0}^2 = M_{\pi^\pm}^2 - \frac{16\rho^2}{f^2} \overline{W}'_{68}, \quad (3.22)$$

at maximal twist. If instead the pion mass splitting is taken to be of the same order as the pion masses and hence as leading order effect, this amounts to adopting the *LCE power counting*. Eq. (3.22) then holds for the tree level masses at maximal twist,

$$\begin{aligned} m_{\pi^\pm}^2 &= 2B\mu, \\ m_{\pi^0}^2 &= m_{\pi^\pm}^2 - \frac{16\rho^2}{f^2} \overline{W}'_{68}. \end{aligned} \quad (3.23)$$

Technically, in one-loop computations this means one has to distinguish looping charged pions from neutral pions. Consequently, one naively expects both types of chiral logarithms to occur. Obviously, with μ and a^2 both contributing at leading order, hence spawning interaction vertices, one can expand $\mathscr{L}_m$ and $\mathscr{L}_{a^2}$ to four pion fields. The sum of both can then be rewritten as the sum of the usual continuum interaction vertex only with tree level masses given in eq. (3.23), and additional $\mathcal{O}(a^2)$ vertices [30],

$$\mathscr{L}_{m,4\pi} + \mathscr{L}_{a^2,4\pi} = -\frac{1}{24 f^2} m_{\pi^\pm}^2 \pi^4 - \frac{2\rho^2}{f^4} \overline{W}'_{68} \cos^2 \omega \pi^4 + \frac{8}{3} \frac{\rho^2}{f^4} \overline{W}'_{68} \sin^2 \omega \pi^2 \pi_3^2, \quad (3.24)$$

with $\pi^2 = \sum_a \pi^a \pi^a$ and $\pi^4 = \left(\pi^2\right)^2$. The non-analytic part of the one-loop calculation is then obtained by reiterating the continuum results with $\mathcal{O}(a^2)$-shifted tree level masses replacing the continuum tree level masses, plus working out the contributions from the additional vertices given in eq. (3.24). This result is supplemented by the analytic contributions that provide the counterterms to cancel divergences accompanying the chiral logarithms.

The charged pion mass to one loop in two flavor tmWChPT at maximal twist reads [30]

$$M_{\pi^\pm}^2 = m_{\pi^\pm}^2 \left[1 + \frac{1}{32\pi^2 f^2} m_{\pi^0}^2 \log \frac{m_{\pi^0}^2}{\mu^2} - \frac{8}{f^2} m_{\pi^\pm}^2 \left(2L_4 + L_5 - 4L_6 - 2L_8\right) + C_1 \rho^2\right]. \quad (3.25)$$

The correct continuum result [11] is obtained in the limit $\rho \to 0$, implying a vanishing pion mass splitting $m_{\pi^0}^2 \to m_{\pi^\pm}^2$. Somewhat surprisingly, only the neutral pion log is present in the result. The remainder of this work is devoted to performing a similar analysis in the case of 2+1+1 dynamical flavors.

3.4.2. Inclusion of a Dynamical Strange Quark

Three scenarios to include the strange quark as dynamical flavor with twisted masses in the light (u, d)-sector were explored [33], that are briefly recapitulated in the following.

The simplest way to include a dynamical strange quark is to leave the strange quark untwisted. The respective $\mathcal{O}(a)$ terms could be removed through addition of a Sheikholeslami-Wohlert term. However, kaon operators composed of a twisted and an untwisted fermion would require extra effort to extract continuum physics.
If the strange quark is to be twisted, an accompanying twist partner is required. The natural choice is to take the next heavier quark, the charm quark, to serve as twist partner. In order to parametrize non-degenerate strange and charm quark masses, the quark mass term of the heavy (s, c)-doublet in the twisted basis is given by[5]

$$\bar{\Psi}_h \left(m_h^{(q)} + \mathrm{i}\gamma_5 \mu_h^{(q)} \sigma_a + \delta^{(q)} \sigma_3 \right) \Psi_h, \tag{3.26}$$

whereby the direction along which the twist is implemented remains to be discussed. Again, in the continuum the mass term could be untwisted to yield a standard QCD mass term. By comparison with the ordinary diagonal quark mass matrix, one thus identifies the respective quark masses

$$m_{s,c}^{(q)} = \sqrt{\left(m_h^{(q)}\right)^2 + \left(\mu_h^{(q)}\right)^2} \pm \delta^{(q)}, \tag{3.27}$$

such that $m_s^{(q)} < m_c^{(q)}$ implies $\delta^{(q)} < 0$.
One choice for the direction σ_a in eq. (3.26) is the *parallel choice* $\sigma_a = \sigma_3$ implementing the twist in the same direction as the quark mass splitting. This approach was pursued in [34] and leads to a non-real fermion determinant, preventing unquenched simulations with four dynamical flavors as long as currently known algorithms are employed.
In contrast the *perpendicular choice* $\sigma_a \neq \sigma_3$ leads to a real fermion determinant, but mixes flavors. Still, choosing $\sigma_a = \sigma_1$ amounts to the setup now commonly used (see e.g. [35, 18]). In addition to enabling unquenched simulations with dynamical strange and charm quarks, implementing the twist orthogonally implies an exact symmetry of the action under an appropriately chosen parity transformation, that in turn implies kaon mass degeneracy [36].
In a first attempt to construct the ChPT to describe the setup employed in current simulations, we hence start from lattice QCD with four Wilson quarks and mass matrix

$$\tilde{M} = \left(\tilde{M}_l \oplus \tilde{M}_h\right) = \begin{pmatrix} \tilde{M}_l & 0 \\ 0 & \tilde{M}_h \end{pmatrix},$$

with 2×2 light and heavy sector mass matrices $\tilde{M}_{l,h}$ given by

$$\begin{aligned} \tilde{M}_l &= m^{(q)} + \mathrm{i}\mu_l^{(q)} \gamma_5 \sigma_3 \\ \tilde{M}_h &= m^{(q)} + \mathrm{i}\mu_h^{(q)} \gamma_5 \sigma_1 + \delta^{(q)} \sigma_3, \end{aligned}$$

respectively. Note that the same untwisted mass $m^{(q)}$ is used in both the light and the heavy sector in current simulations. Following the standard procedure of transferring the explicit chiral symmetry breaking pattern to the effective theory through spurion

[5] Note, that we prefer to implement the quark mass splitting diagonally in contrast to [33], since this amounts to the common setup in recent simulations. For the following argument, this does not play a role.

analysis in principle yields the desired ChPT. However, setting up the theory this way treats D mesons as pseudo Goldstone bosons. The thereby implicit perturbative expansion in the masses is not sensible at the physical masses of the D mesons. Still, let us briefly recall some of the features of the naive ChPT for 2+1+1 flavors that were worked out in the literature [13]. The name alludes to the setup of two degenerate light quarks and two non-degenerate heavier quarks.
In analogy to the construction of two flavor tmWChPT the theory is set up using the ChPT mass matrix

$$\chi = 2B(M_l \oplus M_h), \tag{3.28}$$

where the 2×2 light and heavy sector submatrices read

$$\begin{aligned} M_l &= m + \mathrm{i}\mu_l\sigma_3 &&= m_l' \mathrm{e}^{\mathrm{i}\phi_l\sigma_3}, \\ M_h &= m + \mathrm{i}\mu_h\sigma_1 + \delta\sigma_3 &&= m_h' \mathrm{e}^{\mathrm{i}\phi_h\sigma_1} + \delta\sigma_3. \end{aligned}$$

There is now one twisted mass $\mu_{l,h}$ for each sector, and equivalently two radial masses and twist angles defined as a straightforward generalization from their definition in the case of two flavors with twisted masses, particularly

$$m'_{l,h} = \sqrt{m^2 + \mu_{l,h}^2}. \tag{3.29}$$

We will use both parametrizations of the mass matrix in terms of Cartesian and polar coordinates.
The physical fields are linear combinations of the fields π^a [13],

$$\Sigma_p = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta_8 + \frac{1}{\sqrt{12}}\eta_{15} & \pi^+ & K^+ & \bar{D}^0 \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta_8 + \frac{1}{\sqrt{12}}\eta_{15} & K^0 & D^- \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta_8 + \frac{1}{12}\eta_{15} & D_s^- \\ D^0 & D^+ & D_s^+ & -\frac{3}{\sqrt{12}}\eta_{15} \end{pmatrix}$$

and are as usual incorporated by expanding around the ground state Σ_0 of the theory as in eq. (3.9). The respective Lagrangian is just the one constructed before.
The particular choice for the mass matrix suggests for the ground state to be of the form

$$\Sigma_0 = \Sigma_l \oplus \Sigma_h, \tag{3.30}$$

with the ansatz

$$\Sigma_l = \mathrm{e}^{\mathrm{i}\omega_l\sigma_3}, \qquad \Sigma_h = \mathrm{e}^{\mathrm{i}\omega_h\sigma_1}.$$

Although the ground state itself is a direct sum of a light and heavy part, terms from $\mathscr{L}_{m^2}$, $\mathscr{L}_{ma}$ and $\mathscr{L}_{a^2}$ induce a coupling between both sectors in the potential energy, since there are contributions composed of a product of two traces.
In the GSM regime, which implies only $\mathscr{L}_m$ contributing to the leading order potential energy, and the other terms amounting to higher order corrections, the respective vacuum angles are given by [13]

$$\begin{aligned} \omega_l &= \phi_l - \frac{8}{f^2}\frac{\rho\sin\phi_l}{2Bm_l'}\left[2Bm_l'\overline{W}_{68} + 2Bm_h' 2\overline{W}_6 + \rho\cos\phi_l 2\overline{W}'_{68} + \rho\cos\phi_h 4\overline{W}'_6\right], \\ \omega_h &= \phi_h - \frac{8}{f^2}\frac{\rho\sin\phi_h}{2Bm_h'}\left[2Bm_h'\overline{W}_{68} + 2Bm_l' 2\overline{W}_6 + \rho\cos\phi_h 2\overline{W}'_{68} + \rho\cos\phi_l 4\overline{W}'_6\right]. \end{aligned} \tag{3.31}$$

The meson tree level masses in this theory read [13]

$$\begin{aligned} m_{\pi^\pm}^2 = m_{\pi^0}^2 &= 2Bm_l' \equiv m_\pi^2, \\ m_{K,D}^2 &= B\left(m_l' + m_{s,c}\right), \\ m_{D_s}^2 &= 2Bm_h'. \end{aligned}$$

Consistent with eq. (3.27), the tree level meson masses in the respective ChPT are determined by their quark content after identifying

$$m_{s,c} = m_h' \pm \delta.$$

The heavy sector radial mass m_h' is hence the average of the strange and charm quark mass, and δ is half their mass splitting.
The η_8 and η_{15} states are not the mass eigenstates of the theory and subject to so-called mixing of flavor neutral mesons [13]. η_8, η_{15} and the SU(4) singlet referred to as η_1 are linear combinations of the respective mass eigenstates η, η_c and η'. The flavor-neutral π^0 does not mix due to degenerate up and down quark masses and hence isopin symmetry. However, η' is too heavy to appear as dynamical degree of freedom in ordinary ChPT and can be thought of as having been integrated out. η-η' mixing is discussed in [12].
In this naively set up ChPT, the meson masses to one loop read [13]

$$\begin{aligned} M_{\pi^\pm}^2 = m_\pi^2 + \frac{8}{f^2}\Big(& m_\pi^4[4L_6 + 2L_8 - 2L_4 - L_5] + 2m_\pi^2 m_{D_s}^2[2L_6 - L_4] \\ & + \rho m_\pi^2 \cos\phi_l[4\overline{W}_6 + 2\overline{W}_8 - 2\overline{W}_4 - \overline{W}_5] \\ & + \rho m_\pi^2 \cos\phi_h[2\overline{W}_6 - 2\overline{W}_4] \\ & + \rho m_{D_s}^2 \cos\phi_l \overline{W}_6 \\ & + \rho^2\cos^2\phi_l[4\overline{W}_6' + 2\overline{W}_8'] \\ & + \rho^2\cos\phi_l\cos\phi_h 4\overline{W}_6'\Big) \\ & + \text{loop}_\pi. \end{aligned} \tag{3.32}$$

$$\begin{aligned} M_K^2 = m_K^2 + \frac{4}{f^2}\Big(& m_K^4[-8L_4 - 2L_5 + 16L_6 + 4L_8] + 4m_K^2(m_D^2 - m_K^2)[2L_6 - L_4] \\ & + \rho m_K^2(\cos\phi_l + \cos\phi_h)[-4\overline{W}_4 - \overline{W}_5 + 8\overline{W}_6 + 2\overline{W}_8] \\ & + \rho(m_D^2 - m_K^2)(\cos\phi_l + \cos\phi_h)2\overline{W}_6 \\ & + \rho^2\left(\cos\phi_l + \cos\phi_h\right)^2[4\overline{W}_6' + \overline{W}_8'] \\ & - \rho^2\left(\sin^2\phi_l + \sin^2\phi_h\right)\overline{W}_8'\Big) \\ & + \text{loop}_K. \end{aligned}$$

The respective loop contributions are given in [13] and include both η and η_c chiral logs, alluding to the problems in constructing ChPT the way outlined above. η_c is way too heavy to appear as degree of freedom in a sensible ChPT, as are all the D mesons. The important thing to note here is that the above loop contributions reduce to their well-known continuum form [12], when the η_c is thought of as being too heavy

to appear as dynamical degree of freedom similarly to the η'. Making η_c heavy implies η_8 and η_{15} decoupling in the theory in the sense of a vanishing mixing, and we are left solely with a dynamical η_8.
To conclude this section, we stress that the naive ChPT for $N_f = 2+1+1$ flavor with twisted masses outlined above is not applicable for the phenomenologically relevant case with $M_D \gg M_K$, since it treats heavy D mesons as pseudo Goldstone bosons.

4. Chiral Perturbation Theory for 2+1+1 Wilson Quarks with Twisted Masses

4.1. Construction of a Charmless Chiral Perturbation Theory

In this section we construct the ChPT to describe twisted mass lattice QCD simulations with four dynamical flavors as performed by the *European Twisted Mass Collaboration (ETMC)*. The respective theory that we will call charmless ChPT in the following has to be constructed such that it does not treat the D mesons as pseudo Goldstone bosons.

4.1.1. Matching Theories at Lagrangian Level

In order to illustrate how we proceed in its construction, consider standard SU(3) continuum ChPT [12] and suppose we are only interested in energies and momenta well below the kaon mass. The kaons and η meson degrees of freedom then decouple from the theory. In the spirit of an effective theory, they can be integrated out and contribute to the LECs of SU(2) ChPT, whose results have to be reproduced.
The actual matching is performed by setting the respective mesonic degrees of freedom to zero,

$$\Sigma_p^{(3)} = \exp\left(\frac{2\mathrm{i}}{f_{(3)}}\pi\right), \qquad \pi = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 & \pi^+ & 0 \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{4.1}$$

where the additional superscript[1] is introduced to denote quantities in the respective theories. Since the ground state in continuum ChPT is just the SU(N_f) identity, we insert

$$\Sigma_{(3)} = \Sigma_p^{(3)} = \begin{pmatrix} \Sigma_{(2)} & \\ & 1 \end{pmatrix}, \tag{4.2}$$

where $\Sigma_{(2)}$ is the standard meson field matrix of SU(2) ChPT, into the Lagrangian of SU(3) ChPT in order to perform the matching. For notational convenience, we re-express the SU(3) mass matrix as

$$M_{(3)} = \begin{pmatrix} M_{(2)} & \\ & m_s \end{pmatrix}, \tag{4.3}$$

[1] We use superscripts and subscripts equivalently for typographic convenience.

where M_2 denotes the 2×2 mass matrix in the (u, d)-sector. From

$$\partial_\mu \Sigma_{(3)} = \begin{pmatrix} \partial_\mu \Sigma_{(2)} & \\ & 0 \end{pmatrix}, \tag{4.4}$$

we conclude that the kinetic part in the leading order Lagrangian and the NLO terms proportional to L_1, L_2 and L_3 indeed reduce to their SU(2) counterparts. In contrast, terms without derivatives produce extra terms when calculating the traces, due to the extra 1 in the lower right hand corner of $\Sigma_{(3)}$ in eq. (4.2). This can be seen for instance in the mass term with $\chi = 2BM$ as usual, that can be written as[2]

$$\left\langle \chi^\dagger_{(3)} \Sigma_{(3)} + \Sigma^\dagger_{(3)} \chi_{(3)} \right\rangle_3 = \left\langle \chi^\dagger_{(2)} \Sigma_{(2)} + \Sigma^\dagger_{(2)} \chi_{(2)} \right\rangle_2 + 4B_{(3)} m_s. \tag{4.5}$$

The LO mass term hence reduces to the SU(2) mass term plus a constant, which is irrelevant and can be dropped. NLO terms are more interesting, though. Consider the L_4 term that can be rewritten using eq. (4.5),

$$\begin{aligned} &L_4 \left\langle \partial_\mu \Sigma_{(3)} \partial_\mu \Sigma^\dagger_{(3)} \right\rangle \left\langle \chi^\dagger_{(3)} \Sigma_{(3)} + \Sigma^\dagger_{(3)} \chi_{(3)} \right\rangle = \\ &\qquad L_4 \left\langle \partial_\mu \Sigma_{(2)} \partial_\mu \Sigma^\dagger_{(2)} \right\rangle \left\langle \chi^\dagger_{(2)} \Sigma_{(2)} + \Sigma^\dagger_{(2)} \chi_{(2)} \right\rangle + 4B_{(3)} m_s L_4 \left\langle \partial_\mu \Sigma_{(2)} \partial_\mu \Sigma^\dagger_{(2)} \right\rangle. \end{aligned}$$

The additional term has the form of the SU(2) kinetic term. One thus ends up with an effective kinetic term,

$$\mathscr{L}_{p^2} = \frac{f^2_{(3)}}{4} \left(1 + 16 L_4 \frac{B_{(3)} m_s}{f^2_{(3)}} \right) \left\langle \partial_\mu \Sigma_{(2)} \partial_\mu \Sigma^\dagger_{(2)} \right\rangle.$$

Demanding that this kinetic term be equivalent to its SU(2) ChPT counterpart, one reads off the LEC $f_{(2)}$ of SU(2) ChPT, whereby the analytic part of its leading order functional dependence on the strange quark mass is made explicit,

$$f_{(2)} = f_{(3)} \left(1 + 8 L_4 \frac{B_{(3)} m_s}{f^2_{(3)}} \right). \tag{4.6}$$

This is exactly the analytic part of the matching of the LO parameter $f_{(2)}$ found from equating results for the pion decay constant calculated in SU(2) and SU(3) ChPT [12]. Similarly, using the *building block* eq. (4.5) to rewrite the L_6 term, we find, apart from an overall constant that is dropped,

$$\begin{aligned} &-L_6 \left\langle \chi^\dagger_{(3)} \Sigma_{(3)} + \Sigma^\dagger_{(3)} \chi_{(3)} \right\rangle^2 = \\ &\qquad - L_6 \left\langle \chi^\dagger_{(2)} \Sigma_{(2)} + \Sigma^\dagger_{(2)} \chi_{(2)} \right\rangle^2 - 8B_{(3)} m_s L_6 \left\langle \chi^\dagger_{(2)} \Sigma_{(2)} + \Sigma^\dagger_{(2)} \chi_{(2)} \right\rangle. \end{aligned}$$

[2] The trace subscripts indicate traces over SU(3) and SU(2) matrices respectively acting in flavor space. In the following the flavor trace subscript will be dropped, as the names of the involved fields clarify, which trace is meant.

Again, requiring the SU(2) mass term to match the effective mass term from SU(3) ChPT, we read off

$$\begin{aligned} B_{(2)} &= B_{(3)} \left(\frac{f_{(3)}}{f_{(2)}}\right)^2 \left(1 + \frac{32 B_{(3)} m_s}{f_{(3)}^2} L_6\right) \\ &= B_{(3)} \left(1 + \frac{16 B_{(3)} m_s}{f_{(3)}^2} \left(2L_6 - L_4\right)\right), \end{aligned}$$

where the latter equality holds up to the order considered. We again reproduce the analytic part of the matching found from equating pion masses in SU(2) and SU(3) ChPT [12]. Finally, all other NLO terms are found to reduce to their SU(2) counterparts plus irrelevant constants. We thus conclude that for continuum ChPT

$$\mathscr{L}_{\text{cont}}^{\text{SU(3)}}(f_{(3)}, B_{(3)}) \to \mathscr{L}_{\text{cont}}^{\text{SU(2)}}(f_{(2)}, B_{(2)}) + \text{constants},$$

where the arrow indicates the substitution given in eq. (4.2).
In the upshot, the reduction from higher N_f ChPT to lower N_f ChPT can be performed already at Lagrangian level. After appropriate absorption of the heavy flavor mass dependence in the LECs of lower N_f ChPT, we have completely undone the expansion in the heavy quark mass and end up with the light flavor ChPT. The fact that the heavy quark mass dependence can always be absorbed by appropriate redefinition of LECs merely reflects the fact that at any order all terms compatible with the underlying symmetries are present.

4.1.2. Building Blocks for the Construction of Charmless tmWChPT

The approach to reverting the expansion in a heavy quark flavor will now be employed to construct charmless ChPT, nevertheless initially incorporating a strange quark and its twist partner, the charm quark, in order to correctly capture the effects of chirally rotated masses. The rationale is as follows: We start from 2+1+1 flavors that are sufficiently light such that ChPT holds. We then reduce the theory by absorbing the charm quark dependence in LO LECs in analogy to what we have done in the last section regarding the strange quark. Thereafter we can have a heavy charm quark without conflicting with the premises of a sensible ChPT.
Since the reduction to charmless ChPT is to be performed in the physical basis, we first rewrite the four flavor Lagrangian in terms of the physical fields. As outlined in section 3.4, a nontrivial ground state can be reshuffled to the mass matrix in the respective terms, whereas it enters explicitly in lattice terms, c.f. eqs. (3.17) - (3.19). Starting from the $N_f = 2{+}1{+}1$ mass matrix with twisted masses given by eq. (3.28) and the respective ansatz for the ground state in terms of the vacuum angles $\omega_{l,h}$, we find that the physical mass matrix $\chi_p = \tilde{\chi}_l \oplus \tilde{\chi}_h$ remains a direct sum of

$$\begin{aligned} \tilde{\chi}_l &= 2B \begin{pmatrix} (m + \mathrm{i}\mu_l)(\cos\omega_l - \mathrm{i}\sin\omega_l) & 0 \\ 0 & (m - \mathrm{i}\mu_l)(\cos\omega_l + \mathrm{i}\sin\omega_l) \end{pmatrix}, \\ \tilde{\chi}_h &= 2B \begin{pmatrix} m\cos\omega_h + \mu_h \sin\omega_h + \delta & \mathrm{i}(-m\sin\omega_h + \mu_h\cos\omega_h) \\ \mathrm{i}(-m\sin\omega_h + \mu_h\cos\omega_h) & m\cos\omega_h + \mu_h\sin\omega_h - \delta \end{pmatrix}. \end{aligned} \tag{4.7}$$

Note that the off-diagonal element

$$2Bm\sin\omega_h - 2B\mu_h\cos\omega_h$$

in the heavy sector M can be rewritten as an $\mathcal{O}(a^2)$ term using the (heavy sector) gap equation of the four flavor theory. In the $\overline{W}_8$ term, the off-diagonal element is redistributed to the diagonal when computing the product with ground state and physical field matrix insertions. The $\overline{W}_8$ term is an $\mathcal{O}(a)$ term originally, and hence if at all additionally contributes at $\mathcal{O}(a^3)$. In the GSM regime, this is a correction beyond the order considered. In the LCE regime, the coefficient of the respective term in $\mathscr{L}_{a^3}$, that is not known anyway, is only modified. The off-diagonal entry in the heavy sector of the four flavor mass matrix can thus be neglected in the course of constructing the charmless theory.
In order to reduce the four flavor theory to its charmless counterpart, we now drop the heavy D, D_s and η_{15} meson fields. We hence insert

$$\Sigma_p = \begin{pmatrix} \Sigma_{(3)} & \\ & 1 \end{pmatrix} \tag{4.8}$$

into the Lagrangian of WChPT with twisted masses. The rather nontrivial matching behavior compared to matching the continuum ChPT as sketched before arises from the fact, that the block structure of the ground state in eq. (3.30) differs from the matching block structure in eq. (4.8). In other words, the ground state mixes strange and charm quark contributions, that have to be disentangled in order to be able to identify the physically heavy D meson fields that are to be dropped.
In the course of reducing the theory, one is thus confronted with working out the matrix products encountered in the tmWChPT Lagrangian. To this end, note that the ground state (eq. (3.30)) can be rewritten to mimic the block structure of eq. (4.8),

$$\Sigma_0 = \begin{pmatrix} & \tilde{\Sigma}_l & & 0 \\ & & & 0 \\ & & & \mathrm{i}\sin\omega_h \\ 0 & 0 & \mathrm{i}\sin\omega_h & \cos\omega_h \end{pmatrix},$$

where we introduced

$$\tilde{\Sigma}_l = \begin{pmatrix} \cos\omega_l + \mathrm{i}\sin\omega_l & 0 & 0 \\ 0 & \cos\omega_l - \mathrm{i}\sin\omega_l & 0 \\ 0 & 0 & \cos\omega_h \end{pmatrix}. \tag{4.9}$$

Two prominent matrix products comprised of the matrix-valued ground state and the reduced matrix incorporating the dynamical physical fields are then found to be

$$\Sigma_p\Sigma_0 = \begin{pmatrix} & & & \mathrm{i}\sin\omega_h\left(\Sigma_{(3)}\right)_{1,3} \\ & \Sigma_{(3)}\tilde{\Sigma}_l & & \mathrm{i}\sin\omega_h\left(\Sigma_{(3)}\right)_{2,3} \\ & & & \mathrm{i}\sin\omega_h\left(\Sigma_{(3)}\right)_{3,3} \\ 0 & 0 & \mathrm{i}\sin\omega_h & \cos\omega_h \end{pmatrix} \tag{4.10}$$

and

$$\Sigma_p \Sigma_0 \Sigma_p = \begin{pmatrix} \Sigma_{(3)} \tilde{\Sigma}_l \Sigma_{(3)} & \mathrm{i} \sin \omega_h \left(\Sigma_{(3)} \right)_{k,3} \\ \mathrm{i} \sin \omega_h \left(\Sigma_{(3)} \right)_{3,k} & \cos \omega_h \end{pmatrix}, \tag{4.11}$$

where $\left(\Sigma_{(3)}\right)_{k,3}$ and $\left(\Sigma_{(3)}\right)_{3,k}$ denote the third column and row of $\Sigma_{(3)}$.
With these identities at hand, the essential building block for the reduction of lattice terms can readily be worked out. Again, let the reduction by the replacement according to eq. (4.8) in the Lagrangian be indicated by an arrow. We then find[3],

$$\begin{aligned} \left\langle \Sigma + \Sigma^\dagger \right\rangle_{2+1+1} &= \left\langle \Sigma_p \Sigma_0 + \Sigma_0^\dagger \Sigma_p^\dagger \right\rangle_{2+1+1} \\ &\to \left\langle \Sigma_{(3)} \tilde{\Sigma}_l + \tilde{\Sigma}_l^\dagger \Sigma_{(3)}^\dagger \right\rangle_{2+1} + 2 \cos \omega_h . \end{aligned} \tag{4.12}$$

The other building block is the mass term. It can be reduced according to the prescription

$$\begin{aligned} \left\langle \chi^\dagger \Sigma + \Sigma^\dagger \chi \right\rangle &= \left\langle \chi_p^\dagger \Sigma_p + \Sigma_p^\dagger \chi_p \right\rangle \\ &\to \left\langle \chi_3^\dagger \Sigma_{(3)} + \Sigma_{(3)}^\dagger \chi_3 \right\rangle , \end{aligned} \tag{4.13}$$

where

$$\begin{aligned} \chi_3 = 2B \operatorname{diag}\Big[&(m + \mathrm{i}\mu_l)(\cos \omega_l - \mathrm{i} \sin \omega_l), \\ &(m - \mathrm{i}\mu_l)(\cos \omega_l + \mathrm{i} \sin \omega_l), \\ &m \cos \omega_h + \mu_h \sin \omega_h + \delta \Big] \\ = 2B \operatorname{diag}\Big[&m_l' \left(\cos\left(\phi_l - \omega_l\right) + \mathrm{i} \sin\left(\phi_l - \omega_l\right)\right), \\ &m_l' \left(\cos\left(\phi_l - \omega_l\right) - \mathrm{i} \sin\left(\phi_l - \omega_l\right)\right), \\ &m_h' \cos\left(\phi_h - \omega_h\right) + \delta \Big] \end{aligned} \tag{4.14}$$

is obtained from truncation of the mass matrix in the physical basis χ_p. In eq. (4.13), we have not given the constant term related to the charm quark mass. The charm quark dependence is thought of as having been absorbed by redefinition of LO LECs, as has been shown to work in the section on reducing ChPT at Lagrangian level.
Quite trivially, one additionally checks, that

$$\begin{aligned} \left\langle \Sigma - \Sigma^\dagger \right\rangle &= \left\langle \Sigma_p \Sigma_0 - \Sigma_0^\dagger \Sigma_p^\dagger \right\rangle \\ &\to \left\langle \Sigma_{(3)} \tilde{\Sigma}_l - \tilde{\Sigma}_l^\dagger \Sigma_{(3)}^\dagger \right\rangle , \end{aligned} \tag{4.15}$$

since the additional cosine on the diagonal of eq. (4.10) cancels after subtraction of the Hermitian conjugate, and

$$\left\langle \chi^\dagger \Sigma - \Sigma^\dagger \chi \right\rangle \to \left\langle \chi_3^\dagger \Sigma_{(3)} - \Sigma_{(3)}^\dagger \chi_3 \right\rangle$$

by analogy with eq. (4.13).

[3] Again, in the following the flavor trace subscript will be dropped. Field names unambiguously identify the dimension of matrices in the flavor traces.

4.1.3. Lattice Effects in Charmless ChPT

Now, the matching behavior of terms in $\mathscr{L}_{p^2a}$, $\mathscr{L}_{ma}$ can readily be worked out:

$$
\begin{aligned}
&\overline{W}_4\rho\left\langle\partial_\mu\Sigma\partial_\mu\Sigma^\dagger\right\rangle\left\langle\Sigma+\Sigma^\dagger\right\rangle\\
&\qquad\to\overline{W}_4\rho\left\langle\partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)}\right\rangle\left\langle\Sigma_{(3)}\tilde{\Sigma}_l+\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right\rangle+2\overline{W}_4\rho\cos\omega_h\left\langle\partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)}\right\rangle,\\
&\overline{W}_5\rho\left\langle\partial_\mu\Sigma\partial_\mu\Sigma^\dagger\left(\Sigma+\Sigma^\dagger\right)\right\rangle\\
&\qquad\to\overline{W}_5\rho\left\langle\partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)}\left(\Sigma_{(3)}\tilde{\Sigma}_l+\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right)\right\rangle,\\
&\overline{W}_6\rho\left\langle\chi^\dagger\Sigma+\Sigma^\dagger\chi\right\rangle\left\langle\Sigma+\Sigma^\dagger\right\rangle\\
&\qquad\to\overline{W}_6\rho\left\langle\chi_3^\dagger\Sigma_{(3)}+\Sigma^\dagger_{(3)}\chi_3\right\rangle\left\langle\Sigma_{(3)}\tilde{\Sigma}_l+\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right\rangle+2\overline{W}_6\rho\cos\omega_h\left\langle\chi_3^\dagger\Sigma_{(3)}+\Sigma^\dagger_{(3)}\chi_3\right\rangle,\\
&\overline{W}_7\rho\left\langle\chi^\dagger\Sigma-\Sigma^\dagger\chi\right\rangle\left\langle\Sigma-\Sigma^\dagger\right\rangle\\
&\qquad\to\overline{W}_7\rho\left\langle\chi_3^\dagger\Sigma_{(3)}-\Sigma^\dagger_{(3)}\chi_3\right\rangle\left\langle\Sigma_{(3)}\tilde{\Sigma}_l-\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right\rangle,\\
&\overline{W}_8\rho\left\langle\chi^\dagger\Sigma\Sigma+\Sigma^\dagger\Sigma^\dagger\chi\right\rangle\\
&\qquad\to\overline{W}_8\rho\left\langle\chi_3^\dagger\Sigma_{(3)}\tilde{\Sigma}_l\Sigma_{(3)}+\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\chi_3\right\rangle.
\end{aligned}
$$

Terms in the $\mathscr{L}_{a^2}$ Lagrangian are found to reduce as follows,

$$
\begin{aligned}
&\overline{W}'_6\rho^2\left\langle\Sigma+\Sigma^\dagger\right\rangle^2\\
&\qquad\to\overline{W}'_6\rho^2\left\langle\Sigma_{(3)}\tilde{\Sigma}_l+\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right\rangle^2+4\overline{W}'_6\rho^2\cos\omega_h\left\langle\Sigma_{(3)}\tilde{\Sigma}_l+\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right\rangle,\\
&\overline{W}'_7\rho^2\left\langle\Sigma-\Sigma^\dagger\right\rangle^2\\
&\qquad\to\overline{W}'_7\rho^2\left\langle\Sigma_{(3)}\tilde{\Sigma}_l-\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\right\rangle^2,\\
&\overline{W}'_8\rho^2\left\langle\Sigma\Sigma+\Sigma^\dagger\Sigma^\dagger\right\rangle=\overline{W}'_8\rho^2\left\langle\Sigma_0\Sigma_p\Sigma_0\Sigma_p+\Sigma_p^\dagger\Sigma_0^\dagger\Sigma_p^\dagger\Sigma_0^\dagger\right\rangle\\
&\qquad\to\overline{W}'_8\rho^2\left\langle\tilde{\Sigma}_l\Sigma_{(3)}\tilde{\Sigma}_l\Sigma_{(3)}+\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\right\rangle-2\overline{W}'_8\rho^2\sin^2\omega_h\left(\Sigma_{(3)}+\Sigma^\dagger_{(3)}\right)_{3,3}.
\end{aligned}
$$

The last term exhibits a nontrivial reduction, that can be understood by multiplying eq. (4.11) with Σ_0 and taking the trace. The single element $\left(\Sigma_{(3)}+\Sigma^\dagger_{(3)}\right)_{3,3}$ can alternatively be written as

$$
\left(\Sigma_{(3)}+\Sigma^\dagger_{(3)}\right)_{3,3}=\left\langle \mathrm{P}_s\left(\Sigma_{(3)}+\Sigma^\dagger_{(3)}\right)\right\rangle,
$$

where we introduced the projector

$$
\mathrm{P}_s=\mathrm{diag}(0,0,1).
$$

The charmless tmWChPT Lagrangian associated to lattice effects up to order $\mathcal{O}(a^2)$ hence reads

$$\begin{aligned}
\mathscr{L}_{p^2a} + \mathscr{L}_{ma} =& + \overline{W}_4 \rho \left\langle \partial_\mu \Sigma_{(3)} \partial_\mu \Sigma^\dagger_{(3)} \right\rangle \left\langle \Sigma_{(3)} \tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right\rangle \\
& + \overline{W}_5 \rho \left\langle \partial_\mu \Sigma_{(3)} \partial_\mu \Sigma^\dagger_{(3)} \left(\Sigma_{(3)} \tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right) \right\rangle \\
& - \overline{W}_6 \rho \left\langle \chi_3^\dagger \Sigma_{(3)} + \Sigma^\dagger_{(3)} \chi_3 \right\rangle \left\langle \Sigma_{(3)} \tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right\rangle \\
& - \overline{W}_7 \rho \left\langle \chi_3^\dagger \Sigma_{(3)} - \Sigma^\dagger_{(3)} \chi_3 \right\rangle \left\langle \Sigma_{(3)} \tilde{\Sigma}_l - \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right\rangle \\
& - \overline{W}_8 \rho \left\langle \chi_3^\dagger \Sigma_{(3)} \tilde{\Sigma}_l \Sigma_{(3)} + \Sigma^\dagger_{(3)} \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \chi_3 \right\rangle \\
& + 2\overline{W}_4 \rho \cos\omega_h \left\langle \partial_\mu \Sigma_{(3)} \partial_\mu \Sigma^\dagger_{(3)} \right\rangle \\
& - 2\overline{W}_6 \rho \cos\omega_h \left\langle \chi_3^\dagger \Sigma_{(3)} + \Sigma^\dagger_{(3)} \chi_3 \right\rangle, \\
\mathscr{L}_{a^2} =& - \overline{W}'_6 \rho^2 \left\langle \Sigma_{(3)} \tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right\rangle^2 \\
& - \overline{W}'_7 \rho^2 \left\langle \Sigma_{(3)} \tilde{\Sigma}_l - \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right\rangle^2 \\
& - \overline{W}'_8 \rho^2 \left\langle \tilde{\Sigma}_l \Sigma_{(3)} \tilde{\Sigma}_l \Sigma_{(3)} + \Sigma^\dagger_{(3)} \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \tilde{\Sigma}^\dagger_l \right\rangle \\
& - 4\overline{W}'_6 \rho^2 \cos\omega_h \left\langle \Sigma_{(3)} \tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l \Sigma^\dagger_{(3)} \right\rangle \\
& + 2\overline{W}'_8 \rho^2 \sin^2\omega_h \left(\Sigma_{(3)} + \Sigma^\dagger_{(3)} \right)_{3,3}.
\end{aligned} \tag{4.16}$$

Obviously, it is supplemented by terms that would not be present if one started from SU(2+1) WChPT with twisted masses in the light sector.
Absorbing the charm quark dependence in the continuum Lagrangian works completely analogous to the reduction from three flavor ChPT to two flavor ChPT. The charmless continuum Lagrangian is hence just the ordinary ChPT Lagrangian [11], however, with LO LECs differing from the ones entering SU(4) ChPT,

$$\begin{aligned}
\mathscr{L}_2 =& \frac{f^2}{4} \left\langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \right\rangle - \frac{f^2}{4} \left\langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \right\rangle \\
\mathscr{L}_4 =& - L_1 \left\langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \right\rangle^2 - L_2 \left\langle \partial_\mu \Sigma_3 \partial_\nu \Sigma_3^\dagger \right\rangle \left\langle \partial_\mu \Sigma_3 \partial_\nu \Sigma_3^\dagger \right\rangle - L_3 \left\langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \partial_\nu \Sigma_3 \partial_\nu \Sigma_3^\dagger \right\rangle \\
& + L_4 \left\langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \right\rangle \left\langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \right\rangle + L_5 \left\langle \partial_\mu \Sigma_3 \partial_\mu \Sigma_3^\dagger \left(\chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \right) \right\rangle \\
& - L_6 \left\langle \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \right\rangle^2 - L_7 \left\langle \chi_3^\dagger \Sigma_3 - \Sigma_3^\dagger \chi_3 \right\rangle^2 - L_8 \left\langle \chi_3^\dagger \Sigma \chi_3^\dagger \Sigma_3 + \Sigma_3^\dagger \chi_3 \Sigma_3^\dagger \chi_3 \right\rangle.
\end{aligned} \tag{4.17}$$

The L_1, L_2 and L_3 terms do not contribute to meson masses or decay constants to one loop, as their expansion in terms of meson fields starts only at $\mathcal{O}(\pi^4)$, and any loop diagram built from these vertices is of higher order than considered.

4.2. Meson Masses in the Generically Small Masses Regime

With the charmless ChPT Lagrangian at hand, we are now equipped to tackle some sample calculation in the framework of this theory.

4.2.1. Ground State and Tree Level Masses

In order to conform with the literature [13], we parametrize the mass matrix by the respective radial masses and twist angles. The vacuum angle in the light sector obtained from minimizing the potential energy then reads

$$\omega_l = \phi_l - \frac{8}{f^2}\frac{\rho \sin\phi_l}{2Bm'_l}\left[2Bm'_l\overline{W}_{68} + 2Bm_s\overline{W}_6 + \rho\cos\phi_l 2\overline{W}'_{68} + \rho\cos\omega_h 4\overline{W}'_6\right]. \tag{4.18}$$

In order to compare to the respective vacuum angle obtained from minimizing the four flavor potential and subsequently dropping the charm quark, recall that

$$\begin{aligned} m'_h &= \tfrac{1}{2}(m_s + m_c) \\ \delta &= \tfrac{1}{2}(m_s - m_c) \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} m_s &= m'_h + \delta \\ m_c &= m'_h - \delta \end{aligned} \quad . \tag{4.19}$$

Therefore, loosely speaking, making the charm quark heavy in the sense of ChPT while keeping the strange quark mass fixed at its physical value corresponds to sending both m'_h and δ to infinity such that their difference remains fixed. Thus, the replacement

$$m'_h \to \frac{1}{2}m_s \tag{4.20}$$

describes the matching prescription for explicit removal of the charm quark dependence from results of the four flavor theory. Indeed, the light vacuum angle given in eq. (3.31) reduces to the one of eq. (4.18) under this replacement.
The heavy sector vacuum angle is determined solely by the mass term. A nontrivial ground state appears only when lattice effects and mass terms are of comparable sizes and hence compete in the minimization of the potential. A heavy charm quark, however, readily implies

$$\omega_h = \phi_h. \tag{4.21}$$

It is unclear, whether a heavy charm quark suppresses the $\mathcal{O}(a^2)$ contributions to the light vacuum angle. Taking the respective limit in the potential of the four flavor theory contradicts the assertion of a sufficiently light charm quark needed for the theory to be sensible in the first place. We may either write down a four flavor ChPT or make the charm quark heavy. The two are not compatible.
We stick to the light sector gap equation given in eq. (4.18) since it leaves the light sector physics intact regardless of the masses in the heavy sector. This appears reasonable due to the following rationale: If we start from the four flavor theory and decide to discard mesons including the charm or the strange quark as dynamical degrees of freedom, we expect to recover standard two flavor twisted mass WChPT. This is only true if we keep the $\mathcal{O}(a^2)$ terms in the light sector gap equation. Although we thus choose to use the gap equation (4.18), we stress that this step is not based on a physically rigorous argument.
Having determined the ground state, the LO masses can be read off after expanding the Lagrangian in terms of meson fields,

$$\begin{aligned} m_\pi^2 &= 2Bm'_l, \\ m_K^2 &= B\left(m'_l + m_s\right), \\ m_\eta^2 &= \frac{2}{3}B\left(m'_l + 2m_s\right). \end{aligned} \tag{4.22}$$

Again, more precisely the field π^8 is related to the η_8 meson. The mass eigenstates, the η and η' mesons, are obtained from the mixing of the flavor-neutral η_8 meson and η_1 related to the anomalous $\mathrm{U}(1)_A$ symmetry. We will not address η-η' mixing [12] any further and will abbreviate η_8 as η in all the following results.

These tree level results of course coincide with the results obtained in the four flavor theory [13].

4.2.2. Meson Masses to One Loop

Since the leading order Lagrangian is just the continuum Lagrangian, it is immediately clear, that the nonanalytic one loop contributions have the same form as in the continuum result. However, recall that the tree level masses in (4.22) already include an $\mathcal{O}(a)$ shift.

All one loop diagrams contributing to the meson masses to one loop are tadpole diagrams built from four pion vertices from the LO Lagrangian. How contributions to the masses are calculated from the Lagrangian is discussed in App. B. Thereby occurring divergent loop integrals are conveniently regularized using dimension regularization (see App. A). The NLO Lagrangian provides counterterms to cancel all divergences by appropriate renormalization of the respective NLO LECs.

The charged pion mass reads

$$\begin{aligned} M^2_{\pi^\pm} = m_\pi^2 + \frac{8}{f^2}\Big(& m_\pi^4[4L_6 + 2L_8 - 2L_4 - L_5] + m_\pi^2(2m_K^2 - m_\pi^2)[-L_4 + 2L_6] \\ & + \rho m_\pi^2 \cos\phi_l [4\overline{W}_6 + 2\overline{W}_8 - 2\overline{W}_4 - \overline{W}_5] \\ & + \rho m_\pi^2 \cos\phi_h [2\overline{W}_6 - 2\overline{W}_4] \\ & + \rho(2m_K^2 - m_\pi^2)\cos\phi_l \overline{W}_6 \\ & + \rho^2 \cos^2\phi_l [4\overline{W}'_6 + 2\overline{W}'_8] \\ & + \rho^2 \cos\phi_l \cos\phi_h 4\overline{W}'_6 \Big) \\ & + \mathrm{loop}_\pi . \end{aligned} \tag{4.23}$$

By construction, this is just the continuum expression supplemented by NLO corrections from $\mathscr{L}_{ma}$ and $\mathscr{L}_{a^2}$. Again, the $\mathcal{O}(a^2)$ terms induce a mass splitting between the charged and the neutral pion that is found to be

$$M^2_{\pi^\pm} - M^2_{\pi^0} = \frac{16\rho^2 \sin^2\phi_l}{f^2}\left[2\overline{W}'_6 + \overline{W}'_8\right]. \tag{4.24}$$

The pion mass splitting is a sole light sector feature. The light sector physics is basically unaltered in our theory, apart from additional contributions from kaons and η. The mass splitting thus coincides with the one in two flavor tmWChPT (c.f. eq. (3.22)).

The degenerate kaon mass is given by

$$
\begin{aligned}
M_K^2 = m_K^2 + \frac{4}{f^2}\Big(& m_K^4[-8L_4 - 2L_5 + 16L_6 + 4L_8] + m_K^2(2m_K^2 - m_\pi^2)[2L_4 - 4L_6] \\
& + \rho m_K^2(\cos\phi_l + \cos\phi_h)[-4\overline{W}_4 - \overline{W}_5 + 8\overline{W}_6 + 2\overline{W}_8] \\
& + \rho(2m_K^2 - m_\pi^2)(\cos\phi_l + \cos\phi_h)[-\overline{W}_6] \\
& + \rho^2\left(\cos\phi_l + \cos\phi_h\right)^2[4\overline{W}_6' + \overline{W}_8'] \\
& + \rho^2\left(\sin^2\phi_l + \sin^2\phi_h\right)[-\overline{W}_8']\Big) \\
& + \mathrm{loop}_K.
\end{aligned}
\tag{4.25}
$$

These masses can be compared to the respective four flavor results given in eq. (3.32). From eq. (4.20), we find that explicit reduction of the four flavor masses amounts to setting

$$
\begin{aligned}
m_{D_s}^2 = 2Bm_h' \to Bm_s &= \frac{1}{2}\left(2m_K^2 - m_\pi^2\right), \\
-\left(m_D^2 - m_K^2\right) = Bm_s - Bm_c \to Bm_s &= \frac{1}{2}\left(2m_K^2 - m_\pi^2\right).
\end{aligned}
$$

The expressions are then found to coincide. This, in a sense, validates the approach presented in this work. Starting from a charmless Lagrangian, we still captured the relevant structure of the four flavor theory and end up with correct expressions for the masses.

It is sensible to express the results in terms of tree level meson masses, since non-perturbatively determined meson masses are the actual observables in lattice simulations, in contrast to the quark masses as mere parameters. Thereby one circumvents the need to specify the definition of the critical quark mass [31] in connection with the $\mathcal{O}(a)$ shift and the mass renormalization.

Additionally, the expressions in eqs. (4.23) - (4.25) reproduce the continuum results [12] in their continuum limit $\rho \to 0$ as expected. To this end, recall that the loop contributions are just the ones from the continuum with $\mathcal{O}(a)$ shifted quark hence tree level meson masses, that tend to their continuum counterparts in the respective limit. The one loop masses simplify considerably in the case of maximal twist,

$$\cos\phi_l = 0 = \cos\phi_h.$$

There are then no $\mathcal{O}(ma)$ and $\mathcal{O}(p^2a)$ contributions to the masses, confirming automatic $\mathcal{O}(a)$-improvement [28, 31] in tmWChPT.

4.3. Meson Masses in the Large Cutoff Effects Regime

The pion mass splitting entering at next to leading order in the GSM regime becomes even more important in the LCE regime by construction. Since $\mathcal{O}(a^2)$ terms are promoted to leading order, the tree level masses of the charged pions and the neutral pion already differ by the amount given in eq. (4.24). Therefore, one has to distinguish between looping charged pions and neutral pions in the computation of meson masses to one loop. In the ChPT for two light degenerate Wilson fermions with twisted masses, it was established that indeed only the neutral pion enters the chiral logs in the charged pion mass (c.f. eq. (3.25)).

4.3.1. Approximate Gap Equation and Tree Level Masses

Let us briefly return to the four flavor theory to see that even in the regime of practical interest, charmless ChPT captures all the relevant information. The potential energy in the LCE regime is given by

$$V = -\mathscr{L}_m - \mathscr{L}_{a^2}.$$

The gap equations for the light and heavy sector of the four flavor theory are completely symmetric,

$$2B\mu_{l,h}\cos\omega_{l,h} = \sin\omega_{l,h}\left(2Bm'_{l,h} + 16\frac{\rho^2}{f^2}\overline{W}'_{68}\cos\omega_{l,h} + 32\frac{\rho^2}{f^2}\overline{W}'_{6}\cos\omega_{h,l}\right).$$

Again the last term couples light and heavy sector. The coupling at $\mathcal{O}(a^2)$ has already been recognized in the GSM regime, though as a next to leading order effect. Note that the gap equation does not include any dependence on the mass difference δ between the strange and charm quark.

With respect to phenomenological applications, we want to have

$$m'_l \sim \rho^2 \ll m'_h,$$

since the heavy charm quark implies a large m'_h according to eq. (4.19). Put differently, working in the LCE regime amounts to having light quark masses of order $\mathcal{O}(a^2)$ while still keeping a GSM-like heavy sector. We can then fall back to the respective discussion above and conclude that in charmless ChPT the light sector gap equation is essentially the gap equation found in two flavor tmWChPT, once the heavy sector is tuned to maximal twist.

The calculations carried out in the two flavor setup [30] can thus readily be carried over. Expanding the whole leading order Lagrangian and using the light sector gap equation, one derives the pion tree level masses to read

$$\begin{aligned} m^2_{\pi^\pm} &= \frac{2B\mu_l}{\sqrt{1-\cos^2\omega_l}} \\ m^2_{\pi^0} &= m^2_{\pi^\pm} + \underbrace{\left(-\frac{16\rho^2}{f^2}\left(1-\cos^2\omega_l\right)\overline{W}'_{68}\right)}_{=\Delta m^2_\pi}. \end{aligned} \tag{4.26}$$

The degenerate Kaon tree level mass is given by

$$\begin{aligned}
m_K^2 = & \frac{2B}{2}\left(m\cos\omega_l + \mu_l \sin\omega_l + m\cos\omega_h + \mu_h\sin\omega_h + \delta\right) \\
& + 4\frac{\rho^2}{f^2}(\cos\omega_l + \cos\omega_h)^2(4\overline{W}_6' + \overline{W}_8') - 4\frac{\rho^2}{f^2}\overline{W}_8'(\sin^2\omega_l + \sin^2\omega_h) \\
= & \frac{1}{2}\frac{2B\mu_l}{\sqrt{1-\cos^2\omega_l}} + \frac{2B}{2}(\delta + m\cos\omega_h + \mu_h\sin\omega_h) \\
& + 16\frac{\rho^2}{f^2}\cos\omega_h^2\overline{W}_6' + 8\frac{\rho^2}{f^2}\cos\omega_l\cos\omega_h(2\overline{W}_6' + \overline{W}_8') - 4\frac{\rho^2}{f^2}\overline{W}_8'(\sin^2\omega_l + \sin^2\omega_h),
\end{aligned} \tag{4.27}$$

where, again, the light sector gap equation has been employed in the derivation.
The first line of course agrees with the tree level result in the GSM regime, supplemented by the additional $\mathcal{O}(a^2)$ terms given in the second line.
Additionally, the η tree level mass can readily be computed. It satisfies the continuum Gell-Mann-Okubo formula evaluated with pion and kaon tree level masses including $\mathcal{O}(a^2)$ corrections, plus explicit $\mathcal{O}(a^2)$ terms,

$$m_\eta^2 = \frac{1}{3}\left(4m_K^2 - m_{\pi^\pm}^2\right) - \frac{16\rho^2}{3f^2}(\cos\omega_l - \cos\omega_h)^2\left(2\overline{W}_7' + \overline{W}_8'\right). \tag{4.28}$$

For $\cos\omega_l = \cos\omega_h$, the η mass obeys the continuum Gell-Mann-Okubo relation. Even if the respective twist angles differed by $\mathcal{O}(a)$, this would correspond to promoting the correction to higher than leading order.
Recall that the mass given above describes the unphysical η_8 rather than the physical η.

4.3.2. Rewriting the Leading Order Lagrangian

In the loop calculation in the GSM regime, the calculation has simplified considerably due to the fact, that the leading order Lagrangian coincided with the continuum Lagrangian. The masses to one loop were therefore given by the nonanalytic continuum results, supplemented by analytic terms, than can readily be computed. It thus looks promising to first rewrite the leading order Lagrangian once expanded to four meson fields in terms of the vertices that an ordinary mass term in continuum SU(3) ChPT would spawn, however, now with the $\mathcal{O}(a^2)$ shifted tree level masses $m_{\pi^\pm}^2$ and m_K^2 given in eqs. (4.26) and (4.27), plus additional $\mathcal{O}(a^2)$ four pion vertices. The meson masses to one loop are then trivially the continuum expressions (with tree level masses including the $\mathcal{O}(a^2)$ shift) plus additional chiral logs proportional to a^2, supplemented by a vast number of analytic contributions from the NLO and NNLO Lagrangian. We hence generalize the approach outlined in [30].
Therefore, the mass matrix χ_3 can be rewritten as a function of the tree level meson masses given in eq. (4.26) and (4.27) instead of the quark masses,

$$\chi_3\Big(m, \mu_{l,h}, \omega_{l,h}\Big) = \chi_3\left(m_{\pi^\pm}^2, m_K^2\right) + \Big[\mathcal{O}\left(a^2\right)\text{-terms}\Big]\Big(\omega_{l,h}\Big). \tag{4.29}$$

Note that the neutral pion tree level mass and the η tree level mass are given by linear combinations of the charged pion mass and the kaon mass plus $\mathcal{O}(a^2)$ terms, and the functional dependence of χ_3 sketched above suffices to parametrize the mass matrix completely. After expanding the leading order Lagrangian to four meson fields, we find

$$
\begin{aligned}
\mathscr{L}_{m,4\pi} + \mathscr{L}_{a^2,4\pi} = \overline{W}_6'\frac{\rho^2}{f^4}\Big(& - 4\cos^2\omega_l \pi_l^2\pi^2 + \frac{16}{3}\sin^2\omega_l\pi_3^2\pi^2 \\
& - 4\cos\omega_l\cos\omega_h \pi_l^2\pi_h^2 \\
& - (\cos\omega_l + \cos\omega_h)^2\pi_h^4 \\
& + \frac{2}{3}(\cos^2\omega_l - \cos^2\omega_h)\pi_8^2\pi_h^2 \\
& + \frac{4}{3}\Big(\cos^2\omega_l - \cos\omega_l\cos\omega_h\Big)\pi_8^2\pi_l^2 \\
& - \frac{1}{9}(\cos\omega_l - \cos\omega_h)^2\pi_8^4\Big) \\
+ \overline{W}_8'\frac{\rho^2}{f^4}\Big(& - 2\cos^2\omega_l\pi_l^2\pi^2 + \frac{8}{3}\sin^2\omega_l\pi_3^2\pi^2 \\
& - \frac{1}{2}(\cos\omega_l + \cos\omega_h)^2\pi_h^4 \\
& - 2\cos\omega_l\cos\omega_h\pi_l^2\pi_h^2 \\
& - 2\Big(\cos^2\omega_l - \cos\omega_l\cos\omega_h\Big)\pi_8^2\pi_l^2 \\
& + \frac{1}{3}\Big(\cos^2\omega_l + 4\cos\omega_l\cos\omega_h - 5\cos^2\omega_h\Big)\pi_8^2\pi_h^2 \\
& + \frac{1}{54}\Big(5\cos^2\omega_h + 14\cos\omega_l\cos\omega_h - 19\cos^2\omega_l\Big)\pi_8^4 \\
& + \frac{1}{2}\sin^2\omega_l\pi_h'^4 + \frac{2}{3\sqrt{3}}\xi\pi_3\pi_8\pi_h'^2\Big) \\
+ \overline{W}_7'\frac{\rho^2}{f^4}\Big(& \frac{16}{3}\cos\omega_l(\cos\omega_h - \cos\omega_l)\pi_8^2\pi_l^2 \\
& + \frac{8}{3}\cos\omega_h(\cos\omega_l - \cos\omega_h)\pi_8^2\pi_h^2 \\
& + \frac{8}{27}\Big(-2\cos^2\omega_l + \cos\omega_l\cos\omega_h + \cos^2\omega_h\Big)\pi_8^4 \\
& + \frac{16}{3}\sin^2\omega_l\pi_3^2\pi_8^2 \\
& + \sin^2\omega_l\pi_h'^4 + \frac{2}{3\sqrt{3}}\xi\pi_3\pi_8\pi_h'^2\Big) \\
+ \text{continuum}, &
\end{aligned}
\tag{4.30}
$$

where

$$
\begin{aligned}
\pi_l^2 &= \sum_{i=1}^{3}\pi_i^2 \\
\pi_h^2 &= \sum_{i=4}^{8}\pi_i^2 \\
\pi^2 &= \pi_l^2 + \pi_h^2 \\
\pi_h'^2 &= \pi_4^2 + \pi_5^2 - \pi_6^2 - \pi_7^2
\end{aligned}
$$

denote prominent combinations of fields stemming from the light- and heavy sector, respectively, and the continuum terms are the standard SU(3) ChPT four pion vertices stemming from the mass term but with tree level masses in the LCE regime.
As far as the $\overline{W}'_6$ and $\overline{W}'_8$ terms are concerned, the two expressions in the first line generalize the corresponding terms found in the two flavor twisted mass case [30]. Particularly, the respective coefficients are identical.
In the $\overline{W}'_8$ and $\overline{W}'_7$ terms, the vertices proportional to

$$\xi = 2 + \cos 2\omega_h + \cos(\omega_h - \omega_l) - 5\cos 2\omega_l + \cos(\omega_h + \omega_l)$$

allude to potential π^0-η_8-mixing. The prefactor ξ vanishes at zero twist, but acquires a nonzero value at maximal twist. In continuum ChPT, the mixing is proportional to the mass difference between the up and down quark, and hence not expected in the current setup either. Indeed, the particular form of the vertex incorporating $\pi_h'^2$ implies that contributions to the two-point function

$$\langle \pi_3 \pi_8 \rangle$$

cancel as long as the fields π_i for $i \in [4,7]$ are mass-degenerate at tree-level. Thus, according to eq. (4.27), there is no π_3-π_8-mixing even to NLO in the current setup, and the respective fields are just π^0 and η_8. Note that the vertices will still contribute for instance to kaon scattering at one loop.
Furthermore, there are similar vertices of the form

$$\pi_{1,2}\pi_8\pi_h'^2$$

in the $\overline{W}'_8$ and $\overline{W}'_7$ terms. Their common prefactor is again a function of $\omega_{l,h}$, and vanishes for any $\omega_l = \omega_h$.
The $\overline{W}'_7$ term vanishes at zero twist,

$$\omega_l = 0 = \omega_h.$$

Working however at

$$\omega_l = \frac{\pi}{2} = \omega_h,$$

one encounters a nontrivial contribution.
The flavor symmetry violating three meson vertex stemming from the mass term generalizes the result of the two flavor calculation [30] in a straightforward manner,

$$\mathscr{L}_{m,3\pi} = \frac{2B}{6f}\pi_3\pi^2\left(\mu_l \cos\omega_l - m\sin\omega_l\right),$$

which can hence, using the gap equation analogously to the SU(2) case, be cast into

$$\mathscr{L}_{m,3\pi} = \frac{16}{3}\frac{\rho^2}{f^2}\sin\omega_l\left(\overline{W}'_{68}\cos\omega_l + \overline{W}'_6\cos\omega_h\right)\pi_3\pi^2.$$

However, three meson vertices are of no particular interest in the current application, since at least two three-meson vertices are needed in order to form a loop diagram contributing to the meson self energy, with the loop adding another $p^2 \sim m$. Their contribution is at least of order $\mathcal{O}\left(\left(a^2\right)^2 p^2\right) \sim \mathcal{O}\left(ma^4\right)$ and thus beyond the order considered here.

The upshot here is that in accordance with the approach of first rewriting the leading order Lagrangian presented in the two flavor case, one can re-express the four pion part of the charmless Lagrangian as a sum of vertices that take the form as in SU(3) continuum ChPT and supplemental $\mathcal{O}(a^2)$ vertices. The findings particularly reproduce the established two flavor results [30].

4.3.3. Meson Masses to One Loop at Maximal Twist

At maximal twist,

$$\cos\omega_l = 0 = \cos\omega_h,$$

there are just three extra vertices from the leading order Lagrangian contributing to the self energy to one loop besides the familiar ones from continuum ChPT,

$$\begin{aligned}\Delta\left[\mathscr{L}_{m,4\pi} + \mathscr{L}_{a^2,4\pi}\right]\Big|_{\text{max. twist}} =& \frac{8}{3}\frac{\rho^2}{f^4}\left(2\overline{W}'_6 + \overline{W}'_8\right)\pi_3^2\pi^2 \\ &+ \frac{1}{2}\frac{\rho^2}{f^4}\left(2\overline{W}'_7 + \overline{W}'_8\right)\pi_h'^4 \\ &+ \frac{16}{3}\frac{\rho^2}{f^4}\overline{W}'_7\pi_3^2\pi_8^2 \\ &+ \frac{4}{\sqrt{3}}\frac{\rho^2}{f^4}\left(2\overline{W}'_7 + \overline{W}'_8\right)\pi_3\pi_8\pi_h'^2.\end{aligned} \tag{4.31}$$

The vertices given in the first three lines lead to additional divergent loop corrections, that are canceled by appropriate redefinition of LECs from the NNLO Lagrangian,

$$\mathscr{L}_{\text{lat, NNLO}} = \mathscr{L}_{p^2a^2} + \mathscr{L}_{ma^2} + \mathscr{L}_{a^4}.$$

The vertices given in the last line do not contribute to the masses at one loop, and are only given for completeness. The full NNLO Lagrangian in the LCE regime of SU(2) ChPT was derived in the literature.[37] However, to obtain these results, SU(2) Cayley-Hamilton relations were employed, that do not hold in SU(4). Additional terms entering the NNLO Lagrangian can easily be constructed. As before, all terms compatible with the symmetries have to be written down in the four flavor theory, and subsequently reduced to yield the NNLO Lagrangian of the charmless theory. We refrain from giving all terms compatible with the symmetry and restrict ourselves to some exemplary terms that are needed to explicitly demonstrate the presence of a sufficient number of linearly independent combinations of LECs to cancel all divergences. To this end, *some* of the allowed terms entering the NNLO Lagrangian, evaluated at maximal twist, read

$$
\begin{aligned}
\mathscr{L}_{p^2a^2} =& a_1\rho^2 \left\langle \partial_\mu\Sigma\partial_\mu\Sigma^\dagger \right\rangle + a_2\rho^2 \left\langle \partial_\mu\Sigma + \partial_\mu\Sigma^\dagger \right\rangle \left\langle \partial_\mu\Sigma + \partial_\mu\Sigma^\dagger \right\rangle \\
&+ a_3\rho^2 \left\langle \Sigma\Sigma + \Sigma^\dagger\Sigma^\dagger \right\rangle \left\langle \partial_\mu\Sigma\partial_\mu\Sigma^\dagger \right\rangle + a_4\rho^2 \left\langle \partial_\mu\Sigma\partial_\mu\Sigma^\dagger\Sigma\Sigma + \Sigma^\dagger\Sigma^\dagger\partial_\mu\Sigma\partial_\mu\Sigma^\dagger \right\rangle \\
\rightarrow& a_1\rho^2 \left\langle \partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)} \right\rangle + a_2\rho^2 \left\langle \partial_\mu\Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\partial_\mu\Sigma^\dagger_{(3)} \right\rangle \left\langle \partial_\mu\Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\partial_\mu\Sigma^\dagger_{(3)} \right\rangle \\
&+ a_3\rho^2 \left\langle \Sigma_{(3)}\tilde{\Sigma}_l\Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)} \right\rangle \left\langle \partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)} \right\rangle \\
&\quad - 2a_3\rho^2 \left\langle P_s(\Sigma_{(3)} + \Sigma^\dagger_{(3)}) \right\rangle \left\langle \partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)} \right\rangle \\
&+ a_4\rho^2 \left\langle \partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)}\Sigma_{(3)}\tilde{\Sigma}_l\Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\partial_\mu\Sigma_{(3)}\partial_\mu\Sigma^\dagger_{(3)} \right\rangle ,
\end{aligned}
\tag{4.32}
$$

$$
\begin{aligned}
\mathscr{L}_{ma^2} =& b_1\rho^2 \left\langle \chi^\dagger\Sigma + \Sigma^\dagger\chi \right\rangle + b_2\rho^2 \left\langle \Sigma\Sigma + \Sigma^\dagger\Sigma^\dagger \right\rangle \left\langle \chi^\dagger\Sigma + \Sigma^\dagger\chi \right\rangle \\
&+ b_3\rho^2 \left\langle \Sigma + \Sigma^\dagger \right\rangle^2 \left\langle \chi^\dagger\Sigma + \Sigma^\dagger\chi \right\rangle \\
\rightarrow& b_1\rho^2 \left\langle \chi_3^\dagger\Sigma_{(3)} + \Sigma^\dagger_{(3)}\chi_3 \right\rangle + b_2\rho^2 \left\langle \Sigma_{(3)}\tilde{\Sigma}_l\Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)} \right\rangle \left\langle \chi_3^\dagger\Sigma_{(3)} + \Sigma^\dagger_{(3)}\chi_3 \right\rangle \\
&- 2b_2\rho^2 \left\langle P_s(\Sigma_{(3)} + \Sigma^\dagger_{(3)}) \right\rangle \left\langle \chi_3^\dagger\Sigma_{(3)} + \Sigma^\dagger_{(3)}\chi_3 \right\rangle \\
&+ b_3\rho^2 \left\langle \Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)} \right\rangle^2 \left\langle \chi_3^\dagger\Sigma_{(3)} + \Sigma^\dagger_{(3)}\chi_3 \right\rangle ,
\end{aligned}
\tag{4.33}
$$

$$
\begin{aligned}
\mathscr{L}_{a^4} =& h_1\rho^4 \left\langle \Sigma\Sigma + \Sigma^\dagger\Sigma^\dagger \right\rangle^2 + h_2\rho^4 \left\langle \Sigma + \Sigma^\dagger \right\rangle^2 \\
\rightarrow& h_1\rho^4 \left[\left\langle \Sigma_{(3)}\tilde{\Sigma}_l\Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)}\tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)} \right\rangle - 2\left\langle P_s(\Sigma_{(3)} + \Sigma^\dagger_{(3)}) \right\rangle \right]^2 \\
&+ h_2\rho^4 \left\langle \Sigma_{(3)}\tilde{\Sigma}_l + \tilde{\Sigma}^\dagger_l\Sigma^\dagger_{(3)} \right\rangle^2 .
\end{aligned}
\tag{4.34}
$$

In principle, there is no need to keep track of individual higher order LECs in the results, since these are undetermined anyway. It is only in order to show that there is a sufficient number of linearly independent combinations that they are stated explicitly for the moment. The identifiers of the LECs are nonstandard, and must particularly not be confused with the respective constants from the two flavor calculation.

It is now easy to compute the meson masses to one loop. One loop diagrams contributing to the self-energy, again, are tadpole diagrams built from four pion vertices of $\mathscr{L}_{p^2}$; the vertices of $\mathscr{L}_m$ and $\mathscr{L}_{a^2}$ have been rewritten in terms of vertices taking the form as in continuum ChPT and some remaining vertices of $\mathcal{O}(a^2)$. Hence, the calculation up to here is just as in the continuum, once the correct tree level masses including the $\mathcal{O}(a^2)$ shift are inserted. Technically, this means one has to keep track of the index of the looping pion, since the neutral pion acquires a tree level mass differing from the charged pion tree level mass by $\mathcal{O}(a^2)$.

In the continuum-like contribution, pion chiral logs now split,

$$\begin{aligned} M_{\pi^\pm}^2 &= m_{\pi^\pm}^2 \left[1 + \frac{1}{6f^2}A_0(\pi^0) - \frac{1}{6f^2}A_0(\eta)\right] + \frac{1}{6f^2}2m_{\pi^0}^2 A_0(\pi^0) \\ &= m_{\pi^\pm}^2 \left[1 + \frac{1}{6f^2}3A_0(\pi^0) - \frac{1}{6f^2}A_0(\eta)\right] + \frac{1}{3f^2}\Delta m_\pi^2 A_0(\pi^0), \\ M_K^2 &= m_K^2 \left[1 + \frac{1}{3f^2}A_0(\eta)\right] + \frac{1}{12f^2}\Delta m_\pi^2 A_0(\pi^0), \end{aligned} \tag{4.35}$$

where $A_0(\pi_a)$, again, refers to the (divergent) loop integral regularized using dimensional regularization. The chiral logs involving the mass of its argument are contained in these expressions (cf. App A).
In the continuum limit,

$$\Delta m_\pi^2 \to 0 \quad \Leftrightarrow \quad m_{\pi^\pm}^2 = m_{\pi^0}^2,$$

the masses in eq. (4.35) reduce to the results given in the literature [12] after appropriate renormalization of the Gasser-Leutwyler coefficients L_i. At maximal twist in tmWChPT, one finds an additional pion chiral log proportional to the pion mass splitting, that has not been present in the continuum nor the untwisted scenario.
The extra vertices given in eq. (4.31) spawn additional contributions,

$$\begin{aligned} \Delta M_{\pi^\pm}^2 &= -\frac{1}{3f^2}\Delta m_\pi^2 A_0(\pi^0), \\ \Delta M_K^2 &= -\frac{1}{3f^2}\Delta m_\pi^2 A_0(\pi^0) + \frac{4\rho^2}{f^4}\left(2\overline{W}'_7 + \overline{W}'_8\right) A_0(K). \end{aligned} \tag{4.36}$$

As for the pion mass expression, the same term is present in the continuum-like contribution, but with opposite sign. The terms hence cancel. With respect to the kaon mass, however, one now finds chiral logs involving the neutral pion, kaons and the η-meson to be present, in contrast to only the η log being present in the continuum expression; there are no charged pion chiral logs present in both, the charged pion and kaon masses. The complete result for the masses reads

$$\begin{aligned} M_{\pi^\pm}^2 = m_{\pi^\pm}^2 \Big[& 1 + \frac{1}{6f^2}3A_0(\pi^0) - \frac{1}{6f^2}A_0(\eta) \\ & + \frac{8}{f^2}m_{\pi^\pm}^2\left(2L_8 + 2L_6 - L_4 - L_5\right) + \frac{16}{f^2}m_K^2\left(2L_6 - L_4\right)\Big] \\ & - 4m_{\pi^\pm}^2\frac{\rho^2}{f^2}\left(a_1 + b_1 - 8b_2 - 8a_3 - 2a_4\right) \\ M_K^2 = m_K^2 \Big[& 1 + \frac{1}{3f^2}A_0(\eta) + \frac{8}{f^2}m_K^2\left(2L_8 + 4L_6 - 2L_4 - L_5\right) + \frac{8}{f^2}m_{\pi^\pm}^2\left(2L_6 - L_4\right)\Big] \\ & - \frac{1}{4f^2}\Delta m_\pi^2 A_0(\pi^0) + \frac{4\rho^2}{f^4}\left(2\overline{W}'_7 + \overline{W}'_8\right) A_0(K) \\ & - 4m_K^2\frac{\rho^2}{f^2}\left(a_1 + b_1 - 16b_2 - 8a_3 - 4a_4\right) + 16m_{\pi^\pm}^2\frac{\rho^2}{f^2}b_2 \\ & - 128\frac{\rho^4}{f^2}h_1. \end{aligned} \tag{4.37}$$

Analytic NNLO terms are quoted incompletely and only exemplarily to illustrate the presence of counterterms for all divergences. Note there are also contributions stemming from $\mathscr{L}_{p^2a}$, $\mathscr{L}_{ma}$ and $\mathscr{L}_{a^3}$. When $\cos\omega_l$ is taken to be of order $\mathcal{O}(a)$ as a result of slight mistuning, they are promoted to NNLO. These terms are not of interest as counterterms and thus not given explicitly either.
The divergent part of the results resides in $A_0(\pi_a)$,

$$A_0(\pi_a) = -\frac{m_a^2}{16\pi^2}\left(\Delta + 1 - \log m_a^2\right),$$

where

$$\Delta = \frac{2}{\epsilon} - \gamma_E + \log 4\pi,$$

diverges in the desired case of $D \to 4$ dimensions, implying $\epsilon \to 0$. These divergences are removed by introducing renormalized LECs, whereby besides the divergence proportional to ϵ^{-1}, the finite part $\log 4\pi - \gamma_E + 1$ is also subtracted by convention. Let

$$A_0'(\pi_a) = \frac{m_a^2}{16\pi^2}\log m_a^2,$$
$$\Delta' = -\frac{1}{16\pi^2}(\Delta + 1)$$

denote the finite and to-be subtracted parts of A_0, respectively, and $L_{46} = 2L_6 - L_4$, $L_{58} = 2L_8 - L_5$[4]. Expressing the η tree level mass through the pion and kaon masses, cf. eq (4.28), and rearranging the expressions for the masses in order to demonstrate renormalizability explicitly, one finds

$$\begin{aligned}
M_{\pi^\pm}^2 = m_{\pi^\pm}^2\Big[1 &+ \frac{1}{6f^2}3A_0'(\pi^0) - \frac{1}{6f^2}A_0'(\eta) \\
&+ \frac{m_{\pi^\pm}^2}{f^2}\left(8(L_{46}+L_{58}) + \frac{5}{9}\Delta'\right) + \frac{m_K^2}{f^2}\left(16L_{46} - \frac{2}{9}\Delta'\right)\Big] \\
&+ m_{\pi^\pm}^2\frac{\rho^2}{f^2}\left(-4(a_1 + b_1 - 8b_2 - 8a_3 - 2a_4) + \frac{\Delta m_\pi^2}{2\rho^2}\Delta'\right), \\
M_K^2 = m_K^2\Big[1 &+ \frac{1}{3f^2}A_0'(\eta) \\
&+ \frac{m_{\pi^\pm}^2}{f^2}\left(8L_{46} - \frac{1}{9}\Delta'\right) + \frac{m_K^2}{f^2}\left(8(2L_{46}+L_{58}) + \frac{4}{9}\Delta'\right)\Big] \\
&+ \frac{4\rho^2}{f^4}\left(2\overline{W}_7' + \overline{W}_8'\right)A_0'(K) - \frac{1}{4f^2}\Delta m_\pi^2 A_0'(\pi^0) \\
&+ \frac{\rho^2 m_{\pi^\pm}^2}{f^2}\left(16b_2 - \frac{\Delta m_\pi^2}{4\rho^2}\Delta'\right) \\
&+ \frac{\rho^4}{f^2}\left(-128h_1 - \frac{\Delta m_\pi^4}{4\rho^4}\Delta'\right) \\
&+ \frac{\rho^2 m_K^2}{f^2}\left(-4(a_1 + b_1 - 16b_2 - 8a_3 - 4a_4) + \frac{4}{f^2}\left(2\overline{W}_7' + \overline{W}_8'\right)\Delta'\right),
\end{aligned}$$

[4] These combinations of LECs keep appearing throughout the following equations. Abbreviations are however nonstandard.

where it can now readily be checked that the various combinations of LECs suffice to cancel all divergences. Summarizing linearly independent combinations of (unknown) LECs, and abbreviating $\overline{W}'_{78} = 2\overline{W}'_7 + \overline{W}'_8$, one finally arrives at

$$\begin{aligned}
M_{\pi^\pm}^2 = m_{\pi^\pm}^2 \Big[1 &+ \frac{1}{32\pi^2 f^2} m_{\pi^0}^2 \log \frac{m_{\pi^0}^2}{\mu^2} - \frac{1}{96\pi^2 f^2} m_\eta^2 \log \frac{m_\eta^2}{\mu^2} + \frac{8 m_{\pi^\pm}^2}{f^2} \left(L_{46} + L_{58} \right) \\
&+ \frac{16 m_K^2}{f^2} L_{46} + C_1 \rho^2 \Big], \\
M_K^2 = m_K^2 \Big[1 &+ \frac{1}{48\pi^2 f^2} m_\eta^2 \log \frac{m_\eta^2}{\mu^2} + 8 \frac{m_{\pi^\pm}^2}{f^2} L_{46} + 8 \frac{m_K^2}{f^2} \left(2L_{46} + L_{58} \right) \Big] \\
&+ \frac{\rho^2}{4\pi^2 f^4} \overline{W}'_{78} m_K^2 \log \frac{m_K^2}{\mu^2} - \frac{1}{64\pi^2 f^2} \Delta m_\pi^2 m_{\pi^0}^2 \log \frac{m_{\pi^0}^2}{\mu^2} \\
&+ C_2 \frac{\rho^2 m_{\pi^\pm}^2}{f^2} + C_3 \frac{\rho^2 m_K^2}{f^2} + C_4 \frac{\rho^4}{f^2}.
\end{aligned} \tag{4.38}$$

Note the correct result is recovered in the continuum limit,

$$\rho \to 0, \qquad m_{\pi^0}^2 \to m_{\pi^\pm}^2, \qquad \Delta m_\pi^2 \to 0,$$

and the expression matches the result found in the two flavor theory with large isospin breaking [30], after replacing (in analogy to eq. (4.20), now for a strange quark too heavy to appear in the theory)

$$m_K^2 \to \frac{1}{2} m_{\pi^\pm}^2. \tag{4.39}$$

The additional η chiral log simply is to be discarded, as η involving strangeness is not a dynamical degree of flavor in SU(2) ChPT.
The calculation of the neutral pion mass works completely analogous. The continuum-like contribution reads

$$\begin{aligned}
M_{\pi^0}^2 = m_{\pi^\pm}^2 &\left[1 + \frac{1}{f^2} A_0(\pi^\pm) - \frac{1}{2f^2} A_0(\pi^0) - \frac{1}{6f^2} A_0(\eta) \right] \\
&+ \Delta m_\pi^2 \left[1 + \frac{2}{3f^2} A_0(\pi^\pm) + \frac{1}{3f^2} A_0(K) \right],
\end{aligned}$$

and the contribution from the additional vertices is given by

$$\Delta M_{\pi^0}^2 = -\frac{1}{3f^2} \Delta m_\pi^2 \left[2A_0(\pi^\pm) + 6A_0(\pi^0) + 4A_0(K) + A_0(\eta) \right].$$

The complete neutral pion mass is the sum of these individual contributions and the respective analytic corrections, that provide the counterterms to cancel all divergences,

$$
\begin{aligned}
M_{\pi^0}^2 = m_{\pi^\pm}^2 & \left[1 + \frac{1}{f^2}A_0(\pi^\pm) - \frac{1}{2f^2}A_0(\pi^0) - \frac{1}{6f^2}A_0(\eta)\right] \\
& + \Delta m_\pi^2 \left[1 - \frac{2}{f^2}A_0(\pi^0) - \frac{1}{f^2}A_0(K) - \frac{1}{3f^2}A_0(\eta)\right] \\
& + \frac{8}{f^2}m_{\pi^\pm}^4(L_{46}+L_{58}) - \frac{8}{f^2}\Delta m_\pi^2 m_{\pi^\pm}^2(L_4+L_5) - \frac{16}{f^2}\Delta m_\pi^2 m_K^2 L_4 \\
& + \frac{16}{f^2}m_{\pi^\pm}^2 m_K^2 L_{46} \\
& - \frac{4\rho^2}{f^2}\left(m_{\pi^\pm}^2 + \Delta m_\pi^2\right)(a_1 + 8a_2 - 8a_3 - 2a_4) + \frac{4\rho^2}{f^2}m_{\pi^\pm}^2(-b_1 + 16b_2 + 16b_3) \\
& + \frac{64\rho^2}{f^2}m_K^2(b_2 + 2b_3) + \frac{32\rho^4}{f^2}(h_2 - 8h_1)\,.
\end{aligned}
$$

Separating finite and to-be subtracted parts of the neutral pion mass and re-expressing it in terms of the charged pion mass, the kaon mass and the mass splitting, one finds

$$
\begin{aligned}
M_{\pi^0}^2 = m_{\pi^\pm}^2 & \left[1 + \frac{1}{f^2}A_0'(\pi^\pm) - \frac{1}{2f^2}A_0'(\pi^0) - \frac{1}{6f^2}A_0'(\eta)\right] \\
& + \Delta m_\pi^2 \left[1 - \frac{2}{f^2}A_0'(\pi^0) - \frac{1}{f^2}A_0'(K) - \frac{1}{3f^2}A_0'(\eta)\right] \\
& + \frac{m_{\pi^\pm}^4}{f^2}\left(8(L_{46}+L_{58}) + \frac{5}{9}\Delta'\right) + \frac{m_{\pi^\pm}^2 m_K^2}{f^2}\left(16L_{46} - \frac{2}{9}\Delta'\right) \\
& + \frac{\rho^2 m_K^2}{f^2}\left(64(b_2+2b_3) - \frac{\Delta m_\pi^2}{\rho^2}\frac{13}{9}\Delta'\right) \\
& + \frac{\rho^2 m_{\pi^\pm}^2}{f^2}\left(4(-b_1+16b_2+16b_3) - \frac{\Delta m_\pi^2}{\rho^2}\frac{43}{18}\Delta'\right) \\
& + \frac{\rho^4}{f^2}\left(32(h_2-8h_1) - \frac{\Delta m_\pi^4}{\rho^4}2\Delta'\right).
\end{aligned}
$$

It is readily checked, that the renormalization of the continuum part is consistent with the conditions obtained from renormalizing the charged pion and kaon mass. Furthermore, as now terms including the LECs a_2, b_3 and h_2 are present, that did not contribute in the charged pion mass or the kaon mass, there is a sufficient number of linearly independent NNLO LECs to cancel all occurring divergences. The somewhat awkward coefficients multiplying the divergences occurring in the $\mathcal{O}(ma^2)$ terms reflect the arbitrary choice to expand the neutral pion mass in terms of the charged pion mass and the pion mass splitting.

The fact, that all divergences can be canceled by appropriate renormalization of higher order LECs is of course a consequence of the construction principle of the effective field theory. It is still comforting to see renormalizability worked out explicitly also in the charmless theory.

Eventually, the neutral pion mass reads

$$
\begin{aligned}
M_{\pi^0}^2 = m_{\pi^\pm}^2 \Bigg[1 &+ \frac{1}{32\pi^2 f^2}\left(2m_{\pi^\pm}^2 \log\frac{m_{\pi^\pm}^2}{\mu^2} - m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2}\right) - \frac{1}{96\pi^2 f^2} m_\eta^2 \log\frac{m_\eta^2}{\mu^2} \\
&+ 8\frac{m_{\pi^\pm}^2}{f^2}\left(L_{46} + L_{58}\right) + 16\frac{m_K^2}{f^2} L_{46} + \tilde{C}_1 \rho^2 \Bigg] \\
+\Delta m_\pi^2 \Bigg[1 &- \frac{1}{8\pi^2 f^2} m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2} - \frac{1}{16\pi^2 f^2} m_K^2 \log\frac{m_K^2}{\mu^2} \\
&- \frac{1}{48 f^2} m_\eta^2 \log\frac{m_\eta^2}{\mu^2} + \tilde{C}_2 m_K^2 + \tilde{C}_3 \rho^2 \Bigg].
\end{aligned}
\tag{4.40}
$$

The neutral pion mass involves all kinds of chiral logs, particularly both, neutral pion and charged pion chiral logs. Again, in both, the continuum limit [12], and the limit of a heavy strange quark [30], this expression yields the correct results.
For completeness, we give the η_8-mass to one loop, as well. The continuum-like contribution reads

$$
\begin{aligned}
M_\eta^2 = m_\eta^2 &\left[1 + \frac{1}{f^2} A_0(K) - \frac{2}{3f^2} A_0(\eta) \right] \\
&+ m_{\pi^\pm}^2 \left[-\frac{2}{6f^2} A_0(\pi^\pm) - \frac{1}{6f^2} A_0(\pi^0) + \frac{1}{3f^2} A_0(K) + \frac{1}{6f^2} A_0(\eta) \right],
\end{aligned}
$$

which reproduces the continuum results in the respective limit. The contribution from the additional vertices is given by

$$
\begin{aligned}
\Delta M_\eta^2 &= \frac{16}{3f^4}\left[2\overline{W}_6' + \overline{W}_8' + 2\overline{W}_7'\right] \rho^2 A_0(\pi^0) \\
&= -\frac{1}{3f^2} \Delta m_\pi^2 A_0(\pi^0) + \frac{16}{3f^4} \rho^2 2\overline{W}_7' A_0(\pi^0).
\end{aligned}
$$

The complete η_8 mass is the sum of these individual contributions and the respective analytic corrections, that provide the counterterms to cancel all divergences. The analytic continuum part remains unaltered. By construction, there exist counterterms all occurring divergences and we hence refrain from quoting them explicitly.

$$
\begin{aligned}
M_\eta^2 = m_\eta^2 &\left[1 + \frac{1}{16\pi^2 f^2} m_K^2 \log\frac{m_K^2}{\mu^2} - \frac{1}{24\pi^2 f^2} m_\eta^2 \log\frac{m_\eta^2}{\mu^2} \right] \\
+ m_{\pi^\pm}^2 &\Bigg[-\frac{2}{96\pi^2 f^2} m_{\pi^\pm}^2 \log\frac{m_{\pi^\pm}^2}{\mu^2} - \frac{1}{96\pi f^2} m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2} \\
&\qquad + \frac{1}{48\pi^2 f^2} m_K^2 \log\frac{m_K^2}{\mu^2} + \frac{1}{96\pi^2 f^2} m_\eta^2 \log\frac{m_\eta^2}{\mu^2} \Bigg] \\
&- \frac{1}{48\pi^2 f^2} \Delta m_\pi^2 m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2} + \frac{2}{3\pi^2 f^4} \rho^2 \overline{W}_7' m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2} \\
&+ C_1' \frac{\rho^2 m_{\pi^\pm}^2}{f^2} + C_2' \frac{\rho^2 m_K^2}{f^2} + C_3' \frac{\rho^4}{f^2} \\
&+ \text{continuum analytic.}
\end{aligned}
\tag{4.41}
$$

Eq. (4.41) can be rewritten in terms of the continuum result and additional chiral logs,

$$\begin{aligned} M_\eta^2 = \quad & \text{continuum result} \\ & - \frac{1}{96\pi^2 f^2}\Delta m_\pi^2 \left(2m_{\pi^0}^2 + m_{\pi^\pm}^2\right) \log\frac{m_{\pi^0}^2}{\mu^2} + \frac{2}{3\pi^2 f^4}\rho^2 \overline{W}_7' m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2} \\ & + \text{analytic.} \end{aligned} \tag{4.42}$$

In this expression, the correct continuum limit is evident. Again, there are additional chiral logs as pure lattice effects.

4.4. Decay Constants to One Loop

Another application of the charmless theory is in computing decay constants to one loop. Again, the nonanalytic behavior, namely the chiral logs, may differ from continuum results. The decay constants f_a of pseudoscalar Goldstone bosons are defined by the meson to vacuum matrix element mediated by the axial vector current A_μ^a [11],

$$\left\langle 0 \,\middle|\, A_\mu^a \,\middle|\, \pi^b(p) \right\rangle = \mathrm{i}\delta^{ab} p_\mu f_b, \tag{4.43}$$

whereby the field renormalization Z needed when evaluating the left-hand side of eq. (4.43) has been determined while computing the masses to one loop at maximal twist,

$$\begin{aligned} Z_{\pi^\pm} &= 1 - \frac{8}{f^2}\left(m_{\pi^\pm}^2(2L_4 + L_5) + L_4\left(2m_K^2 - m_{\pi^\pm}^2\right)\right) + \mathcal{O}(a^2) \\ &\quad + \frac{1}{3f^2}\left(A_0(\pi^\pm) + A_0(\pi^0) + A_0(K)\right), \\ Z_{\pi^0} &= 1 - \frac{8}{f^2}\left(m_{\pi^\pm}^2(2L_4 + L_5) + L_4\left(2m_K^2 - m_{\pi^\pm}^2\right)\right) + \mathcal{O}(a^2) \\ &\quad + \frac{1}{3f^2}\left(2A_0(\pi^\pm) + A_0(K)\right), \\ Z_K &= 1 - \frac{4}{f^2}\left(2(2L_4 + L_5)m_K^2 + 2L_4 m_{\pi^\pm}^2\right) + \mathcal{O}(a^2) \\ &\quad + \frac{1}{12f^2}\left(2A_0(\pi^\pm) + A_0(\pi^0)\right) + \frac{1}{2f^2}A_0(K) + \frac{1}{4f^2}A_0(\eta). \end{aligned} \tag{4.44}$$

The continuum analytic part of $Z_{\pi^\pm}$ and Z_{π^0} coincide of course. Note however the different chiral logs entering the respective expressions. The analytic $\mathcal{O}(a^2)$ contributions stem from $\mathscr{L}_{p^2a^2}$, that contributes to the masses at one loop in the Aoki regime. It will only shift the respective analytic contributions to the decay constant and is hence not given explicitly. Note that there are no contributions proportional to a, alluding to $\mathcal{O}(a)$-improvement at maximal twist.
In principle one has to construct the most general expression transforming as an axial vector using the building blocks involved in the construction of the respective Lagrangian [17]. Equivalently one can follow the procedure of introducing sources in the Lagrangian and constructing the axial current through appropriate functional derivatives with respect to these sources (e.g. [29]). Afterwards, the reduction eliminating the degrees of freedom involving charm is to be performed as outlined for the Lagrangian.

The nonanalytic behavior of the decay constants is entirely governed by the LO axial current. No matter what power counting scheme one works in, it is given by [17]

$$A^a_{\mu,\mathrm{LO}} = \frac{f^2}{2}\left\langle T^a\left(\Sigma^\dagger\partial_\mu\Sigma - \Sigma\partial_\mu\Sigma^\dagger\right)\right\rangle, \tag{4.45}$$

and we do not have to construct the complete axial current if we are solely interested in the nonanalytic behavior. As discussed in [17] the lattice axial vector is subject to renormalization that depends on the particular enforced Ward identity on the lattice, leading to differences of $\mathcal{O}(a)$ in the currents. Since the currently used conditions to fix the lattice axial vector current are not accessible in the framework of ChPT, the only meaningful quantities are those in which the axial vector renormalization cancels. To one loop, discarding the axial vector renormalization the decay constant is just given by the continuum result supplemented by analytic contributions at order $\mathcal{O}(a^2)$. We do not expect analytic contributions at $\mathcal{O}(a)$ due to automatic $\mathcal{O}(a)$-improvement at maximal twist. The only peculiarity arises when working in the LCE regime featuring the pion mass splitting at leading order by construction. As in the computation of the meson masses to one loop, we then have to keep track of the pions propagating in loops.

To one loop, one finds

$$\begin{aligned}
\left\langle 0\left| A^{\pi^\pm}_{\mu,\mathrm{LO}}\right|\pi^\pm(p)\right\rangle &= \mathrm{i}\sqrt{Z_{\pi^\pm}}p_\mu f\left[1-\frac{2}{3f^2}\left(A_0(\pi^\pm)+A_0(\pi^0)+A_0(K)\right)\right],\\
\left\langle 0\left| A^{\pi^0}_{\mu,\mathrm{LO}}\right|\pi^0(p)\right\rangle &= \mathrm{i}\sqrt{Z_{\pi^0}}p_\mu f\left[1-\frac{2}{3f^2}\left(2A_0(\pi^\pm)+A_0(K)\right)\right],\\
\left\langle 0\left| A^{K}_{\mu,\mathrm{LO}}\right|K(p)\right\rangle &= \mathrm{i}\sqrt{Z_{K}}p_\mu f\left[1-\frac{1}{6f^2}\left(2A_0(\pi^\pm)+A_0(\pi^0)+6A_0(K)+3A_0(\eta)\right)\right].
\end{aligned}$$

Hence, by comparison with eq. (4.43), and including the field renormalization, one finds

$$\begin{aligned}
\frac{f_{\pi^\pm}}{f} &= 1-\frac{1}{2f^2}\left(A_0(\pi^\pm)+A_0(\pi^0)+A_0(K)\right)\\
&\qquad + \text{cont. analytic} + \mathcal{O}(a^2),\\
\frac{f_{\pi^0}}{f} &= 1-\frac{1}{2f^2}\left(2A_0(\pi^\pm)+A_0(K)\right)\\
&\qquad + \text{cont. analytic} + \mathcal{O}(a^2),\\
\frac{f_K}{f} &= 1-\frac{1}{8f^2}(2A_0(\pi^\pm)+A_0(\pi^0))-\frac{3}{4f^2}A_0(K)-\frac{3}{8f^2}A_0(\eta)\\
&\qquad + \text{cont. analytic} + \mathcal{O}(a^2).
\end{aligned} \tag{4.46}$$

The decay constants in eq. (4.46) reproduce the respective results in the continuum limit, and both a neutral pion log and a charged pion log appear in the charged pion decay constant, whereas only a charged pion log enters the neutral pion decay constant. If the pion decay constant is determined directly through the axial current in contrast to using the indirect method via the pseudoscalar density [11], we find after renormalization of LECs

$$\begin{aligned}\frac{f_K}{f_{\pi^\pm}} = 1 + \frac{1}{128\pi^2 f^2}(2m_{\pi^\pm}^2 \log\frac{m_{\pi^\pm}^2}{\mu^2} + 3m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2}) - \frac{1}{64\pi^2 f^2} m_K^2 \log\frac{m_K^2}{\mu^2} \\ - \frac{3}{128\pi^2 f^2} m_\eta^2 \log\frac{m_\eta^2}{\mu^2} + \text{cont. analytic} + \mathcal{O}(a^2).\end{aligned} \tag{4.47}$$

This result again has the correct continuum limit [12] and clarifies that indeed the neutral pion log contributes.

5. Level of Impact Estimation

All calculations so far have been performed for infinite volumes. However, finite volume corrections are under control from a theoretical point of view and can readily be included [38]. The relevant case in practice is a finite space-time with extent $L^3 \times T$ in the three spatial and the one temporal direction, respectively. Assuming a large time extent compared to the spatial extent and imposing periodic boundary conditions, the two scalar integrals A_0 and A_1 are replaced by their finite volume counterparts. The correction due to the finite volume can then be expressed in terms of the Euclidean position space propagator in infinite volume,

$$G^{(\mathrm{L})}(x) = G(x) + \sum_{\vec{n} \neq \vec{0}} G(x + L\vec{n}). \tag{5.1}$$

The meaning of eq. (5.1) is intuitively clear; in order to propagate to a given point on the lattice with periodic boundary conditions, a particle can not only propagate directly along the shortest distance, but may additionally circle around the periodic system to end up at the very same point. $\vec{n} \in \mathbb{Z}^3 \backslash \{\vec{0}\}$ hence counts the number of additional orbits along any of the three spatial directions. Since the propagator in position space asymptotically decreases exponentially with the particle mass, it is clear, that finite volume corrections will be most important for light particles.
Writing the propagator in position space that is related to the modified Bessel function of the second kind K_1, eventually finite volume corrections are properly incorporated, once one replaces the chiral logs [38],

$$\log \frac{m^2}{\mu^2} \to \log \frac{m^2}{\mu^2} + \delta_1(mL), \tag{5.2}$$

in the results for the meson masses to one loop. The correction is given by

$$\delta_1 = \frac{4}{mL} \sum_{\vec{n} \neq \vec{0}} \frac{K_1\left(|\vec{n}|\, mL\right)}{|\vec{n}|}. \tag{5.3}$$

The degeneracy in the sum of eq. (5.3) can be exploited to rewrite the respective correction as

$$\delta_1 = \frac{4}{mL} \sum_{n=1}^{\infty} \frac{g_n K_1\left(\sqrt{n} mL\right)}{\sqrt{n}} \tag{5.4}$$

with respective multiplicities g_n [39].
For sufficiently large mL, the correction behaves as

$$\delta_1 \sim \mathrm{e}^{-mL}, \tag{5.5}$$

emphasizing the need to incorporate finite volume corrections for light looping particles. Similar to the SU(2) tmWChPT scenario [30], it is the very presence of the neutral pion chiral log instead of the charged pion log in the charged pion mass, and the previously even absent pion log in the kaon mass, that might have significant impact on the analysis of current data from twisted mass simulations, since the neutral pion is the lightest pseudoscalar meson, and hence triggers the largest finite volume corrections.
Current charged pion masses are in the range $270\,\text{MeV} \lesssim M_{\pi^\pm} \lesssim 510\,\text{MeV}$ [18]; the ratio of the neutral pion mass and the charged pion mass in different twisted mass ensembles indicate a non-negligible isospin breaking (cf. Tab. 5.1). In the language of tmWChPT, this is indeed explained by asserting that present-day simulations are already performed in the LCE regime, i.e. in a regime where at least the light quark masses become comparable to a^2.
In order to estimate the impact of the neutral pion log on the kaon mass squared, we evaluate part of the respective correction,

$$\begin{aligned}\Delta_\infty M_K^2 &= -\frac{1}{64\pi^2 f^2}\Delta m_\pi^2 m_{\pi^0}^2 \log\frac{m_{\pi^0}^2}{\mu^2},\\ \Delta_{(\mathrm{FV})} M_K^2 &= -\frac{1}{64\pi^2 f^2}\Delta m_\pi^2 m_{\pi^0}^2\ \delta_1\left(m_{\pi^0} L\right),\end{aligned}\tag{5.6}$$

noting that only the approximately known charged and neutral pion masses and the decay constant in the chiral limit enter. The relative impact on the kaon mass is then given by

$$\Delta M_K/M_K = \frac{1}{2}\frac{\Delta_\infty M_K^2 + \Delta_{(\mathrm{FV})} M_K^2}{M_K^2}.\tag{5.7}$$

Estimations for the various ensembles examined by the ETMC are depicted in Table 5.1.
Although finite volume correction and overall chiral log expose different signs and thus partially cancel, we estimate the previously disregarded neutral pion log to alter the kaon mass by the same order of magnitude as the currently quoted statistical error. This conclusion remains valid, even if the neutral pion mass is varied by up to ten percent to amount for the uncertainty in its determination from simulations.
Additionally, the expression for the kaon mass in tmWChPT involves another chiral log without counterpart in continuum ChPT, namely the kaon log. Since $\overline{W}_7'$ has not been determined to date, its impact can hardly be estimated without actually performing the simultaneous fit using the updated expressions for the meson masses to one loop to the whole set of data from numerical studies. Superficially, the numerical prefactor suggests, the log might have significant impact.
Following these rather crude estimations, the previously disregarded neutral pion log is expected to affect the analysis of data obtained in twisted mass QCD simulations to an extent comparable to current statistical and systematic uncertainties. The fact that current data analysis, though neglecting the new terms, appears to work out sufficiently well might be due to the parametric space explored to date. In the parameter space currently examined, the new logs and their respective finite volume corrections tend to cancel each other. This situation may change once different pion masses, lattice spacings or volumes are examined.

Ensemble	β	$aM_\pm$	aM_0	aM_K	$M_0/M_\pm$	af	$M_\pm L$	$M_0 L$	$\delta_1(M_0 L)$	$\Delta_\infty M_K^2/M_K^2$	$\Delta_{\text{FV}} M_K^2/M_K^2$	$\lvert\Delta M_K/M_K\rvert$ [%]	$\left\lvert\Delta M_{K,\text{stat}}/M_K\right\rvert$ [%]
A30.32		0.1234	0.0611	0.2515	0.50	0.0456	3.9	2.0	3.14	-0.00207	0.00162	0.02	0.12
A40.32		0.1415	0.0811	0.2567	0.57	0.0480	4.5	2.6	0.95	-0.00318	0.00088	0.12	0.09
A40.24		0.1445	0.0694	0.2588	0.48	0.0464	3.5	1.7	6.20	-0.00319	0.00525	0.10	0.16
A60.24	1.90	0.1727	0.1009	0.2670	0.58	0.0507	4.1	2.4	1.39	-0.00522	0.00240	0.14	0.19
A80.24		0.1987	0.1222	0.2771	0.61	0.0539	4.8	2.9	0.56	-0.00685	0.00145	0.27	0.22
A100.24		0.2215	0.1570	0.2881	0.71	0.0560	5.3	3.8	0.13	-0.00779	0.00047	0.37	0.12
A80.24s		0.1982	0.1512		0.76		4.8	3.6	0.18				
A100.24s		0.2215	0.1863	0.2650	0.84	0.0555	5.3	4.5	0.05	-0.00654	0.00017	0.32	0.34
B25.32		0.1064	0.0605	0.2124	0.57	0.0405	3.4	1.9	3.91	-0.00228	0.00234	0.00	0.24
B35.32		0.1249	0.0710	0.2184	0.57	0.0429	4.0	2.3	1.69	-0.00334	0.00162	0.09	0.13
B55.32	1.95	0.1540	0.1323	0.2280	0.86	0.0464	4.9	4.2	0.07	-0.00345	0.00011	0.17	0.15
B75.32		0.1808	0.1557	0.2375	0.86	0.0488	5.8	5.0	0.03	-0.00462	0.00007	0.23	0.13
B85.24		0.1931	0.1879	0.2448	0.97	0.0495	4.6	4.5	0.05	-0.00116	0.00003	0.06	0.18
D15.48		0.0695	0.0561		0.81		3.3	2.7	0.79				
D20.48	2.10	0.0797	0.0651		0.82		3.8	3.1	0.39				
D30.48		0.0978	0.0860		0.88		4.7	4.1	0.08				
D45.32sc		0.1198	0.0886		0.74		3.8	2.8	0.66				

Table 5.1.: Meson masses from twisted mass lattice QCD simulations [40, 18] in different ensembles, derived quantities, including the finite volume correction factor $\delta_1(M_0L)$ (eq. (5.4), series truncated at $n = 20$), and estimates of the neutral pion log impact including its finite volume correction (eqs. (5.6) and (5.7)). In our convention, $f \approx 93$ MeV and $\mu \approx 1$ GeV, hence $a\mu \approx 0.456, 0.405, 0.304$ for $\beta = 1.9, 1.95, 2.1$, respectively. $\Delta M_{K,\text{stat}}/M_K$ is the relative statistical error quoted for the kaon masses.

On the other hand, the existence of $\overline{W}'_7$ terms entering actual observables might enable the determination of its value, once appropriate precision is achieved.

6. Conclusion

Quantum Chromodynamics (QCD) is widely believed to be the correct theory describing strong interaction. Prominent features of QCD include analytically proven asymptotic freedom for the currently known six quark flavors realized in nature, as well as confinement at low energies. Confinement refers to the experimentally confirmed observation, that the dynamical degrees of freedom of QCD, quarks and gluons, are not observed as free particles at low energies. Instead, the appropriate degrees of freedom at low energies are bound states of quarks and gluons, so-called hadrons. Lattice Calculations strongly support the notion that this phenomenon is correctly predicted by QCD. Both asymptotic freedom and confinement are manifestations of the running coupling of QCD. The coupling increases at low energies, rendering conventional perturbative methods to explore the low-energy dynamics of QCD useless.

Chiral Perturbation Theory (ChPT) as the effective theory of QCD in the low-energy regime provides a description of the respective dynamics that can be handled with perturbative methods. As in all effective theories, the effect of fields that are not kept as dynamical degrees of freedom is encoded in a set of parameters entering the theory. They can be determined by matching quantities computed in both the effective theory and the underlying theory. In ChPT, they are called Low Energy Constants (LECs).

To date, lattice QCD is the only non-perturbative formulation of QCD. The continuous space-time that QCD is defined on is replaced by a finite Euclidean grid referred to as lattice. Once an appropriate implementation of fermions representing the quarks has been chosen, the resemblance of the path integral formalism in Quantum Field Theory to statistical mechanics allows for the treatment of lattice QCD via Monte Carlo methods.

The lattice effects can be incorporated systematically in ChPT, providing a framework to study the continuum and infinite volume limits, both of which are fundamentally inaccessible to lattice QCD calculations. Comparing correlation functions from lattice QCD and ChPT, the Low Energy Constants of ChPT can be fixed.

The construction of ChPT as the theory describing the low-energy regime of QCD is based on symmetry considerations. While the massless QCD Lagrangian exhibits a global symmetry under seperate transformations of left- and right-handed components of the fermionic matter fields, hadron phenomenology does not confirm that the full chiral symmetry is realized in nature. Particularly, the presence of some extraordinarily light hadrons compared to the residual hadronic scale cannot be explained. The full chiral symmetry exhibited by the massless QCD Lagrangian is thus believed to be spontaneously broken down to a subgroup. One possible mechanism for the spontaneous symmetry breaking is by a nonvanishing quark condensate. Whether or not the quark condensate is the dominant trigger of the phase transition does not affect the construction of ChPT.

According to the Goldstone theorem, a massless (Goldstone-)boson is spawned for every spontaneously broken continuous symmetry. The observed hadron spectrum can be made plausible once the lightest hadrons are reinterpreted as pseudo Goldstone bosons of the spontaneously broken chiral symmetry, that still acquire a small mass due to the additional explicit chiral symmetry breaking by nonvanishing though small quark masses. Soft pion processes can then be studied using perturbation theory in the effective field theory.

Starting from a Lagrangian comprising all terms compatible with the symmetry of the underlying theory one obtains the most general scattering matrix elements that obey the respective symmetries and additional properties of a good Quantum Field Theory such as locality and cluster decomposition. The explicit symmetry breaking of the full chiral symmetry by quark masses is carried over to the effective theory by spurion analysis. This ensures that the symmetry is broken in ChPT in the same way as in QCD. The effective theory then is a joint expansion in hadron momenta and quark masses. Therefore one has to impose a power-counting scheme to organize the expansion consistently.

In order to establish the connection to lattice QCD with a given fermion implementation, all of which violate different symmetries of continuum QCD, the lattice effects have to be made explicit in an effective continuum theory. The expansion of the lattice QCD action near the continuum limit in powers of the lattice spacing is accomplished by Symanzik's effective theory. Since the approach again relies on symmetry arguments, different fermion implementations lead to different Symanzik effective theories. These can then be translated to the ChPT framework based on the chiral symmetry breaking pattern of the additional terms in the Symanzik effective theory. Again, a power counting scheme weighting the relative impact of all sources of symmetry breaking has to be imposed.

Recently, a formulation of lattice QCD with Wilson fermions has emerged, featuring automatic $\mathcal{O}(a)$-improvement when the original QCD mass term is rotated chirally. This twisted-mass formulation has been studied numerically over the past decade and can as well be examined in the framework of ChPT. The appropriate inclusion of lattice effects in this lattice QCD formulation leads to ChPT for Wilson fermions with twisted masses (tmWChPT), which generalizes ChPT for Wilson fermions (WChPT). Including the charm quark at its physical mass in the expansion in the framework of ChPT contradicts the premise of a small perturbation by nonvanishing quark masses. Therefore, D mesons must not occur in ChPT results.

In recent simulations including two mass-degenerate light quark flavors resembling the up and down quark plus two non-degenerate flavors (strange and charm quarks), referred to as 2+1+1 simulations, a twofold twist of masses is implemented in the light and heavy sector separately. To capture the effects of twisted masses in the heavy sector, we start from a 2+1+1 flavor tmWChPT. We then proceed to perform the reduction from the 2+1+1 flavor theory to the charmless theory in analogy to how three flavor ChPT relates to two flavor ChPT. In the course of matching additional terms altering the dynamics remain compared to the naively set up 2+1 tmWChPT with twisted masses in the light sector.

As a first important result of our work, the reduction already at Lagrangian level is shown to work by reproducing the reduction from three to two flavor in continuum ChPT. Additionally, comparing formal predictions of the 2+1+1 flavor theory to the

respective expressions obtained from charmless theory in the GMS-regime, agreement up to terms involving charm degrees of freedom is found.
As an application, we calculate the charged and neutral pion masses, the kaon mass and the η_8 mass to one loop in the LCE regime, that is likely to describe the numerical simulations carried out by the European Twisted Mass Collaboration. The nonanalytic behavior, so-called chiral logs, are governed by looping mesons in the one-loop diagrams. The neutral pion is significantly lighter than the charged pions in recent simulations, alluding to isospin violation correctly predicted by tmWChPT. Therefore, finite volume corrections altering the chiral logs are much more important for neutral pion chiral logs compared to charged pion chiral logs. Particularly, pion chiral logs enter the kaon mass that do not have a counterpart in continuum ChPT. Their respective relative impact is estimated to be of the same order of magnitude as the systematic error claimed in current twisted mass data analysis. We show that decay constants as first actual observables also include neutral pion logs altering their finite volume dependence. Therefore, analysis of numerical data will have to take the newly derived formulae into consideration in upcoming evaluations when even higher precision is accessible.

A. Dimensional Regularization

In the course of computing the meson self-energy to one loop, one is confronted with evaluating integrals of the form

$$A_0(m) = \int \frac{\mathrm{d}^D k}{(2\pi)^D} \frac{1}{k^2 + m^2},$$
$$A_1(m) = \int \frac{\mathrm{d}^D k}{(2\pi)^D} \frac{k^2}{k^2 + m^2},$$

that are divergent for $D \to 4$ space-time dimensions. One hence employs a regulator to evaluate the integrals and postpone the treatment of the divergences. They are later on removed by renormalization.
The integrals can be computed using (see e.g. [41], eq. (65))

$$\int \frac{\mathrm{d}^D k}{(2\pi)^D} \frac{1}{(k^2 + L)^n} = \frac{1}{(4\pi)^{D/2}} \frac{\Gamma(n - D/2)}{\Gamma(n)} L^{-n+D/2},$$

and expanding around $0 = \epsilon = 4 - D$, where the following properties of the Γ function hold

$$\Gamma(x) = 1/x - \gamma_E + \mathcal{O}(x),$$
$$\Gamma(-1 + x) = -1/x + \gamma_E - 1 + \mathcal{O}(x).$$

Here, γ_E is the Euler-Mascheroni constant. Hence, the initial divergence of the integrals is recovered as pole in the expansion of the Γ function, and one obtains

$$\begin{aligned}
A_0(m) &= (4\pi)^{-2+\epsilon/2} \frac{\Gamma(-1 + \epsilon/2)}{\Gamma(1)} m^{2(1-\epsilon/2)} \\
&= \frac{1 + \frac{\epsilon}{2} \log 4\pi}{16\pi^2} \left(-\frac{2}{\epsilon} + \gamma_E - 1\right) m^2 (1 - \epsilon \log m) + \mathcal{O}(\epsilon) \\
&= \frac{m^2}{16\pi^2} \left(-\frac{2}{\epsilon} + \gamma_E - 1 - \log 4\pi + 2 \log m\right) + \mathcal{O}(\epsilon) \\
&= -\frac{m^2}{16\pi^2} \left(\Delta + 1 - \log m^2\right),
\end{aligned}$$

where

$$\Delta = \frac{2}{\epsilon} - \gamma_E + \log 4\pi,$$

and

$$\begin{aligned}
A_1(m) &= \int \frac{\mathrm{d}^D k}{(2\pi)^D} \frac{k^2 + m^2 - m^2}{k^2 + m^2} \\
&= \underbrace{\frac{\text{const}}{\Gamma(0)}}_{\to 0} - m^2 A_0(m).
\end{aligned}$$

B. Feynman Rules and Contributions to Meson Masses to One Loop

With the accurate Lagrangian up to a prescribed order at hand, one is confronted with computing the contributions to the self-energy in terms of (Euclidean) Feynman rules. Let $V_r^{a,b,c,d}[p_1, p_2, p_3, p_4]$ denote the Euclidean Feynman rules for the four-pion vertices occurring in the expansion of the leading order Lagrangian up to four meson fields, where a, b, c, d denote meson field indices, r simply indicates the different vertices, and all momenta are oriented as incoming. Their contribution to the self-energy of field π^a then reads

$$\frac{1}{2}\sum_{b=1}^{8}\int \frac{\mathrm{d}^4 k}{(2\pi)^4}\frac{1}{k^2+m_b^2}\sum_r V_r^{a,b,b,a}[p,k,-k,-p], \tag{B.1}$$

where the sum over r extends over all vertices, and the tadpole diagram's overall symmetry factor is included. Up to proportionality constants, the vertices in the integrand of eq. (B.1) are of one of the following forms,

$$p^2, \quad (p+k)^2, \quad \text{const},$$

where terms including no momenta, for example stemming from the mass term, are referred to as constant. The truncated Green's function can thus be re-written as

$$\begin{aligned} &\frac{1}{2}\sum_{b=1}^{8} c_0^{a,b}(p^2)A_0(m_b) + c_1^{a,b}A_1(m_b) \\ &= \frac{1}{2}\sum_{b=1}^{8}\left(c_0^{a,b}(p^2) - c_1^{a,b}m_b^2\right)A_0(m_b), \end{aligned} \tag{B.2}$$

in terms of the two scalar integrals $A_0(m_b)$ and $A_1(m_b)$ discussed in App. A. Obviously, the two integrals distinguish the cases of whether the derivative occurring in the interaction vertices acts on the external or the looping meson. The propagator accordingly always involves the mass of the looping particle.

The actual translation of terms in the Lagrangian to their contribution to the truncated two-point function of particle a can be handled by means of expression replacements in computer algebra systems. The replacement rules for the four pion vertices stemming from the leading order Lagrangian, that contribute via tadpole diagrams, read

$$\begin{aligned} \partial_\mu\pi_a\partial^\mu\pi_a\,\pi_b\pi_b &\to \overbrace{(-)}^{\text{eucl.}}4ip\,(-ip)A_0(m_b), \\ \pi_a\pi_a\,\partial_\mu\pi_b\partial^\mu\pi_b &\to (-)\;4A_1(m_b), \\ \pi_a\pi_a\,\pi_b\pi_b &\to (-)\;4A_0(m_b), \\ \pi_a\pi_a\,\pi_a\pi_a &\to (-)\;24A_0(m_a), \\ \partial_\mu\pi_a\pi_a\,\partial^\mu\pi_b\pi_b &\to 0, \end{aligned}$$

where the $4 = 2 \cdot 2$ and $24 = 4!$ reflect the different ways of contracting external fields with the vertex. The overall symmetry factor $\frac{1}{2}$ of the tadpole diagram has to be kept in mind. The last term does not contribute to the one-loop diagram, as the sum of all possible contractions always vanishes,

$$\begin{aligned} &V^{a,b,b,a}_{\partial_\mu \pi_a \pi_a \, \partial^\mu \pi_b \pi_b}[p, p+k, -(p+k), -p] \\ &\quad \propto p(p+k) + p[-(p+k)] + (-p)(p+k) + (-p)[-(p+k)] = 0. \end{aligned}$$

The above expressions have to be Wick-rotated back to Minkowski-space, and then give contributions to the meson self-energy $\Sigma(p^2)$. This part of the self-energy is supplemented by analytic contributions stemming from the next to leading order Lagrangian. The respective vertices contribute only at tree-level, the respective replacements thus trivially read

$$\begin{aligned} \pi_a \pi_a &\to \overbrace{(-)}^{\text{eucl.}} 2 \\ \partial_\mu \pi_a \partial^\mu \pi_a &\to (-)\, 2ip\,(-ip) \end{aligned}$$

Having computed the meson self-energy, the meson mass to one loop, M_a^2, is given by the pole of the propagator, hence as solution of the equation

$$p^2 - m_a^2 + \Sigma_a\left(p^2\right) = 0$$

at $p^2 = M_a^2$. The self-energy can always be writen as

$$\Sigma_a(p^2) = Ap^2 + Bm_a^2 + C,$$

where the respective coefficients are of the orders

$$A, B = \mathcal{O}(p^2), \qquad C = \mathcal{O}(p^4),$$

or of equivalent order in terms of m and a, according to the prescribed power-counting scheme. The meson mass accurate to $\mathcal{O}(p^4)$ is then given by

$$M_a^2 = m_a^2(1 - B - A) - C.$$

The wave-function renormalization Z_{π_a} is then given by,

$$Z_{\pi_a} = 1 - \left.\frac{\mathrm{d}\Sigma_a}{\mathrm{d}p^2}\right|_{p^2 = M_a^2} = 1 - A.$$

The divergence of the scalar integral A_0 in the limit $D \to 4$ calls for renormalization of the theory. The appropriate counterterms are provided by the next to leading order Lagrangian. Indeed, by construction, appropriate renormalization of NLO LECs renders the theory finite. The finite part of A_0, the chiral logarithms, remain in the expressions for the meson masses to one loop.

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