Chiral perturbation theory for twisted mass QCD at small quark mass

Satoru Ueda\textsuperscript{a} and Sinya Aoki\textsuperscript{b,c}

\textsuperscript{a}KEK Theory Center, High Energy Accelerator Research Organization (KEK), Tsukuba 305-0801, Japan
\textsuperscript{b}Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan
\textsuperscript{c}Center for Computational Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan

E-mail: sueda@post.kek.jp, saoki@het.ph.tsukuba.ac.jp

ABSTRACT: We study the lattice cutoff ($a$) and quark mass dependences of pion masses and decay constants in the $N_f = 2$ twisted mass QCD, using the Wilson chiral perturbation theory to the next leading order (NLO). In order to investigate the region near zero quark mass, we introduce the power counting scheme where $O(a^2, am)$ terms are included in the tree level effective Lagrangian. At the NLO of this power counting scheme, we calculate the charged pion mass and decay constant as a function of the lattice cutoff as well as the twisted quark mass at the maximal twist. In this paper, we adopt two different definitions for the maximal twist. We confirm that the difference between the two appears as the $O(a^2)$ effects so that the automatic $O(a)$ improvement is realized for both definitions.
1 introduction

The twisted mass lattice QCD (tmlQCD) [1–3] has several advantages for numerical simulations, one of which is the automatic $O(a)$ improvement at the maximal twist [3–5]. The tmlQCD becomes free from $O(a)$ lattice spacing errors, by simply setting the twist angle to its maximum value $\omega = \pi/2$.

This automatic $O(a)$ improvement of the tmlQCD has been investigated in quench simulations by the XLF Collaboration [6–9] and Abedel-Rehime et al.[10, 11], while the unexpected first order phase transition has been found in full QCD simulations by DESY group [12–14]. Recently the European Twisted mass Collaboration (ETMC) has started
the large-scale full QCD simulations at the maximal twist with $N_f = 2$ [15, 16] and $N_f = 2 + 1 + 1$ [17, 18].

The chiral perturbation theory (ChPT) [19–22], which is a low energy effective theory of QCD describing the dynamics of Nambu-Goldstone(NG) bosons, plays an important role to extrapolate physical observables such as NG boson masses and decay constants calculated in lattice QCD simulations at heavier quark masses to the physical quark mass point. Furthermore, not only the quark mass dependence but also the scaling violation for the Wilson quark action are described by the Wilson ChPT (WChPT), which includes effects of non-zero lattice spacing $a$ [23–25]. Since $O(a)$ contribution can be absorbed into the quark mass term $m$, an inclusion of the lattice spacing effect in the ChPT is rather non-trivial, so that $O(a^2)$ terms dominate in the small quark mass region. For QCD with the ordinary Wilson quark, several physical observables have been calculated in the WChPT at the next leading order (NLO), while only the leading order (LO) results exist in the WChPT for the tmQCD\(^1\) \(^2\). In this paper, we therefore present results of pion masses and decay constants in the WChPT at the NLO, including $O(a^2, am)$ terms in the LO Lagrangian.

In Sec. 2, we consider the power counting scheme in detail and give results at LO. In Sec. 3, we calculate the one loop contribution for pion masses and decay constants, and show that divergences of these quantities at one loop can be renormalized by the NLO counter terms. We present the pion masses and decay constants at NLO arbitrary value of the twist angle. In Sec. 4, we consider the automatic $O(a)$ improvement at the maximal twist, using the NLO calculation. We summarize our paper in Sec. 5. Details of NLO calculations are given in appendix. A.

2 Analysis at ”leading order”

2.1 Power counting and Lagrangian

In the ordinary continuum ChPT [19–22], the quark mass $m$, equivalently the meson momentum $p^2$, is considered as the expansion parameter, so that $O(M)$ terms consist of the LO Lagrangian where $M = m$ or $p^2$. At the NLO order, local counter terms of $O(M^2)$ cancel the divergences of these quantities at one loop can be renormalized by the NLO terms.

In addition to $M$, the lattice spacing $a$ appears as the expansion parameter in the chiral perturbation theory for lattice QCD. Due to the explicit breaking of the chiral symmetry in the Wilson quark action, the lattice spacing effects start at $O(a)$. Therefore it is natural to treat $O(a)$ term as the LO contribution such that $a \sim M$. In the WChPT, this LO $O(a)$ term can be absorbed into the mass term by

$$m \rightarrow \tilde{m} = m + O(a), \quad (2.1)$$

\(^1\)There exists the NLO ChPT calculations without $O(a^2, am)$ terms for $N_f = 2$ [26–28], $N_f = 3$ [26, 28], and $N_f = 2 + 1 + 1$ [30].

\(^2\)In ref. [31], NLO chiral log terms have been calculated with a similar power counting scheme, but in this paper we calculate and consider the renormalization at NLO in detail and the general case.
Table 1. Power counting scheme in this paper. We treat \( O(\tilde{M}) \) (LO) and \( O(a^2, a\tilde{M}) \) (SLO) as the tree level Lagrangian. We introduce NLO and NSLO terms as local counter terms to cancel divergence of one loop contributions.

\[
\begin{array}{|c|c|c|c|}
\hline
\text{tree level} & \text{LO} & \text{SLO} & \text{NSLO} \\
\text{one loop} & \text{NLO} & \text{O}(\tilde{M}^2) & \text{O}(a^2M, a\tilde{M}^2) \\
\hline
\end{array}
\]

so that no extra contributions to the continuum ChPT appear in the WChPT at this order. This power counting, however, is not correct in the region where \( \tilde{m} \) is small, since the NG boson mass \( m_\pi \) at the LO is given by

\[
m_\pi^2 = 2B\tilde{m}, \tag{2.2}
\]

which becomes tachyon for negative \( \tilde{m} \). One has to add \( O(a^2) \) terms to the LO Lagrangian for the stability of the vacuum to avoid the appearance of the tachyon\(^2\). This LO Lagrangian is still insufficient due to the following reason. While 1-loop contributions from this LO Lagrangian generate \( O(\tilde{M}^2, \tilde{M}a^2, a^4) \) terms where \( \tilde{M} = \tilde{m} \) or \( p^2 \), terms odd in \( a \) such as \( O(\tilde{M}a) \) are never generated from 1-loop contributions. Hereafter we ignore \( O(a^4) \) terms since they are small in present lattice QCD simulations.

From the above consideration, a physical observable \( X \) in general depends on both quark mass \( \tilde{m} \) and \( a \) as

\[
X(\tilde{m}, a) = \tilde{m}X_0(\tilde{m}) + \tilde{m}aX_1(\tilde{m}) + a^2X_2(\tilde{m}) + O(a^3), \tag{2.3}
\]

where we ignore small \( a^3 \) or higher contributions. We therefore set up the WChPT to calculate \( X_0(\tilde{m}) \), \( X_1(\tilde{m}) \) and \( X_2(\tilde{m}) \) order by order in \( \tilde{m} \). For this purpose, in addition to leading order \( O(\tilde{M}) \) terms, we consider \( O(\tilde{M}a, a^2) \) terms as the tree level Lagrangian. We call \( O(\tilde{M}a, a^2) \) terms the sub-leading order (SLO) terms to distinguish the \( \tilde{m} \) from LO terms. The one-loop contributions generate an additional factor of \( \tilde{M} \) to the tree level Lagrangian, LO plus SLO. Divergences from these one-loop contributions must be canceled by NLO \( O(\tilde{M}^2) \) and NSLO \( O(a^2M, a\tilde{M}^2) \) terms. We stress again that higher order contributions such as \( a^2\tilde{M}^2 \) are neglected here.

For the twisted mass fermion \([1, 2]\), there are two mass parameters, untwisted quark mass \( \tilde{m} \) and twisted quark mass \( \mu \), which are denoted as \( m = \tilde{m}, \mu \). Therefore \( \tilde{M} \) in this case represents \( \tilde{m}, \mu \) or \( p^2 \). In table 1, we summarize our power counting scheme.

\(^3\)In the continuum ChPT, no tachyon appears for all \( m \), since \( \tilde{m} \to |m| \) in the mass formula, thanks to the chiral symmetry, which is absent in the WChPT.
### 2.2 Tree-level Lagrangian

The tree-level effective Lagrangian for $N_f = 2$ tmlQCD, which include LO and SLO, is given by

\[
\mathcal{L}_{\text{LO}} = \frac{f_0^2}{4} \langle D_\mu \Sigma D_\mu \Sigma \rangle - \frac{f_0^2}{4} \langle \Sigma \chi^\dagger + \chi \Sigma \rangle - \frac{f_0^2}{4} \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma \rangle \tag{2.4}
\]

\[
\mathcal{L}_{\text{SLO}} = W_{45} \langle D_\mu \Sigma D_\mu \Sigma \rangle \langle (\Sigma - \Sigma_0) \hat{A}^\dagger + \hat{A} (\Sigma - \Sigma_0) \rangle \\
- W_{68} \langle \Sigma \chi^\dagger + \chi \Sigma \rangle \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma \rangle - W_{68}' \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma \rangle^2, \tag{2.5}
\]

where $D_\mu \Sigma$ is covariant derivative with the left and right source current $l_\mu$ and $r_\mu$ defined by

\[
D_\mu \Sigma = \partial_\mu \Sigma - i l_\mu \Sigma + i \Sigma r_\mu, \tag{2.6}
\]

\[
D_\mu \Sigma^\dagger = \partial_\mu \Sigma^\dagger + i \Sigma^\dagger l_\mu - i r_\mu \Sigma. \quad \tag{2.7}
\]

After the construction of the Lagrangian, spurion fields $\chi$ and $\hat{A}$ should be set to

\[
\chi \rightarrow 2B_0 M = 2B_0 (m + i \tau^3 \mu), \quad \hat{A} \rightarrow 2W_0 a. \tag{2.8}
\]

The coefficients $f_0, B_0, W_{0,45,68}$ and $W_{68}'$ in eqs. (2.4), (2.5) and (2.8) are the low energy constants, and their dimension are $[f_0] = [B_0] = 1, [W_0] = 3$, and $[W_{45,68}] = [W_{68}] = 0$. The $SU(2)$ matrix fields $\Sigma(x)$ for NG bosons is defined by

\[
\Sigma = \Sigma_0^{1/2} \Sigma_{ph} \Sigma_0^{1/2}, \tag{2.9}
\]

\[
\Sigma_{ph} = \exp \left[ i \pi_a(x) \tau^a \right], \tag{2.10}
\]

where $\Sigma_0$ is a vacuum expectation value of $\Sigma(x), \tau^a$ is the Pauli matrices and $\pi_a(x)$ is the pseudo scalar NG field.

As already mentioned, the $O(a)$ term, $\langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma \rangle$ can be absorbed to $O(m)$ term, $\langle \Sigma \chi^\dagger + \chi \Sigma \rangle$ by the replacement that

\[
2B_0 \tilde{m} = 2B_0 m + 2W_0 a. \tag{2.11}
\]

Replacing the mass parameter $m$ with shifted mass $\tilde{m}$, we obtain

\[
\mathcal{L}_{\text{LO+SLO}} = \frac{f_0^2}{4} \left[ 1 + \frac{c_0 a}{4} \langle (\Sigma - \Sigma_0) + (\Sigma - \Sigma_0)^\dagger \rangle \right] \langle D_\mu \Sigma D_\mu \Sigma \rangle \\
- f_0^2 \frac{2B_0 \tilde{m}}{4} \langle \Sigma + \Sigma^\dagger \rangle - \frac{2B_0 \mu}{4} \langle i (\Sigma - \Sigma^\dagger) \tau^3 \rangle \\
+ \frac{\tilde{c}_2 a^2 2B_0 \tilde{m}}{16} \langle \Sigma + \Sigma^\dagger \rangle^2 - \tilde{c}_2 a^2 B_0 \mu \langle \Sigma + \Sigma^\dagger \rangle \langle i (\Sigma - \Sigma^\dagger) \tau^3 \rangle, \tag{2.12}
\]

where the coefficients $c$’s are defined by

\[
c_0 = 32W_{45} \frac{W_0}{f_0^2}, \quad c_2 = -64(W_{68}' - W_{68}) \frac{W_0^2}{f_0^2}, \quad \tilde{c}_2 = 32W_{68} \frac{W_0}{f_0^2}. \tag{2.13}
\]
2.3 Gap equation and pseudo scalar meson mass

We first determine the vacuum in the Lagrangian (2.12). Parametrizing the vacuum expectation value of $\Sigma$ as

$$\Sigma_0 = \exp[i\phi \tau^3] = \cos \phi + i\tau^3 \sin \phi,$$

the vacuum energy becomes

$$V(\phi) = -f_0^2[2B_0\tilde{m} \cos \phi + 2B_0\mu \sin \phi - (c_2a^2 - \tilde{c}_2aB_0\tilde{m}) \cos^2 \phi + \tilde{c}_2a2B_0\mu \cos \phi \sin \phi].$$

The vacuum expectation value corresponds to the minimal point of this vacuum energy (2.15) $\phi_0$, which is determined by solving the gap equation,

$$2B_0\tilde{m} \sin \phi_0 - (c_2a^2 - \tilde{c}_2aB_0\tilde{m}) \sin 2\phi_0 = 2B_0\mu \cos \phi_0 + \tilde{c}_2a2B_0\mu \cos 2\phi_0.$$  

We next expand the Lagrangian in terms of the component fields $\pi$ as

$$\mathcal{L}_{\text{LO+SLO}} = \mathcal{L}_{\text{LO+SLO}}^{(2)} + \mathcal{L}_{\text{LO+SLO}}^{(3)} + \cdots,$$

where $\mathcal{L}_{\text{LO+SLO}}^{(n)}$ represents the $O(\pi^n)$ terms in the tree-level Lagrangian. With the components fields $\pi_a$, the $O(\pi^2)$ Lagrangian $\mathcal{L}_{\text{LO+SLO}}^{(2)}$ is given by

$$\mathcal{L}_{\text{LO+SLO}}^{(2)} = \frac{1}{2} \left( \partial_\mu \pi_a \right)^2 + \frac{m_{\pi,a}^2}{2} (\pi_a)^2.$$  

where the tree-level pion mass $m_{\pi,a}^2$ is written as

$$m_{\pi,a}^2 = \begin{cases} 
(m_\pi^\pm)^2 = m_\pi^2 & (a = 1, 2) \\
(m_\pi^0)^2 = m_\pi^2 + \Delta m_\pi^2 & (a = 3) 
\end{cases}.$$  

$$m_\pi^2 = 2B_0m' - 2c_2a^2 \cos^2 \phi_0 + 2\tilde{c}_2a(2B_0m') \cos \phi_0,$$

$$\Delta m_\pi^2 = 2c_2a^2 \sin^2 \phi_0 + 2\tilde{c}_2a(2B_0\mu') \sin \phi_0.$$  

Here $m_\pi \equiv m_\pi^\pm$ ($m_\pi^0$) denotes the charged (neutral) pion mass, and the short-handed notation for mass parameter is given by

$$\begin{pmatrix} m' \\
\mu' \end{pmatrix} = \begin{pmatrix} \cos \phi_0 & \sin \phi_0 \\
-\sin \phi_0 & \cos \phi_0 \end{pmatrix} \begin{pmatrix} \tilde{m} \\
\mu \end{pmatrix}.$$  

Using this notation, the gap equation (2.16) is written as

$$2B_0\mu' = -c_2a^2 \sin 2\phi + \tilde{c}_2a(2B_0m' \sin \phi - 2B_0\mu' \cos \phi).$$

Using this recursively, $a\mu'$ terms is found to be be of higher order, so that we can replace the $\mu'$ term with $a^2$, $am'$ terms.

We now discuss the lattice cutoff $a$ as well as quark masses $\tilde{m}$, $\mu$ dependences of vacuum condensation $\cos \phi_0$ and pion masses. Let us consider the case that the coefficient $\tilde{c}_2 = 0$. In this case, there are two possible phase diagrams[24], depending on the sign of a coefficient
c_2$. Solving the gap equation (2.16) and minimizing the potential energy (2.15), we obtain the dependence of $\cos \phi_0$ on the untwisted quark mass $\tilde{m}$. For $c_2 > 0$, figure 1 shows the form of $\cos \phi_0$ as a function of $2B_0 \tilde{m}/c_2 a^2$ at $2B_0 \mu/c_2 a^2 = 0, 1, 2,$ and 3. Corresponding pion masses are shown in figure 2. In the untwisted theory ($\mu = 0$), there are second order transitions at $2B_0 \tilde{m}/c_2 a^2 = \pm 2$, as shown by the kinks in figure 1 and by the vanishing pion masses in figure 2. The parity-flavor breaking phase, defined by the condition that $\cos \phi_0 \neq \pm 1$, lies between these two second order phase transition points, and two Nambu-Goldstone bosons associated with the flavor breaking appear in this phase[32–34]. Once $2B_0 \mu$ becomes non-zero, however, the transition turns into a crossover, and pion masses always stay non-zero due to the explicit flavor breaking by non-zero $\mu$. For $c_2 > 0$, the charged pion is heavier than the neutral pion, due to the $O(a^2)$ effect. If we change the value of the twisted mass continuously at fixed $|2B_0 \tilde{m}/c_2 a^2| < 2$, there appears the first order phase transition while crossing the parity-breaking phase at $\mu = 0$.

For $c_2 < 0$, figure 3 shows $\cos \phi_0$ and pion masses as a function of $2B_0 \tilde{m}/c_2 a^2$ at the several fixed values of $2B_0 \mu$. Figures 3-a and 3-b show the results for untwisted theory at $\mu = 0$. The condensate $\cos \phi_0$ jumps from $\Sigma_0 = 1$ for $2B_0 \tilde{m} > 0$ to $\Sigma_0 = -1$ for $2B_0 \tilde{m} < 0$. This is the first order transition without the flavor breaking, so that all pions remain

**Figure 1.** Vacuum angle $\cos \phi_0$ as a function of $\tilde{m}$ for $c_2 > 0$ and $2B_0 \mu/c_2 a^2 = 0, 1, 2, 3$.

**Figure 2.** Pion masses as a function of $\tilde{m}$ for $c_2 > 0$ and $2B_0 \mu/c_2 a^2 = 0, 1, 2, 3$.
massive and degenerate. The effect of non-zero twisted mass $\mu$ generates a non-zero value of $\tau^3$ component, $\sin \phi_0 = \sqrt{1 - \cos^2 \phi}$. There still remains the first order phase transition
at which $\sin \phi_0$ flips sign between $\pm (1 - |2B_0\mu/2c_2a^2|)$. The first order phase transition disappears at $|2B_0\mu/2c_2a^2| = 2$ and it turns into a cross-over at $|2B_0\mu/2c_2a^2| > 2$. Due to the explicit flavor breaking, the neutral pion($\pi^0$) is lighter than charged pions($\pi^\pm$).

These qualitative features remain true even for the case that $\tilde{c}_2 \neq 0$. In figure 4(Left) we show results for $c_2 > 0$ at $\mu = 0$. In this case the 2nd order transition points of the parity-flavor breaking phase move toward more negative values as the $\tilde{c}_2 a$ increases. Pion masses are degenerate and their slopes increase (decrease) in the right(left) of the phase transition points in the symmetric phase, while charge pions become massless NG bosons and the neutral pion is massive in the broken phase. On the other hand, in the case that $c_2 < 0$ and $\mu = 0$, the first order phase transition line does not move at all and the pion mass is still degenerate, as shown in figure 4(Right). The slope of both pion masses increase (decrease) in the positive (negative) $\tilde{m}$ region.
2.4 Vertices

Since the twisted mass term $\mu$ explicitly break the parity symmetry, terms including odd powers of pion fields, $\mathcal{L}_{LO+SLO}^{(2n+1)}$ with $n = 1, 2, \ldots$, exist in addition to those with even powers, $\mathcal{L}_{LO+SLO}^{(2n)}$. For $\pi^3$ terms, one finds

$$\mathcal{L}_{LO+SLO}^{(3)} = -\frac{c_0 a}{2 f_0} \sin \phi_0 \pi_3 (\partial_\mu \pi_a)^2$$

$$+ \frac{1}{6 f_0} [2 B_0 \mu' + 8 c_2 a^2 \cos \phi_0 \sin \phi_0 - 4 \tilde{c}_2 a (2 B_0 m' \sin \phi_0 - 2 B_0 \mu' \cos \phi_0)] \pi^2 \pi_3,$$

(2.24)

while for the $O(\pi^4)$ Lagrangian we have

$$\mathcal{L}_{LO+SLO}^{(4)} = \frac{1}{6 f_0^2} \left[ (\pi a \partial_\mu \pi_a)^2 - \left( 1 + \frac{3}{2} c_0 a \cos \phi_0 \right) \pi^2 (\partial_\mu \pi_a)^2 \right]$$

$$- \frac{1}{24 f_0^2} [2 B_0 m' - 8 c_2 a^2 \cos^2 \phi_0 + \tilde{c}_2 a (2 B_0 m' \cos \phi_0) \pi^2]$$

$$- \frac{1}{24 f_0^2} [8 c_2 a^2 \sin^2 \phi_0 + \tilde{c}_2 a (2 B_0 \mu') \sin \phi_0] \pi^2 (\pi_3)^2.$$

(2.25)

2.5 Axial current and “decay constants” in twist base

The quark bilinear operators are defined through the derivatives of the Lagrangian with respect to source terms as

$$S^0 = \bar{\psi} \psi = \frac{\delta}{\delta s} \mathcal{L}, \quad P^a = \bar{\psi} \gamma^a \tau^a \frac{\partial}{\partial \psi} = -i \frac{\delta}{\delta p^a} \mathcal{L},$$

$$V^a_\mu = \bar{\psi} \gamma_\mu \tau^a \frac{\delta}{\delta \psi} = \frac{i}{2} \left( \frac{\delta}{\delta p_\mu} + \frac{\delta}{\delta l_\mu} \right) \mathcal{L}, \quad A^a_\mu = \bar{\psi} \gamma_\mu \gamma^a \frac{\partial}{\partial \psi} = \frac{i}{2} \left( \frac{\delta}{\delta p_\mu} - \frac{\delta}{\delta l_\mu} \right) \mathcal{L}.$$

(2.26)

Applying these derivatives to the tree-level Lagrangian (2.5), we obtain the axial current as

$$A^a_\mu = -\langle \tau^a (\Sigma \partial_\mu \Sigma^\dagger - \Sigma^\dagger \partial_\mu \Sigma) \rangle$$

$$= \begin{cases} 
if_0 \partial_\mu \pi_a \cos \phi_0 & (a = 1, 2) 
if_0 \partial_\mu \pi_a & (a = 3)
\end{cases},$$

(2.28)

(2.29)

where in second line, we expand the $\Sigma$ in terms of pion fields $\pi_a$ up to the $O(\pi)$ order. Since the pseudo scalar “decay constant” $f_{PS}$ in twist base is defined from the expectation value of $A^a_\mu$ between the vacuum and one NG boson state as

$$\langle 0 | A^a_\mu(x) | p_b(p) \rangle = f_{PS}^b p_\mu e^{-ipx} \delta_{ab},$$

(2.30)

we obtain

$$f_{PS}^b = \begin{cases} 
f_0 \cos \phi_0 & (a = 1, 2) 
f_0 & (a = 3)
\end{cases}$$

(2.31)
at this order. Note that this decay constants is in twist base, and we need the vector current for calculate it in physical base.

The $\pi^3$ terms in the axial current $A^a_\mu$, needed at the NLO calculation, is given by

$$ (A_{\mu}^{1,2})^{(3)}_{\text{LO+SLO}} = -if \left[ \frac{2}{3f_0^2} \pi^2 \partial_\mu \pi_a - \frac{1}{3f_0^2} \pi_a \partial_\mu \pi^2 + \frac{c_0 a \cos \phi_0}{2f_0^2} \pi^2 \partial_\mu \pi_a \right] \cos \phi_0$$

$$ - if \frac{c_0 a \sin^2 \phi_0}{f_0^2} \pi^3 (\pi_a \partial_\mu \pi_3 - \pi_3 \partial_\mu \pi_a),$$

$$ (A_{\mu}^{3})^{(3)}_{\text{LO+SLO}} = -if \left[ \frac{2}{3f_0^2} \pi^2 \partial_\mu \pi_a - \frac{1}{3f_0^2} \pi_a \partial_\mu \pi^2 + \frac{c_0 a \cos \phi_0}{2f_0^2} \pi^2 \partial_\mu \pi_a \right].$$

(2.32)

(2.33)

3 "next leading order" analysis

3.1 NLO and NSLO Lagrangian

The NLO and NSLO Lagrangians are given by

$$ \mathcal{L}_{\text{NLO}} = \mathcal{L}_{p^2 m, m^2} + \mathcal{L}_{a p^2 m, a^2 m} \quad \mathcal{L}_{\text{NSLO}} = \mathcal{L}_{ap^2 m, am^2} + \mathcal{L}_{a^2 p^2, a^2 m}. $$

(3.1)

We here do not include the $O(p^4, ap^4)$ terms, since they do not contribute to pion masses and decay constants at this order. The $O(p^2 m, m^2)$ terms are the ordinal NLO terms in continuum ChPT[19-22] and are given by

$$ \mathcal{L}_{p^2 m, m^2} = L_{45} \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle \langle D_\mu \Sigma D_\mu \Sigma^\dagger \rangle - L_{68} \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle^2. $$

(3.2)

In $O(p^2 m, m^2)$ terms, we follow the notation of [28]. The relation of the low energy constants in the notations between [21] l and [28] L is given by

$$ L_{45} = l_4/8, L_{68} = (l_3 + l_4)/16. $$

The $O(ap^2, am^2)$ and $O(a^2 p^2, a^2 m)$ terms describe the lattice artifacts and they are constructed as usual using the spurion analysis as

$$ \mathcal{L}_{ap^2 m, am^2} = \langle D_\mu \Sigma D_\mu \Sigma^\dagger \rangle \left[ V_1 \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle + V_2 \langle \hat{A} \hat{\chi}^\dagger + \hat{\chi} \hat{A}^\dagger \rangle \right] $$

$$ + V_3 \langle D_\mu \Sigma \hat{A}^\dagger + \hat{A} D_\mu \Sigma^\dagger \rangle \langle D_\mu \Sigma \hat{\chi}^\dagger + \hat{\chi} D_\mu \Sigma^\dagger \rangle $$

$$ + V_4 \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle + V_5 \langle \hat{A} \hat{\chi}^\dagger + \hat{\chi} \hat{A}^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle $$

$$ + V_6 \langle \hat{A} \hat{\chi}^\dagger + \hat{\chi} \hat{A}^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle $$

$$ + \tilde{V}_{23} \langle D_\mu \Sigma \hat{A}^\dagger D_\mu \Sigma \hat{\chi}^\dagger + D_\mu \Sigma \hat{\chi} D_\mu \Sigma^\dagger \hat{A} \rangle + \tilde{V}_{3a} \langle D^2 \Sigma \hat{A}^\dagger + \hat{A} D^2 \Sigma^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle $$

$$ + \tilde{V}_{3m} \langle D^2 \Sigma \hat{\chi}^\dagger + \hat{\chi} D^2 \Sigma^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle, $$

(3.3)

$$ \mathcal{L}_{a^2 p^2, a^2 m} = \langle D_\mu \Sigma D_\mu \Sigma^\dagger \rangle \left[ X_1 \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma^\dagger \rangle^2 + X_2 \langle \hat{A} \hat{\chi}^\dagger + \hat{\chi} \hat{A}^\dagger \rangle^2 \right] $$

$$ + X_3 \langle \Sigma \hat{A}^\dagger + \hat{A} \Sigma^\dagger \rangle^2 \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle + X_5 \langle \hat{A} \hat{\chi}^\dagger + \hat{\chi} \hat{A}^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle $$

$$ + X_6 \langle \hat{A} \hat{\chi}^\dagger + \hat{\chi} \hat{A}^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle $$

$$ + \tilde{X}_{23} \langle D_\mu \Sigma \hat{A}^\dagger D_\mu \Sigma \hat{\chi}^\dagger + D_\mu \Sigma \hat{\chi} D_\mu \Sigma^\dagger \hat{A} \rangle $$

$$ + \tilde{X}_{3a} \langle D^2 \Sigma \hat{A}^\dagger + \hat{A} D^2 \Sigma^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle $$

$$ + \tilde{X}_{3m} \langle D^2 \Sigma \hat{\chi}^\dagger + \hat{\chi} D^2 \Sigma^\dagger \rangle \langle \Sigma \hat{\chi}^\dagger + \hat{\chi} \Sigma^\dagger \rangle, $$

(3.4)
where the $V_i(i = 1, \ldots, 6)$, $\tilde{V}_i(i = 23, 3a, 3m)$, $X_i(i = 1, \ldots, 6)$, and $\tilde{X}_i(i = 23, 3)$ are additional low energy constants.

Here we introduce the nineteen parameters in NLO Lagrangian but our aim is not to determine these parameters. We instead investigate quark and lattice spacing dependences of physical observables using these parameters. In the physical observable, these parameters always appear as the same linear combinations, so that the number of independent fit parameters are much smaller.

Expanding $\Sigma$ in terms of component fields $\pi$, $O(\pi)$ and $O(\pi^2)$ terms of NLO+NSLO Lagrangian $\mathcal{L}^{(1)}_{\text{NLO+NSLO}}$ and $\mathcal{L}^{(2)}_{\text{NLO+NSLO}}$ are given by

\[
\mathcal{L}^{(1)}_{\text{NLO+NSLO}} = C^1_{\text{NLO}}\pi^2, \quad \text{(3.5)}
\]

\[
\mathcal{L}^{(2)}_{\text{NLO+NSLO}} = \frac{1}{2} \left( C^{2p,a}_{\text{NLO}}(\partial_\mu \pi_a)^2 + C^{2a}_{\text{NLO}}\pi^2 \right). \quad \text{(3.6)}
\]

The coefficients $C_{\text{NLO}}$'s are given by

\[
C^1_{\text{NLO}} = \frac{8}{f_0} \left[ -(2B_0m')(2B_0\mu')4L_{68} - a(2B_0m')^2(8V'_4 + V'_5) \sin \phi_0 
+ a(2B_0m')(2B_0\mu')(16V'_4 + 2V'_6) \cos \phi_0 - a(2B_0\mu')^2(V'_5 + 2V'_6) \sin \phi_0 
- a^2(2B_0m')(8X'_4 + X'_6) \sin 2\phi_0 
+ a^2(2B_0\mu')(4X'_4 + X'_5 + X'_6) + (4X'_4 - X'_6) \cos 2\phi_0 \right], \quad \text{(3.7)}
\]

\[
C^{2p,a}_{\text{NLO}} = \frac{16}{f_0} \left[ 2B_0m'L_{45} + a \left\{ 2B_0m'(4V'_4 + V'_2 - V'_2/2) \cos \phi_0 - 2B_0\mu'(V'_2 - V'_2/2) \sin \phi_0 \right. 
+ a^2 \left\{ (2X'_4 + X'_2/2 - X'_2/2) / 2 \right. 
+ a \left\{ (2B_0\mu')(2V'_3 + V'_3 - 2V'_3a - 2V'_3a) / 2 \right. 
- a^2(X'_3 + X'_3/2 - X'_3) \sin \phi_0 
- a^2(X'_3 + X'_3/2 - X'_3) \sin \phi_0 \right. \right\} \delta_{a3} \right\}, \quad \text{(3.8)}
\]

\[
C^{2a}_{\text{NLO}} = -\frac{16}{f_0} \left[ -(2B_0m')^22L_{68} + a \left\{ (2B_0m')^2(12V'_4 + V'_2/2 + V'_6) \cos \phi_0 
- (2B_0m')(2B_0\mu')V'_3 \sin \phi_0 + (2B_0\mu')V'_3/2 \cos \phi_0 \right. 
+ a^2(2B_0m') \left\{ (6X'_4 + X'_2/2 + X'_2/2) + (6X'_4 + X'_2/2)/2 \cos 2\phi_0 - a^2(2B_0\mu')X'_2/2 \sin 2\phi_0 \right. 
+ \left\{ (2B_0\mu')^22L_{68} - a8V'_4 \left\{ (2B_0\mu')^2 \cos \phi_0 + 2(2B_0m')/(2B_0\mu') \sin \phi_0 \right. 
- 4X'_4a^2 \left\{ (2B_0m')(1 - \cos 2\phi) - 2(2B_0\mu') \sin 2\phi_0 \right. \right\} \delta_{a3} \right\}, \quad \text{(3.9)}
\]

where we use the normalized coefficients $V'_i = 2W_0V_i$, $\tilde{V}'_i = 2W_0\tilde{V}_i$, $X'_i = (2W_0)^2X_i$ and $\tilde{X}'_i = (2W_0)^2\tilde{X}_i$. Note again that, since the twisted mass term explicitly breaks the parity symmetry, odd power terms appear. In particular, the $O(\pi)$ terms, together with 1-loop contributions, must be canceled by the redefinition of the vacuum angle $\phi_0$ as

\[
\phi_R = \phi_0 + \Delta \phi, \quad \text{(3.10)}
\]

where $\Delta \phi$ is the NLO contribution.
3.2 The vacuum expectation value and pion masses

Due to the presence of three-point vertices (2.24), the tadpole diagrams $\mathcal{L}^{(1)}_{1\text{loop}}$ contribute to vacuum expectation value at 1-loop,

$$\mathcal{L}^{(1)}_{1\text{loop}} = \frac{1}{f_0} (A_\pm I_\pm + A_0 I_0) \pi_3,$$

$$A_\pm = c_2 a^2 \sin 2\phi_0 + (c_0 - \tilde{c}_2) a (2B_0 m') \sin \phi_0,$$

$$A_0 = \frac{3}{2} c_2 a^2 \sin 2\phi_0 + \frac{1}{2} (c_0 - 3\tilde{c}_2) a (2B_0 m') \sin \phi_0,$$

where $I_a$ is given by

$$I_a = \int \frac{d^4 p}{(2\pi)^4} \frac{1}{p^2 + (m_\pi^0)^2}.$$

See the detail of the calculation in Appendix A. This contribution diverges and therefore must be renormalized by $O(\pi)$ terms in $\mathcal{L}^{(1)}_{\text{NLO+NSLO}}$, together with the redefinition of the vacuum angle $\phi_R$. Explicitly the renormalization condition becomes

$$\frac{\partial}{\partial \phi} \mathcal{L}^{(1)}_{\text{LO+SLO}} \bigg|_{\phi=\phi_0} \Delta \phi + \mathcal{L}^{(1)}_{1\text{loop}} + \mathcal{L}^{(1)}_{\text{NLO+NSLO}} = 0,$$

which leads to the renormalized vacuum angle $\phi_R = \phi_0 + \Delta \phi$ as

$$\phi_R = \phi_0 - \frac{1}{(m_\pi^0)^2} \left[ A_\pm L_\pm + A_0 L_0 - \frac{8}{f_0^2} \left\{ a(2B_0 m')^2 C_1 + a^2 (2B_0 m') C_2 \right\} \right].$$

The first term is the tree-level contribution for vacuum angle, while the second and third terms are chiral logarithm contributions from the charged and neutral pion, respectively. The last two terms are the polynomial contributions from the NLO Lagrangian. The chiral logarithm for the pion loop is defined by

$$L_a = \frac{(m_\pi^a)^2}{16\pi^2 f_0^2} \log \left( \frac{m_\pi^a}{\mu_{\text{CHPT}}} \right)^2,$$

and the coefficients of the chiral logarithm, $A_a^n$, are given in eqs.(3.12) and (3.13). The coefficients of the NLO polynomial term, $C_1$ and $C_2$, are some combinations of the renormalized NLO low energy constants.

In the similar way, we obtain the result for the pion masses as

$$(m_\pi^a)^2_{\text{NLO}} = (m_\pi^a)^2_{\text{LO}} \bigg|_{\phi_0 \to \phi_0 + \Delta \phi}$$

$$+ \sum_{b=\pm,0} \left( m_\pi^2 B_b^a + a^2 Q_b^a \right) L_b$$

$$- \frac{16}{f_0^2} \left\{ E_1^a (2B_0 m')^2 + E_2^a a (2B_0 m')^2 + E_3^a a^2 (2B_0 m') \right\}.$$

This is one of the main results of this paper. The first term is the tree-level form for pion mass but with the vacuum angle obtained at NLO. The second line represents the chiral
logarithm while the polynomial terms for the NLO Lagrangian are given in the last line. Each coefficient of the chiral logarithms is given by

\begin{align}
B^\pm_\pm &= a(2c_0 - 4\tilde{c}_2) \cos \phi_0, & B^0_\pm &= \frac{1}{2} + a(c_0 - \tilde{c}_2) \cos \phi_0, \\
B^0_\pm &= 1 + a(2c_0 - 2\tilde{c}_2) \cos \phi_0, & B^0_0 &= \frac{1}{2} + a(c_0 - 3\tilde{c}_2) \cos \phi_0, \\
Q^\pm_\pm &= 4c_2 \cos^2 \phi_0, & Q^0_0 &= c_2 \cos^2 \phi_0, \\
Q^0_\pm &= 2c_2 \cos^2 \phi_0, & Q^0_0 &= c_2(3 \cos^2 \phi_0 - 4 \sin^2 \phi_0).
\end{align}

and coefficients of polynomial terms \(E_i(i = 1, 2, 3)\) are combinations of the renormalized NLO low energy constants. Our results have not only the same pion mass contributions for the chiral logarithms in [31], but also the additional \(O(\alpha m)\) terms from SLO. Note that \(O(1)\) terms in eqs. (3.19) and (3.20) of course agree with continuum results [19, 20].

3.3 ”Decay constants”

Let us consider the NLO axial currents. Using eq. (2.27), we obtain the ”NLO” (=NLO+NSLO) terms of the axial currents for \(a = 1, 2,\)

\begin{equation}
(A^a_\mu)_{\text{NLO}} = \frac{16i}{f_0} \partial_\mu \pi_a \left\{ \left( (2B_0m') L_{45} + a(2B_0m')(4V'_1 + V'_2 - \tilde{V}'_{23}/2 - 2\tilde{V}'_{3m}) \cos \phi_0 \\
- a(2B_0\mu')(V'_2 - \tilde{V}'_{23}/2 - 2\tilde{V}'_{3m}) \sin \phi_0 \\
+ a^2(2X'_1 + X'_2/2 - X'_3/2 - 2X'_3 + 2X'_1 \cos 2\phi_0) \right) \cos \phi_0 \\
- a(2B_0m')2\tilde{V}'_{3a} \right\},
\end{equation}

and for \(a = 3,\)

\begin{equation}
(A^3_\mu)_{\text{NLO}} = \frac{16i}{f_0} \partial_\mu \pi_3 \left\{ \left( (2B_0m') L_{45} + a(2B_0m')(4V'_1 + V'_2 - \tilde{V}'_{23}/2 - 2\tilde{V}'_{3a} - 2\tilde{V}'_{3m}) \cos \phi_0 \\
- a(2B_0\mu')(V'_2 + 2V'_3 + \tilde{V}'_{23}/2) \sin \phi_0 \\
+ a^2\left( 2X'_1 + X'_2/2 + X'_3 - X'_3 + (2X'_1 - X'_3 - \tilde{X}'_{23}/2 - \tilde{X}'_{3}) \cos 2\phi_0 \right) \right\}.
\end{equation}

From these results, we calculate the “decay constants” for the pseudo-scalar meson at ”NLO”, which are given by

\begin{equation}
f^{\phi S, \text{NLO}} = f^{\phi S, \text{LO}} \bigg|_{\phi = \phi_0 + \Delta \phi} + f^{\phi S, \text{LO}} \left( \sum_{b = \pm, 0} F_b^a L_b \\
+ \frac{16}{f_0} \left\{ (2B_0m') H^a_1 + a(2B_0m') H^a_2 + a^2 H^a_3 \right\} \right) \\
+ \Delta f^\pm (1 - \delta_{3a}).
\end{equation}

This is also one of the main results of this paper. The first term is the tree-level contribution, which includes the vacuum renormalization effects at ”NLO”. The second term represents the chiral logarithms and the polynomial terms for the NLO Lagrangian are in
the second line. In addition, the “decay constant” for the charged pseudo scalar has the additive renormalization term in the last term. Coefficients of the chiral logarithms are given by

\[ F_0^\pm = -\frac{1}{2} (1 + \frac{5}{2} c_0 a \cos \phi_0), \quad F_0^0 = -\frac{1}{4} c_0 a \cos \phi_0, \]

and the formula for the coefficients of the renormalization terms \( H_1(i = 1, 2, 3) \) and \( \Delta f_\pm \) are given in Appendix A. Note again that \( O(1) \) terms in eqs. (3.26) and (3.27) agree with continuum results [19, 20].

3.4 Consistency

Divergences generated by 1-loop contributions must be removed by the "NLO" terms. For this purpose we define the renormalized NLO and NSLO low energy constants as

\[ L_i = L_i^r(\mu_{\chi PT}) + \frac{l_i}{32\pi^2} R, \]
\[ V_i' = V_i^r(\mu_{\chi PT}) + \frac{v_i}{32\pi^2} R, \]
\[ X_i' = X_i^r(\mu_{\chi PT}) + \frac{x_i}{32\pi^2} R, \]

where \( l_i, v_i, x_i \) are renormalize parameters, the argument \( \mu_{\chi PT} \) represents the renormalized scale and \( R = O(1/\epsilon) \) is introduce to cancel 1-loop divergences in the dimensional regularization. We give the detail formulation in appendix A.

The renormalization conditions for the vacuum expectation value leads to

\[ 8(8v_4 + v_5 + 4l_{68}\tilde{c}_2) = 3c_0 - 5\tilde{c}_2, \]
\[ 8(8x_4 + x_6 - 4l_{68}c_2) = 5c_2. \]

In order to cancel the divergences in 1-loop diagrams for pion masses, coefficients should satisfy the following conditions.

\[ 16(l_{45} - 2l_{68}) = 1, \]
\[ 16(12v_4 + v_5/2 + v_6 + 4v_1 + v_2 - \tilde{v}_{23}/2 + 2\tilde{c}_2l_{45}) = -6\tilde{c}_2 + 6c_0, \]
\[ 16(6x_4 + x_5/2 + x_6/2 + 2x_1 + x_2/2 - \tilde{x}_{23}/2 - c_2l_{45}) = 4c_2, \]
\[ 16(6x_4 + x_6/2 + 2x_1 - c_2l_{45}) = 2c_2, \]
\[ 16(4x_4 - x_3 - \tilde{x}_{23}/2 + \tilde{x}_3 - c_2l_{45}) = -6c_2. \]
Similarly from the decay constant, we have

\[ 4l_{45} = 1, \]  
\[ 16\tilde{v}_{3a} = c_0, \]  
\[ 8(2v_1 + v_2/2 - \tilde{v}_{23}/4 - 2\tilde{v}_{3m}) = 2\tilde{c}_2 + 7c_0/4, \]  
\[ 16x_1 = -3c_2, \]  
\[ 16(x_2/4 - \tilde{x}_{23}/4 - 2\tilde{x}_3) = 2c_2, \]  
\[ 16(x_3/2 + \tilde{x}_{23}/4 + 3\tilde{x}_3/2) = -c_2. \]  

A solutions to these conditions can be obtained as

\[ l_{45} = \frac{1}{4}, \quad l_{68} = \frac{3}{32}, \]  
\[ x_1 = -\frac{3}{16}c_2, \]  
\[ x_2 - \tilde{x}_{23} = -c_2, \]  
\[ x_3 + \tilde{x}_{23}/2 = \frac{7}{16}c_2, \]  
\[ x_4 = \frac{1}{8}c_2, \quad x_5 = \frac{5}{4}c_2, \quad x_6 = 0, \]  
\[ \tilde{x}_3 = -\frac{3}{16}c_2. \]  

\[ 16v_1 + 4v_2 - 2\tilde{v}_{23} - 16\tilde{v}_{3m} = \frac{7}{4}c_0 + 2\tilde{c}_2, \]  
\[ 64v_4 + 8v_5 = 3c_0 - 8\tilde{c}_2, \]  
\[ 64v_4 + 8v_6 + 32\tilde{v}_{3m} = -2c_0 - 7\tilde{c}_2, \]  
\[ \tilde{v}_{3a} = \frac{c_0}{16}. \]

Note that results of \( l_{45} \) and \( l_{68} \) agree with the continuum ChPT [19, 20].

### 4 maximal twist

One of the advantage of the tmlQCD is the automatic \( O(a) \) improvement at maximal twist [3, 5]. The ETMC employs the PCAC quark mass to determine the maximal twist in their simulation,

\[
m_{PCAC}(\mu) = \frac{\sum_x \langle \partial_t A_0^a(x,t)P^a(0) \rangle}{2 \sum_x \langle P^a(x,t)P^a(0) \rangle} = 0 \quad (a = 1, 2). \]  

The above condition must be satisfied by tuning the untwisted mass \( m \) at each twisted mass \( \mu \). The untwisted mass which realizes the maximal twist condition is called the critical untwisted quark mass. This definition for the maximal twist is called the PCAC definition. In order to reduce the numerical cost, however, \( m \) for the maximal twist is defined at \( \mu_{min} \), the minimal value of the twisted mass employed in the simulations, such that \( m_{PCAC}(\mu_{min}) = 0 \). This is called as the fixed PCAC definition. In figure 5, both definitions are schematically drawn for \( c_2 < 0 \). In this section, we investigate the difference between two maximal twist conditions, using our WChPT analysis.
Figure 5. The chiral limit for $c_2 < 0$, where the first order phase transition line exists. The untwisted mass $m$ corresponding to the maximal twist depends on twisted mass $\mu$ in the PCAC definition, while $m$ is constant in the fixed PCAC definition.

### 4.1 PCAC quark mass

The PCAC quark mass can be written in the WChPT as

$$m_{\text{PCAC}} = \frac{f_P m_\pi^2}{2Z(0)},$$

(4.2)

where $f_P, m_\pi$ denote the decay constant and mass for the charged pion, and we define $Z(p)$ as

$$\langle 0 | P^a(x) | \pi(p) \rangle = iZ(p)e^{-ipx}.$$  

(4.3)

At "NLO", we have

$$f_{PS,NLO} = f_{PS,LO}\bigg|_{\phi_0 \to \phi_0 + \Delta \phi} (1 + \Delta f) + \Delta f_\pm,$$

(4.4)

$$m_{\pi,NLO}^2 = m_{\pi,LO}^2\bigg|_{\phi_0 \to \phi_0 + \Delta \phi} (1 + \Delta m),$$

(4.5)

$$Z_{NLO}(p) = Z_{LO}(p)\bigg|_{\phi_0 \to \phi_0 + \Delta \phi} (1 + \Delta Z),$$

(4.6)

where the $\Delta_i(i = f, m, Z)$ denote the NLO contribution corresponding to $f_P, m_\pi$ and $Z(p)$. The PCAC quark mass at the NLO is given by

$$m_{\text{PCAC,NLO}} = m_{\text{PCAC,LO}}\bigg|_{\phi_0 \to \phi_0 + \Delta \phi} (1 + \Delta f + \Delta m - \Delta Z),$$

$$+ \frac{m_{\pi,LO}^2}{2Z_{LO}(0)}\bigg|_{\phi_0 \to \phi_0 + \Delta \phi} \Delta f_\pm$$

(4.7)

where

$$m_{\text{PCAC,LO}}\bigg|_{\phi_0 \to \phi_0 + \Delta \phi} = \frac{m_{\pi,LO}^2}{2B_0(1 + c_2 \cos(\phi_0 + \Delta \phi))} \cos(\phi_0 + \Delta \phi).$$

(4.8)
4.2 PCAC definition

The maximal twist condition in the PCAC definition leads to

\[
\cos \phi_0 = O(am') = O(a\mu). \tag{4.9}
\]

This condition simplify the gap equation (2.16), and the critical untwisted quark mass as a function of the twisted mass \( \mu \) is given by

\[
2B_0\bar{m} = -\tilde{c}_2 a 2B_0 \mu + O(a\mu^2). \tag{4.10}
\]

Eq. (4.10) shows that the critical untwisted quark mass \( \bar{m} \) depends linearly on the twisted quark mass \( \mu \). Using eqs. (4.9) and (4.10), the charged pion mass at the NLO is given by

\[
\left( m_\pi^{\pm} \right)^2_{\text{NLO}} = \left( m_\pi^{\pm} \right)^2_{\text{LO}} \left[ 1 + \frac{1}{2} L_0 - \frac{16}{f_0^2} \left( (m_\pi^{\pm})^2 L_c^r + a^2 X_c^r \right) \right], \tag{4.11}
\]

where, the NLO polynomial coefficients \( L_c^r \) and \( X_c^r \) are given by

\[
L_c^r = L_{55}^r - 2L_{68}^r, \tag{4.12}
\]

\[
X_c^r = (X_5^r/2 + X_2^r/2 - \tilde{X}_{23}^r/2), \tag{4.13}
\]

the chiral logarithm \( L_0 \) is defined by eq. (3.17), and the LO pion masses are simplified as

\[
\left( m_\pi^{\pm} \right)^2 = 2B_0 \mu, \tag{4.14}
\]

\[
\left( m_\pi^0 \right)^2 = 2B_0 \mu + a^2 (2c_2 + 2\tilde{c}_2 2B_0 \mu). \tag{4.15}
\]

Eq. (4.11) shows that the charged pion mass is \( O(a) \) improved: the lattice spacing corrections start at \( O(a^2) \). It is important to note that the charged pion mass at the NLO contains the chiral logarithm only from the neutral pion loops but not from the charged pion loops at the maximal twist, as in the continuum ChPT.

Note that the maximal twist by the PCAC quark mass and the charged axial currents give the same constraint for physical observable in this WChPT analysis.

4.3 Fixed PCAC definition

For the fixed PCAC definition, the maximal twist condition and the critical untwisted quark mass are given by

\[
\cos \phi_0 = O(a\mu_{\text{min}}) \tag{4.16}
\]

\[
2B_0\bar{m} = -\tilde{c}_2 a 2B_0 \mu_{\text{min}} + O(a\mu_{\text{min}}^2), \tag{4.17}
\]

where \( \mu_{\text{min}} \) denotes the minimal value of the twisted mass, used for the fixed PCAC definition. Eq. (4.17) shows that the critical untwisted quark mass is constant and does not depend on the twisted mass \( \mu \). Using eqs. (4.16) and (4.17), the charged pion mass at the NLO is given by

\[
\left( m_\pi^{\pm} \right)^2_{\text{NLO}} = \left( m_\pi^{\pm} \right)^2_{\text{LO}} \bigg|_{\phi_0 \to \phi_0 + \Delta \phi} \left[ 1 + \frac{1}{2} L_0 - \frac{16}{f_0^2} \left( (m_\pi^{\pm})^2 L_c^r + a^2 X_c^r \right) \right], \tag{4.18}
\]

\[
\]
where the coefficients $L^r_C$ and $X^r_c$ are defined in eqs. (4.12) and (4.13) and the pion masses are given by

$$\left(\frac{m_{\pi^+}}{m_{\pi^-}}\right)^2_{\phi_0 \to \phi_0 + \Delta \phi} = 2B_0 \mu, \quad (4.19)$$

$$\left(\frac{m_{\pi^0}}{m_{\pi^-}}\right)^2_{\phi_0 \to \phi_0 + \Delta \phi} = 2B_0 \mu + a^2(2c_2 + 2\tilde{c}^2 + 2B_0 \mu_{\text{min}}). \quad (4.20)$$

The charged pion mass (4.18) for the fixed PCAC definition has the same functional form as (4.11) for the PCAC definition. The fixed critical untwisted quark mass effect, however, appears in the $O(a^2)$ terms for the LO neutral pion mass.

It turns out that the charged pion mass is $O(a)$ improved for both PCAC and fixed PCAC definitions, and that the difference between these two definitions appears as the $O(a^2)$ effects. In addition, contrary to the case at the non-maximal twist where the chiral logarithm of the charged pion mass contains effects from both neutral and charged pion loops due to the lattice artifact, it contains only the effect from the neutral pion loop for both definitions as in the continuum ChPT.

5 Conclusions

In this paper, we construct the Wilson chiral perturbation theory for the $N_f = 2$ twisted mass lattice QCD at the small quark mass regime such that $m_q \sim a^2 \Lambda^3$. In order to consider such a regime, we include $O(a^2)$ and $O(am)$ terms at the tree level as the sub-leading order Lagrangian, which induce the non-trivial phase structure and pion mass splitting at the tree-level. Using this effective theory, we investigate the pion mass and decay constant as a function of not only the twisted quark mass but also the lattice cutoff at the next leading order. Our main results are given in Eqs. (3.18) and (3.25). We also confirm that divergences from 1-loop contributions can be consistently removed by the next leading order Lagrangian.

For the comparison of our results with data obtained by numerical simulations, we derive the twisted quark mass dependence of the charged pion mass at the maximal twist. As the definition of the maximal twist, we adopt two different definitions, the PCAS and the fixed PCAC definition, the latter of which is actually employed in the simulations. We have found that the charged pion mass is $O(a)$ improved, so that lattice spacing corrections start at $O(a^2)$ for both two definitions, and that the difference between the two definitions appears as $O(a^2)$ effects. In addition, it should be noted that the chiral logarithm in the charged pion mass comes from the neutral pion loop only, as in the continuum ChPT.

Acknowledgements

We thank for the important comments form Oliver Bar. This work is supported in part by the Grant-in-Aid of MEXT(No. 20340047) and by Grant-in-Aid for Scientific Research on Innovative Areas (No 2004: 20105001, 20105003).
A detail of calculations

A.1 NLO terms

From the spurion analysis, $O(ap^2, am^2)$ terms are given by

\[
O(ap^2 m) \quad \langle \Sigma \hat{A} \dagger + A\Sigma \dagger \rangle \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle \langle D_{\mu} \Sigma D_{\mu} \Sigma \dagger \rangle, \langle \hat{A} \hat{\chi} \dagger + \hat{\chi} \hat{A} \rangle \langle D_{\mu} \Sigma D_{\mu} \Sigma \dagger \rangle, \langle D_{\mu} \Sigma \hat{A} \dagger + A\Sigma \dagger \rangle \langle D_{\mu} \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle, \langle D_{\mu} \Sigma \hat{A} \dagger D_{\mu} \Sigma \dagger + D_{\mu} \Sigma \dagger \hat{A} D_{\mu} \Sigma \dagger \rangle, \langle D^2 \Sigma \hat{A} \dagger + \hat{A} D^2 \Sigma \dagger \rangle \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle, \langle D^2 \Sigma \hat{\chi} \dagger + \hat{\chi} D^2 \Sigma \dagger \rangle \langle \Sigma \hat{A} \dagger + \hat{A} \Sigma \dagger \rangle \rangle_{s_1}
\]

\[
O(2p m^2) \quad \langle \Sigma \hat{A} \dagger + A\Sigma \dagger \rangle \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle, \langle \hat{A} \hat{\chi} \dagger + \hat{\chi} \hat{A} \rangle \langle \Sigma \hat{A} \dagger + \hat{A} \Sigma \dagger \rangle, \langle \hat{A} \hat{\chi} \dagger + \hat{\chi} \hat{A} \rangle \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle.
\]

(A.1)

Here $S_1$, $S_2$, and $S_3$ terms come from the non-commutativity between the covariant derivative $D_{\mu}$ and mass term $\chi$. Therefore they vanish for the degenerated $N_f = 2$ (untwisted) Wilson fermion case. In the $l_\mu = r_\mu = 0$ limit, these terms can be expressed by other terms,

\[
S_1 \rightarrow \frac{1}{2} \left( \langle \partial_{\mu} \Sigma \hat{A} \dagger + A\partial_{\mu} \Sigma \dagger \rangle \langle \partial_{\mu} \Sigma \hat{\chi} \dagger + \hat{\chi} \partial_{\mu} \Sigma \dagger \rangle - \langle \hat{A} \hat{\chi} \dagger + \hat{\chi} \hat{A} \rangle \langle \partial_{\mu} \Sigma \partial_{\mu} \Sigma \dagger \rangle \right),
\]

(A.3)

\[
S_2 \rightarrow - \langle \partial_{\mu} \Sigma \hat{A} \dagger + A\partial_{\mu} \Sigma \dagger \rangle \langle \partial_{\mu} \Sigma \hat{\chi} \dagger + \hat{\chi} \partial_{\mu} \Sigma \dagger \rangle,
\]

(A.4)

\[
S_3 \rightarrow - \langle \partial_{\mu} \Sigma \hat{A} \dagger + A\partial_{\mu} \Sigma \dagger \rangle \langle \partial_{\mu} \Sigma \hat{\chi} \dagger + \hat{\chi} \partial_{\mu} \Sigma \dagger \rangle.
\]

(A.5)

In a similar way to $O(ap^2 m, am^2)$ terms, $O(a^2 p^2, a^2 m)$ terms are given by

\[
O(ap^2 m) \quad \langle \Sigma \hat{A} \dagger + A\Sigma \dagger \rangle^2 \langle D_{\mu} \Sigma D_{\mu} \Sigma \dagger \rangle, \langle \hat{A} \hat{A} \rangle \langle D_{\mu} \Sigma D_{\mu} \Sigma \dagger \rangle, \langle D_{\mu} \Sigma \hat{A} \dagger + A\Sigma \dagger \rangle^2, \langle D_{\mu} \Sigma \hat{A} \dagger D_{\mu} \Sigma \dagger + D_{\mu} \Sigma \dagger \hat{A} D_{\mu} \Sigma \dagger \rangle, \langle D^2 \Sigma \hat{A} \dagger + \hat{A} D^2 \Sigma \dagger \rangle \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle, \langle D^2 \Sigma \hat{\chi} \dagger + \hat{\chi} D^2 \Sigma \dagger \rangle \langle \Sigma \hat{A} \dagger + \hat{A} \Sigma \dagger \rangle \rangle_{s_4}
\]

\[
O(2m^2) \quad \langle \Sigma \hat{A} \dagger + \hat{A} \Sigma \dagger \rangle^2 \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle, \langle \hat{A} \hat{A} \rangle \langle \Sigma \hat{\chi} \dagger + \hat{\chi} \Sigma \dagger \rangle, \langle \hat{A} \hat{\chi} \dagger + \hat{\chi} \hat{A} \rangle \langle \Sigma \hat{A} \dagger + \hat{A} \Sigma \dagger \rangle,
\]

(A.6)

where $S_4$, $S_5$ terms vanish in the untwisted theory. In the $l_\mu = r_\mu = 0$ limit, they become

\[
S_4 \rightarrow \frac{1}{2} \langle \partial_{\mu} \Sigma \hat{A} \dagger + \hat{A} \partial_{\mu} \Sigma \dagger \rangle \langle \partial_{\mu} \Sigma \hat{\chi} \dagger + \hat{\chi} \partial_{\mu} \Sigma \dagger \rangle - \langle \hat{A} \hat{A} \rangle \langle \partial_{\mu} \Sigma \partial_{\mu} \Sigma \dagger \rangle,
\]

(A.8)

\[
S_5 \rightarrow - \langle \partial_{\mu} \Sigma \hat{A} \dagger + \hat{A} \partial_{\mu} \Sigma \dagger \rangle^2.
\]

(A.9)

A.2 Renormalization for a vacuum expectation value

Since there exist three point functions in the Lagrangian (2.24), we have one loop diagrams for a vacuum expectation value. We obtain

\[
\text{vacuum expectation value} = \frac{a^2 B_0 m'(2c_0 - 2\tilde{c} \tilde{c}) \sin \phi_0 + 2c_2 a^2 \sin 2\phi_0}{2f_0} I_{\pm},
\]

(A.10)

\[
\text{vacuum expectation value} = \frac{a^2 B_0 m'(c_0 - 3\tilde{c} \tilde{c}) \sin \phi_0 + 3c_2 a^2 \sin 2\phi_0}{2f_0} I_0,
\]

(A.11)
where the single(double) line represents the charged(neutral) pion, \( I_{\pm/0} \) denotes a contribution from a charged or neutral pion loop, which is given by
\[
I_{\pm/0} = \int \frac{d^4 p}{(2\pi)^2} \frac{1}{p^2 + (m_{\pm/0}^2)^2} = \frac{\langle m_{\pm/0}^2 \rangle}{16\pi^2} \left[ -\frac{2}{\epsilon} + \gamma_E - 1 + \log \left( \frac{m_{\pm/0}^2}{4\pi} \right) \right].
\] (A.12)
where \( \epsilon \) is the dimensional regulator and \( \gamma_E \) is the Euler-Mascheroni constant. One-loop effects to the vacuum expectation value are summarized as
\[
L^{(1)}_{\text{LO+SLO}} = \frac{1}{f_0} (A_{\pm} I_{\pm} + A_0 I_0) \pi_3,
\] (A.13)
\[
A_{\pm} = c_2 a_2^2 \sin 2\phi_0 + (c_0 - \tilde{c}_2) a (2B_0 m') \sin \phi_0,
\] (A.14)
\[
A_0 = \frac{3}{2} c_2 a_2^2 \sin 2\phi_0 + \frac{1}{2} (c_0 - 3\tilde{c}_2) a (2B_0 m') \sin \phi_0.
\] (A.15)

Using the gap equation (2.23), on the other hand, contributions from \( L_{\text{NLO+NSLO}} \) are given by
\[
L^{(1)}_{\text{NLO+NSLO}} = -\frac{8}{f_0} \left[ \frac{a (2B_0 m')^2}{8V_4 + V_5 + 4\tilde{c}_2 L_{68}} \sin \phi_0 \right.
\]
\[
\left. + a^2 (2B_0 m') (8X_4 + X_6 - 4\tilde{c}_2 L_{68}) \sin 2\phi_0 \right] \pi_3.
\] (A.16)

In order to cancel divergences from the 1-loop integral, low energy constants in \( L_{\text{NLO+NSLO}} \) need to be renormalized, and renormalized low energy constants are given by
\[
L_i = L_i'(\mu_{\text{ChPT}}) + \frac{L_i}{32\pi^2} R,
\] (A.17)
\[
V_i' = V_i'(\mu_{\text{ChPT}}) + \frac{V_i}{32\pi^2} R,
\] (A.18)
\[
X_i' = X_i'(\mu_{\text{ChPT}}) + \frac{X_i}{32\pi^2} R,
\] (A.19)
where the argument \( \mu_{\text{ChPT}} \) is a renormalization scale and \( R \) is defined by
\[
R = -\frac{2}{\epsilon} - \log(4\pi) + \gamma_E - 1,
\] (A.20)
which cancels the 1-loop divergence in dimensional regularization. To renormalize the vacuum expectation value correctly, we need renormalization conditions, eqs. (3.31) and (3.32), and the renormalized Lagrangian for \( \pi \) is written as
\[
L^{(1)}_R = \frac{\partial}{\partial \phi} L^{(1)}_{\text{LO+SLO}} \bigg|_{\phi=\phi_0} \Delta \phi + L^{(1)}_{\text{1loop}} + L^{(1)}_{\text{NLO+NSLO}}
\]
\[
= \left[ \langle m_{\pi}^0 \rangle f_0 \Delta \phi + f_0 (A_{\pm} I_{\pm} + A_0 I_0) - \frac{8}{f_0} \left\{ a (2B_0 m')^2 C_1 + a^2 (2B_0 m') C_2 \right\} \right] \pi_3,
\] (A.21)
where the low energy coefficients \( C_1, C_2 \) are given as,
\[
C_1 = (8V_4' + V_5' + 4\tilde{c}_2 L_{68}') \sin \phi_0,
\] (A.22)
\[
C_2 = (8X_4' + X_6' - 4\tilde{c}_2 L_{68}') \sin 2\phi_0.
\] (A.23)
A.3 Renormalization for mass

The 1-loop diagrams, which contribute to the pion mass term, can be classified into two types. The first type are made from a four-point vertex, while the second ones are made from two three-point vertices. As the first type, we have following diagrams.

In the second type, there are three diagrams.

In the same way as tadpole diagrams, the contributions of the first type diagrams are given by

\[
\begin{align*}
I_\pm & = \frac{1}{2f_0^2} \left[ Z_{\pm}^\pm (\partial_\mu \pi_\pm)^2 + (\Delta M_{\pm}^\pm)^2 \pi_\pm^2 \right] I_\pm, \\
I_0 & = \frac{1}{2f_0^2} \left[ Z_0^\pm (\partial_\mu \pi_\pm)^2 + (\Delta M_{\pm}^0)^2 \pi_\pm^2 \right] I_0, \\
I_{\pm 0} & = \frac{1}{2f_0^2} \left[ Z_{\pm 0}^0 (\partial_\mu \pi_0)^2 + (\Delta M_{\pm 0}^0)^2 \pi_0^2 \right] I_\pm, \\
I_{0 0} & = \frac{1}{2f_0^2} \left[ Z_{0 0}^0 (\partial_\mu \pi_0)^2 + (\Delta M_{0 0}^0)^2 \pi_0^2 \right] I_0.
\end{align*}
\]

where each coefficient is given by

\[
\begin{align*}
Z_{\pm}^\pm & = -\frac{1}{3} c_0 a \cos \phi_0, \quad (\Delta M_{\pm}^\pm)^2 = m_\pi^2 \left\{ -\frac{1}{3} + a(c_0 - 4\tilde{c}_2) \cos \phi_0 \right\} + 4c_2 a^2 \cos^2 \phi_0, \\
Z_0^\pm & = -\frac{1}{3} - \frac{c_0 a \cos \phi_0}{2}, \quad (\Delta M_0^\pm)^2 = m_\pi^2 \left\{ \frac{1}{6} + \frac{a(c_0 - 2\tilde{c}_2) \cos \phi_0}{2} \right\} + c_2 a^2 \cos^2 \phi_0, \\
Z_{\pm 0}^0 & = -\frac{2}{3} c_0 a \cos \phi_0, \quad (\Delta M_{\pm 0}^0)^2 = m_\pi^2 \left\{ \frac{1}{3} + a(c_0 - 2\tilde{c}_2) \cos \phi_0 \right\} + c_2 a^2 (2 \cos^2 \phi_0 - \frac{4}{3} \sin^2 \phi_0), \\
Z_{0 0}^0 & = -\frac{c_0 a \cos \phi_0}{2}, \quad (\Delta M_{0 0}^0)^2 = m_\pi^2 \left\{ -\frac{1}{2} + \frac{a(c_0 - 6\tilde{c}_2) \cos \phi_0}{2} \right\} + c_2 a^2 (3 \cos^2 \phi_0 - 4 \sin^2 \phi_0).
\end{align*}
\]
On the other hand, the second type diagrams give SLO\(^2\) effects as

\[
\begin{align*}
&= (\text{SLO})^2 \int d^4p \frac{1}{p^2 + m^2} \frac{1}{p^2 + m^2 + m^2_{\pi}} \\
&= \text{SLO}^2.
\end{align*}
\]

Therefore the second type diagrams are higher order than NLO and we do not consider them in this paper. We then obtain the renormalized Lagrangian for \(\pi^2\) at 1-loop as

\[
\mathcal{L}_R^{(2)} = \mathcal{L}_{\text{LO+SLO}}^{(2)} + \mathcal{L}_{\text{1loop}}^{(2)} + \mathcal{L}_{\text{NLO+NSLO}}^{(2)},
\]

\[
= \frac{1}{2} \left\{ 1 + \frac{Z^a_b B^a_b}{f_0^2} + C^{2p.a}_{\text{NLO}} \right\} (\partial_\mu \pi_\alpha)^2 + \frac{1}{2} \left\{ (m_\pi^2)^2 + \frac{M^a_b B^a_b}{f_0^2} + C^{2a}_{\text{NLO}} \right\} \pi^2. \tag{A.33}
\]

From this result, the renormalized mass is given by

\[
\begin{align*}
(m_\pi^2)^2_{\text{NLO}} &= \left\{ (m_\pi^2)^2 + \frac{M^a_b B^a_b}{f_0^2} + C^{2a}_{\text{NLO}} \right\} \left\{ 1 + \frac{Z^a_b B^a_b}{f_0^2} + C^{2p.a}_{\text{NLO}} \right\}^{-1} \\
&= (m_\pi^2)^2_{\text{LO}} \bigg|_{\phi_0 \to \phi_0 + \Delta \phi} + \sum_{b = \pm} (m_\pi^2 B^a_b + a^2 Q^a_b) L_b \\
&- \frac{16}{f_0^2} \left\{ E_1^a (2B_0 m')^2 + E_2^a a (2B_0 m')^2 + E_3^a a^2 (2B_0 m') \right\}, \tag{A.34}
\end{align*}
\]

where coefficients of the chiral log terms are given in eqs. (3.19)–(3.22), while

\[
E_1^a = L_{45}^r - 2L_{68}^r, \tag{A.35}
\]

\[
E_2^a = (12V_{15}^r + V_{6}^r / 2 + V_{6}^x + 4V_{1}^r / 2 - V_{23}^r / 2) \cos \phi_0, \tag{A.36}
\]

\[
E_3^a = 6X_{1}^r + X_{5}^r / 2 + X_{6}^r / 2 + 2X_{1}^x + X_{1}^x / 2 + X_{1}^x / 2 - c_2 L_{45}^r) \\
+ \cos 2\phi_0 (6X_{1}^r + X_{6}^r / 2 + 2X_{1}^x - c_2 L_{45}^r) \\
- \delta_{a0} (4X_{1}^x - X_{5}^x - X_{23}^x / 2 + X_{1}^x - c_2 L_{45}^r) (1 - \cos 2\phi_0) \tag{A.37}
\]

for NLO low energy constants.

### A.4 Renormalization for decay constant

Since we have \(O(\pi^3)\) terms (2.32, 2.33) in the axial current, the 1-loop contribution to the decay constant of the charged pion is given by

\[
\langle 0 | A^\mu_\pi | \pi_\alpha(p) \rangle_{\text{1loop}} = -f_0 p_\mu C_{1\text{loop}}^{f,a},
\]

\[
C_{1\text{loop}}^{f,a} = \left[ \frac{2}{3} + \frac{c_0 a \cos \phi_0}{2 f_0^2} \right] L_+ + \left( \frac{2}{3} + \frac{3c_0 a \cos \phi_0}{2} \right) L_0 \cos \phi_0 - c_0 a L_0. \tag{A.38}
\]
For the neutral pion,
\[
\langle 0 | A_\mu^a | \pi_a(p) \rangle_{\text{loop}} = - f_{0\mu} C_{1\text{loop}}^{f,3},
\]
\[
C_{1\text{loop}}^{f,3} = \left( \frac{2}{3} f_0^2 + \frac{c_0 a \cos \phi_0}{2 f_0^2} \right) \langle \pi_b \pi_b \rangle - \frac{2}{3 f_0^2} \langle \pi_3 \pi_3 \rangle
\]
\[
= \left( \frac{4}{3} + c_0 a \cos \phi_0 \right) L_\pm + \frac{c_0 a \cos \phi_0}{2} L_0.
\]
(A.39)

Therefore, we obtain the renormalized decay constant
\[
\langle 0 | A_\mu^a | \pi_a(p) \rangle_R = \left\{ 1 + \frac{Z_b^a I_b}{f_0^2} + C_{\text{NLO}}^{2p,a} \right\}^{-1/2} \langle 0 | A_\mu^a | \pi_a(p) \rangle + \langle 0 | A_\mu^a | \pi_a(p) \rangle_{\text{loop}} + \langle 0 | A_\mu^a | \pi_a(p) \rangle_{\text{NLO}},
\]
where the first term is a contribution for the renormalization of the pion field, and the second and third terms represent the 1-loop and the “NLO” contributions, respectively. In the same way as the vacuum expectation value and the pion mass, we obtain the decay constant at NLO as
\[
f_{PS,NLO} = f_{PS,LO} |_{\phi = \phi_0 + \Delta \phi} + f_{PS,LO} \sum_{b=\pm,0} F_b^a L_b
\]
\[
+ \frac{16}{f_0^2} \left\{ \langle 2 B_0 m' \rangle H_1^a + a \langle 2 B_0 m' \rangle H_2^a + a^2 H_3^a \right\}
\]
\[
+ \Delta f_\pm (1 - \delta_{3a}).
\]
(A.40)

where coefficients for the chiral log terms are given in eqs. (3.26) and (3.27), while
\[
H_1^a = L_{35}/2,
\]
\[
H_2^a = 2 V_1^a + V_2^a/2 - \tilde{V}_3^a/4 - 2 \tilde{V}_4^a - 2 \tilde{V}_5^a \delta_{3a},
\]
\[
H_3^a = X_1^a + X_2^a/4 - X_3^a/4 - 2 X_4^a + X_5^a \cos 2\phi_0
\]
\[
+ (X_6^a/2 + X_7^a/4 + 3 X_8^a/2)(1 - \cos 2\phi) \delta_{3a}
\]
(A.42)

for NLO low energy constants. Note here that an additive renormalization term for the decay constant of the charged pion exists:
\[
\Delta f_\pm = - f_0 \left[ - a \langle 2 B_0 m' \rangle 2 V_5^a + c_0 a L_0 \right].
\]
(A.43)

We finally consider the PCAC mass, defined by
\[
m_{\text{PCAC}} = \frac{\sum_x \int \frac{d^4 p}{(2\pi)^3} \langle 0 | \partial_\mu A_\mu^a(x, t) | \pi(p) \rangle \frac{1}{2E_p} \langle \pi(p) | P^a(0) | 0 \rangle}{2 \sum_x \int \frac{d^4 p}{(2\pi)^3} \langle 0 | P^a(x, t) | \pi(p) \rangle \frac{1}{2E_p} \langle \pi(p) | P^a(0) | 0 \rangle}
\]
\[
= \frac{f_{PS} m_\pi^2}{2 Z_{PS}^a},
\]
(A.44)
Using the same spurion analysis as for the axial currents, the pseudo scalar density and its renormalization factor $Z_{PS}^a$ are given by

\[
P^a = i f_0 B_0 (1 + \tilde{c}_2 a \cos \phi_0) \pi_a \quad (a = 1, 2),
\]
\[
Z_{PS}^a = f_0 B_0 (1 + \tilde{c}_2 a \cos \phi_0)
\]

at the tree-level. Therefore the LO PCAC quark mass becomes

\[
m_{PCAC} = \frac{m_2^2 \cos \phi_0}{2B_0(1 + \tilde{c}_2 \cos \phi_0)}.
\]
References

[1] R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz, “A local formulation of lattice QCD without unphysical fermion zero modes,” Nucl. Phys. Proc. Suppl. 83, 941 (2000) [arXiv:hep-lat/9909003].

[2] R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz [Alpha collaboration], JHEP 0108, 058 (2001) [arXiv:hep-lat/0101001].

[3] R. Frezzotti, S. Sint and P. Weisz [ALPHA collaboration], “O(a) improved twisted mass lattice QCD,” JHEP 0107, 048 (2001) [arXiv:hep-lat/0104014].

[4] S. Aoki and O. Bar, “Twisted-mass QCD, O(a) improvement and Wilson chiral perturbation theory,” Phys. Rev. D 70, 116011 (2004) [arXiv:hep-lat/0409006].

[5] S. Aoki and O. Bar, “Automatic O(a) improvement for twisted-mass QCD in the presence of spontaneous symmetry breaking,” Phys. Rev. D 74, 034511 (2006) [arXiv:hep-lat/0604018].

[6] K. Jansen, A. Shindler, C. Urbach and I. Wetzorke [XLF Collaboration], “Scaling test for Wilson twisted mass QCD,” Phys. Lett. B 586, 432 (2004) [arXiv:hep-lat/0312013].

[7] W. Bietenholz et al. [XLF Collaboration], “Going chiral: Overlap versus twisted mass fermions,” JHEP 0412, 044 (2004) [arXiv:hep-lat/0411001].

[8] K. Jansen, M. Papinutto, A. Shindler, C. Urbach and I. Wetzorke [XLF Collaboration], “Light quarks with twisted mass fermions,” Phys. Lett. B 619, 184 (2005) [arXiv:hep-lat/0503031].

[9] K. Jansen, M. Papinutto, A. Shindler, C. Urbach and I. Wetzorke [XLF Collaboration], “Quenched scaling of Wilson twisted mass fermions,” JHEP 0509, 071 (2005) [arXiv:hep-lat/0507010].

[10] A. M. Abdel-Rehim and R. Lewis, “Twisted mass QCD for the pion electromagnetic form factor,” Phys. Rev. D 71, 014503 (2005) [arXiv:hep-lat/0410047].

[11] A. M. Abdel-Rehim, R. Lewis and R. M. Woloshyn, “Spectrum of quenched twisted mass lattice QCD at maximal twist,” Phys. Rev. D 71, 094505 (2005) [arXiv:hep-lat/0503007].

[12] F. Farchioni et al., “Twisted mass quarks and the phase structure of lattice QCD,” Eur. Phys. J. C 39, 421 (2005) [arXiv:hep-lat/0406039].

[13] F. Farchioni et al., “Exploring the phase structure of lattice QCD with twisted mass quarks,” Nucl. Phys. Proc. Suppl. 140, 240 (2005) [arXiv:hep-lat/0409098].

[14] F. Farchioni et al., “Lattice spacing dependence of the first order phase transition for dynamical twisted mass fermions,” Phys. Lett. B 624, 324 (2005) [arXiv:hep-lat/0506025].

[15] C. Alexandrou et al. [European Twisted Mass Collaboration], “Light baryon masses with dynamical twisted mass fermions,” Phys. Rev. D 78, 014509 (2008) [arXiv:0803.3190 [hep-lat]].

[16] R. Baron et al., “Light Meson Physics from Maximally Twisted Mass Lattice QCD,” arXiv:0911.5061 [hep-lat].

[17] R. Baron et al. [ETM Collaboration], “Status of ETMC simulations with Nf=2+1+1 twisted mass fermions,” PoS LATTICE2008, 094 (2008) [arXiv:0810.3807 [hep-lat]].

[18] R. Baron et al. [European Twisted Mass Collaboration], “Computing K and D meson masses with Nf = 2 + 1 + 1 twisted mass lattice QCD,” Comput. Phys. Commun. 182, 299
(2011) [arXiv:1005.2042 [hep-lat]].

[19] J. Gasser, H. Leutwyler, “On The Low-energy Structure Of Qcd,” Phys. Lett. B125, 321 (1983).

[20] J. Gasser, H. Leutwyler, “Low-Energy Theorems as Precision Tests of QCD,” Phys. Lett. B125, 325 (1983).

[21] J. Gasser and H. Leutwyler, “Chiral Perturbation Theory To One Loop,” Annals Phys. 158, 142 (1984).

[22] J. Gasser and H. Leutwyler, “Chiral Perturbation Theory: Expansions In The Mass Of The Strange Quark,” Nucl. Phys. B 250, 465 (1985).

[23] S. R. Sharpe and R. L. Singleton, “Spontaneous flavor and parity breaking with Wilson fermions,” Phys. Rev. D 58, 074501 (1998) [arXiv:hep-lat/9804028].

[24] S. R. Sharpe and J. M. S. Wu, “The phase diagram of twisted mass lattice QCD,” Phys. Rev. D 70, 094029 (2004) [arXiv:hep-lat/0407025].

[25] S. Aoki, “Chiral perturbation theory with Wilson-type fermions including a**2 Nucl. Phys. Proc. Suppl. 128, 9 (2004).

[26] G. Munster and C. Schmidt, “Chiral perturbation theory for lattice QCD with a twisted mass term,” Europhys. Lett. 66, 652 (2004) [arXiv:hep-lat/0311032].

[27] L. Scorzato, “Pion mass splitting and phase structure in twisted mass QCD,” Eur. Phys. J. C 37, 445 (2004) [arXiv:hep-lat/0407023].

[28] S. R. Sharpe and J. M. S. Wu, “Twisted mass chiral perturbation theory at next-to-leading order,” Phys. Rev. D 71, 074501 (2005) [arXiv:hep-lat/0411021].

[29] G. Munster and T. Sudmann, “Twisted mass lattice QCD with non-degenerate quark masses,” JHEP 0608, 085 (2006) [arXiv:hep-lat/0603019].

[30] G. Munster and T. Sudmann, “Twisted mass chiral perturbation theory for 2+1+1 quark flavours,” JHEP 1104, 116 (2011) [arXiv:1103.1494 [hep-lat]].

[31] O. Bar, “Chiral logs in twisted mass lattice QCD with large isospin breaking,” Phys. Rev. D 82, 094505 (2010) [arXiv:1008.0784 [hep-lat]].

[32] S. Aoki, “New phase structure for lattice QCD with Wilson fermions,” Phys. Rev. D 30, 2653 (1984).

[33] S. Aoki, “A solution to the U(1) problem on a lattice,” Phys. Rev. Lett. 57, 3136 (1986).

[34] S. Aoki, “On the phase structure of QCD with Wilson fermions,” Prog. Theor. Phys. Suppl. 122, 179 (1996) [arXiv:hep-lat/9509008].