Automatic $O(a)$ improvement for twisted-mass QCD in the presence of spontaneous symmetry breaking

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Abstract

In this paper we present a proof for automatic $O(a)$ improvement in twisted mass lattice QCD at maximal twist, which uses only the symmetries of the leading part in the Symanzik effective action. In the process of the proof we clarify that the twist angle is dynamically determined by vacuum expectation values in the Symanzik theory. For maximal twist according to this definition, we show that scaling violations of all quantities which have non-zero values in the continuum limit are even in $a$. In addition, using Wilson Chiral Perturbation Theory (WChPT), we investigate this definition for maximal twist and compare it to other definitions which were already employed in actual simulations.
I. INTRODUCTION

It becomes more and more apparent that twisted mass Lattice QCD (tmLQCD) \cite{1,2} is a promising formulation to approach the chiral limit of QCD, despite the fact that the flavor symmetry is explicitly broken. A twisted mass protects the Wilson-Dirac operator against small eigenvalues and therefore solves the problem of exceptional configurations, thus making numerical simulations with small quark masses feasible. Recent studies \cite{3,4,5,6} in the quenched simulation were performed with \( m_\pi/m_\rho \) values as small as 0.3 without running into problems due to exceptional configurations. Even though it will be challenging to reach such small pion masses in dynamical simulations, \( m_\pi/m_\rho < 0.5 \) seems fairly possible \cite{7}.

This numerical advantage of tmLQCD is supplemented by the property of automatic O(\( a \)) improvement at maximal twist \cite{8,9,10}. For a recent review of these and some more results in twisted mass LQCD see Ref. \cite{11}.

Some issues, however, remain to be fully understood. The proof of automatic O(\( a \)) improvement in Ref. \cite{8} makes use of the symmetries \( m_q \equiv m_0 - m_{cr} \rightarrow -m_q \) and \( r \rightarrow -r \), where \( m_0 \) is the bare (untwisted) quark mass, \( r \) is the parameter in the Wilson term and \( m_{cr}(r) \) is the critical quark mass. Maximal twist is defined by setting the bare mass to a critical value, \( m_0 = m_{cr}(r) \). A concrete definition of \( m_{cr}(r) \) is not required in the proof as long as the symmetry property \( m_{cr}(-r) = -m_{cr}(r) \) is satisfied, and tuning to the bare quark mass where the pion mass vanishes has been suggested as one particular choice for \( m_{cr}(r) \) (We call this definition “the pion mass definition” in the following). However, it has been pointed out in Ref. \cite{12} that the condition \( m_{cr}(-r) = -m_{cr}(r) \) is violated for the pion mass definition by non-perturbative effects. Consequently, the O(\( a^2 \)) scaling violation, expected from an O(\( a \)) improved theory, is lost unless the twisted quark mass satisfies the bound \( \mu > a^2 \Lambda_{QCD}^3 \). Instead, terms linear in \( a \) and with fractional powers of \( a \) are predicted by Wilson Chiral Perturbation Theory (WChPT) for very small twisted quark masses. On the other hand, automatic O(\( a \)) improvement is expected to hold if the critical mass is defined through the partially conserved axial vector Ward identity quark mass (PCAC mass definition).

A recent paper \cite{13} comes to a different conclusion. Automatic O(\( a \)) improvement has been proven by the \( m_q \rightarrow -m_q \) symmetry only, without using the symmetry in \( r \). It is claimed that both the pion and the PCAC mass definition guarantee automatic O(\( a \))
improvement, but the remaining $O(a^2)$ effects differ significantly. In particular, the pion mass definition for $m_{cr}$ exhibits cut-off artifacts of $O(a^2/m^2_\pi)$ which are enhanced for small pion masses. These enhanced lattices artifacts are shown to be absent for the PCAC mass definition.

The results in Ref. [12] and Ref. [13] are obviously in disagreement in the small quark mass region where the bound $\mu > a^2 \Lambda^3_{QCD}$ does not hold. Whether this is of relevance for present day simulations with lattice spacings $a \approx 0.1$ fm remains to be seen. A recent scaling analysis [14] of $f_\pi$ in quenched tmLQCD seems consistent with an $O(a^2)$ scaling violation, although its magnitude is rather large. Given the fact that automatic $O(a)$ improvement is a highly acclaimed feature of twisted mass LQCD, it is certainly desirable to study this issue further and find an explanation for these contradicting results.

Closely related is the so-called 'bending phenomenon', observed in quenched simulations [3, 4, 5, 6]. The pion mass, the pion decay constant and the vector meson mass show an unexpected strong non-linear quark mass dependence for small quark masses if the pion mass definition for the critical quark mass is used. This curvature is significantly reduced when the untwisted quark mass is tuned according to the optimal choice proposed in [13]. That this bending is indeed a lattice artifact of the twisted mass formulation is also supported by calculations using the overlap operator on the same gauge field configurations with similarly small pion masses. Here the bending is absent [3].

In this paper we revisit the property of automatic $O(a)$ improvement in twisted mass QCD. We first give an alternative proof for automatic $O(a)$ improvement at maximal twist without using the symmetries of the parameters $m_q$ and $r$. Although our proof is just an improved version of previous ones [8, 13], we can clarify the meaning of “maximal twist” in the process of our proof. We will argue that, in presence of spontaneous symmetry breaking, the twist angle $\theta$ is determined dynamically by the ratio of two vacuum expectation values in the Symanzik theory, namely

$$\cot \theta = \frac{\langle \bar{\psi}\psi \rangle}{\langle \bar{\psi}i\tau_3\psi \rangle}. \quad (1)$$

Provided that the mass parameters of the theory are tuned such that $\theta = \pm \pi/2$, we can show that the scaling violations of observables start with $a^2$, i.e. the theory is $O(a)$ improved.

We also investigate this new definition for maximal twist using Wilson Chiral Perturbation Theory (WChPT) [15, 16] (for a review see Ref. [17]). We explicitly show the absence of
O(a, aµ) contributions in the expressions for the pion mass and decay constant.

We finally compare our new criterion with other definitions of maximal twist, the pion mass and the PCAC mass definition, which were previously employed in numerical simulations. We find that, although these two definitions show asymptotic a² scaling violations, they do not exhibit the expected a² scaling until a becomes small such that the bound µ > a²Λ³ QCD is satisfied.

II. ALTERNATIVE PROOF OF O(a) IMPROVEMENT

A. Main idea for O(a) improvement

The twisted mass lattice QCD action for the 2-flavor theory is given by

\[ S_{tmQCD} = S_G + S_{tm}. \] (2)

The details of the gauge action \( S_G \) are irrelevant in the following, so we leave it unspecified. \( S_{tm} \) denotes the 2-flavor Wilson fermion action with a twisted mass term, which is defined as

\[ S_{tm} = \sum_{x, \mu} \bar{\psi}_L(x) \frac{1}{2} \left[ \gamma_\mu (\nabla_\mu^+ - \nabla_\mu^-) \psi_L - ar\nabla_\mu^+ \nabla_\mu^- \psi_L \right] (x) + \sum_x \bar{\psi}_L(x) M_0 e^{i\theta_0 \gamma_5 \tau_3} \psi_L(x), \] (3)

with

\[ \left( \nabla_\mu^+ \psi_L \right) (x) = \frac{1}{a} \left( U_\mu(x) \psi_L(x + \mu) - \psi_L(x) \right), \] (4)

\[ \left( \nabla_\mu^- \psi_L \right) (x) = \frac{1}{a} \left( \psi_L(x) - U_\mu^\dagger(x - \mu) \psi_L(x - \mu) \right), \] (5)

being the standard forward and backward difference operators. We supplemented the fields with the subscript "L" in order to highlight the fact that these fields are lattice fields. The parameters \( M_0 \) and \( \theta_0 \) denote the bare mass and bare twist angle. Instead of using this exponential notation it is also customary to write

\[ M_0 e^{i\theta_0 \gamma_5 \tau_3} = m_0 + i\mu_0 \gamma_5 \tau_3, \] (6)

where the bare untwisted mass \( m_0 \) and the bare twisted mass \( \mu_0 \) are given by

\[ m_0 = M_0 \cos \theta_0, \quad \mu_0 = M_0 \sin \theta_0. \] (7)

The lattice action \( \square \) is invariant under the following global symmetry transformations \( \square \) :
1. U(1)⊗U(1) vector symmetry

\[ \psi_L \rightarrow e^{i(a_0 + a_3 \tau^3)} \psi_L, \quad \bar{\psi}_L \rightarrow \bar{\psi}_L e^{-i(a_0 + a_3 \tau^3)}. \]

This transformation is part of the U(2) flavor symmetry of the untwisted theory.

2. Extended parity symmetry

\[ P_{1,2}^L : \psi_L \rightarrow \tau^{1,2} P \psi_L, \quad \bar{\psi}_L \rightarrow P \bar{\psi}_L \tau^{1,2}, \tag{8} \]

where \( P \) is the parity transformation, given by

\[ P \psi_L(\vec{x},t) = i \gamma_0 \psi_L(-\vec{x},t), \quad P \bar{\psi}_L(\vec{x},t) = -i \bar{\psi}_L(-\vec{x},t) \gamma_0. \]

For the gauge fields \( P_F \) is equal to the standard parity transformation. Note that ordinary parity \( P \) is not a symmetry unless it is combined with a flavor rotation in the 1 or 2 direction. Alternatively, one can also augment \( P \) with a sign change of the twisted mass term \( \mu_0 \),

\[ \tilde{P} = P \times [\mu_0 \rightarrow -\mu_0], \tag{9} \]

which is also a symmetry of the action.

3. Charge conjugation symmetry

\[ C : \psi_L(x) \rightarrow i \gamma_0 \gamma_2 \bar{\psi}_L(x)^T, \quad \bar{\psi}_L(x) \rightarrow -\psi_L(x)^T i \gamma_0 \gamma_2, \]

together with the charge conjugation transformation for the gauge fields, \( U(x,\mu) \rightarrow U(x,\mu)^* \).

Besides these symmetries the lattice action is also invariant under hypercubic lattice rotations and local gauge transformations.

According to Symanzik [19, 20], the lattice theory can be described by an effective continuum theory. The form of the effective action of this theory is restricted by locality and the symmetries of the underlying lattice theory. Taking into account the symmetries listed above one finds [18]

\[ S_{\text{eff}} = S_0 + a S_1 + a^2 S_2 + \cdots, \tag{10} \]
where the first two terms are given as

\begin{align}
S_0 &= S_{0, \text{gauge}} + \int d^4 x \bar{\psi}(x) \left[ \gamma_\mu D_\mu + M R e^{i \theta} \gamma_5 \tau^3 \right] \psi(x), \\
S_1 &= C_1 \int d^4 x \bar{\psi}(x) \sigma_{\mu \nu} F_{\mu \nu}(x) \psi(x).
\end{align}

(11)

\begin{align}
S_{0, \text{gauge}} \text{ denotes the standard continuum gauge field action in terms of the gauge field tensor } F_{\mu \nu}. \text{ The second term in } S_0 \text{ is the continuum twisted mass fermion action. The mass parameters are renormalized masses, and we assume the renormalization scheme in [1].} \end{align}

(12)

It is worth mentioning that there is no "twisted" Pauli term \( \bar{\psi} \gamma_5 \tau^3 \sigma_{\mu \nu} F_{\mu \nu} \psi \) present in \( S_1 \), since such a term violates the symmetry in eq. (9).

In addition to the effective action we have to specify the direction of the chiral condensate, since chiral symmetry is spontaneously broken. From the fact that the direction of the chiral condensate is completely controlled by the direction of the symmetry breaking external field (i.e. the quark mass) in the continuum theory, we can take

\begin{align}
\langle \bar{\psi}^i \psi^j \rangle_{S_0} &= \frac{v(M_R)}{8} \left[ e^{-i \theta} \gamma_5 \tau^3 \right]^{ji}_{\beta \alpha}, \\
\text{where } \text{lim}_{M_R \to 0} \text{ lim}_{V \to \infty} v(M_R) \neq 0. \end{align}

(13)

Here the vacuum expectation value (VEV) is defined with respect to the continuum action \( S_0 \). To say it differently, the VEV (13) defines the twist angle \( \theta \) in the Symanzik theory. The above condensate is equivalent to

\begin{align}
\langle \bar{\psi} \psi \rangle_{S_0} &= v(M_R) \cos \theta, \\
\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle_{S_0} &= v(M_R) \sin \theta.
\end{align}

(14)

\begin{align}
\text{1 Other choices for the renormalized parameters are of course possible, but at the expense of additional terms in } S_1 \text{ of the effective action [18]. We also assume that use of the leading order equations of motion has been made in order to drop some } O(a) \text{ terms in } S_1. \text{ Without using the renormalization scheme in [1] and equations of motion there would be seven terms present in } S_1 \text{ instead of only one [18]. However, this larger number of terms would not alter the conclusion of this section.} \end{align}

(15)

\begin{align}
\text{2 This property can also be derived from a different point of view. Since parity is conserved at } \mu_0 = 0 \text{ in the lattice theory, } \bar{\psi} \gamma_5 \tau^3 \sigma \cdot F \psi \text{ does not appear without } \mu_0. \text{ This argument can be extended to the case where the parity-flavor symmetry is spontaneously broken for a certain range of the untwisted mass } M_0 \cos \theta_0 \text{ in the lattice theory. In this case, the charged pions become massless Nambu-Goldstone bosons in the lattice theory, associated with this spontaneous symmetry breaking in the zero twisted mass limit. Therefore, it must also become massless in the Symanzik theory in the same limit. This fact also tells us that explicit parity-flavor breaking terms such as } \bar{\psi} i \gamma_5 \tau^3 \sigma_{\mu \nu} F_{\mu \nu} \psi \text{ must be absent in the Symanzik theory without } \mu_0. \end{align}

\begin{align}
\text{3 The computation of this condensate follows standard arguments where one first considers the theory in a finite box with 4- volume } V. \text{ See, for example, the appendix of Ref. [15].}
\end{align}
We now want to argue that the choice $\theta = \pi/2$ (or $-\pi/2$) corresponds to maximal twist. In terms of the mass parameters this is equivalent to $M_R = \mu_R$ and $m_R = 0$. In this case the action and the VEVs become

$$S_0 = S_{0,\text{gauge}} + \int d^4x \bar{\psi} \left[ \gamma_\mu D_\mu + iM_R\gamma_5\tau^3 \right] \psi(x),$$

$$S_1 = C_1 \int d^4x \bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x),$$

$$\langle \bar{\psi}\psi \rangle_{S_0} = 0,$$

$$\langle \bar{\psi}i\gamma_5\tau^3\psi \rangle_{S_0} = v(M_R).$$

It is easy to check that $S_0$, the continuum part of the effective action is invariant under

$$\psi \rightarrow e^{i\omega\gamma_5\tau^{1,2}} \psi, \quad \bar{\psi} \rightarrow \bar{\psi}e^{i\omega\gamma_5\tau^{1,2}},$$

and therefore also under the $\mathbb{Z}_2$ subgroup $T_1$ of this continuous transformation, defined by

$$T_1\psi = i\gamma_5\tau^1\psi, \quad T_1\bar{\psi} = \bar{\psi}i\gamma_5\tau^1.$$

Since $T_1^2 = 1$ in the space of fermion number conserving operators, which contain equal numbers of $\psi$ and $\bar{\psi}$, the eigenvalues of $T_1$ are 1 ($T_1$-even) or $-1$ ($T_1$-odd). The crucial observation is that the VEVs (18) and (19) are also invariant under this transformation. The symmetry (20) (and its discrete subgroup $T_1$) is not spontaneously broken, hence it is an exact symmetry of the continuum theory. The $O(a)$ term

$$aS_1 = aC_1 \int d^4x \bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x),$$

on the other hand, is odd under $T_1$. Therefore non-vanishing physical observables, which must be even under $T_1$, can not have an $O(a)$ contribution, since the $O(a)$ term is odd under $T_1$ and therefore must vanish identically. This is automatic $O(a)$ improvement at maximal twist.\(^5\) Note that non-invariant, i.e. $T_1$-odd quantities, which vanish in the continuum limit, can have $O(a)$ contributions.

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\(^4\) A similar argument using this symmetry has been given independently by S. Sint.\(^{26}\)

\(^5\) This argument does not rely on our particular renormalization scheme and the use of the equations of motion. All possible terms in $S_1$ are $T_1$-odd once the continuum part is invariant under the transformation.
The above argument gives just the main idea of our proof for automatic $O(a)$ improvement, and we will give a detailed proof in the next subsection. However, one of the most important points of our analysis is that the condition for maximal twist and for automatic $O(a)$ improvement is determined dynamically by the VEV $\langle \bar{\psi}_i^\alpha \psi_j^\beta \rangle$ in the Symanzik theory. More explicitly, the symmetry (20) or (21) of the continuum theory must keep the VEV intact, so that the symmetry is not spontaneously broken. This condition seems natural, since the symmetry (20) corresponds to a part of the exact vector symmetry in the continuum QCD at maximal twist. Note that this symmetry refers to the vector symmetry in the so-called twisted basis [2,8]. After rotating to the physical basis the theory is invariant under ordinary vector rotations in the 1 or 2 direction. However, for the proof of $O(a)$ improvement in the next subsection we prefer to stay in the twisted basis.

**B. Proof of $O(a)$ improvement**

Let us consider an arbitrary multi-local lattice operator $O_{\text{lat}}^{t,p,d}(\{x\})$, where $\{x\}$ represents $x_1, x_2, \cdots, x_n$, $d$ is the canonical dimension of the operator, $t = 0, 1$ and $p = 0, 1$ denote transformation properties under $T_1$ and parity $P$:

$$T_1: \quad O_{\text{lat}}^{t,p,d}(\{x\}) \rightarrow (-1)^t O_{\text{lat}}^{t,p,d}(\{x\}),$$

$$P: \quad O_{\text{lat}}^{t,p,d}(\{-x, t\}) \rightarrow (-1)^p O_{\text{lat}}^{t,p,d}(\{-x, t\}).$$

(23)

Here we do not include the dimension coming from powers of the quark mass in the canonical dimension $d$ of operators. For example,

$$O_{\text{lat}}^{01,3}(x) = \bar{\psi}_L i \gamma_5 \tau^3 \psi_L(x), \quad O_{\text{lat}}^{10,3}(x) = \bar{\psi}_L \psi_L(x),$$

$$O_{\text{lat}}^{00,4}(x) = \sum_\mu \bar{\psi}_L \frac{1}{2} \gamma_\mu (\nabla_\mu^+ + \nabla^-_\mu) \psi_L(x),$$

$$O_{\text{lat}}^{10,5}(x) = \sum_\mu \bar{\psi}_L \frac{1}{2} \nabla_\mu^+ \nabla^-_\mu \psi_L(x),$$

(25)

and in terms of these operators the lattice action is given by

$$S_{tm} = \sum_x \left[ O_{\text{lat}}^{00,4}(x) - ar O_{\text{lat}}^{10,5}(x) + m_0 O_{\text{lat}}^{10,3}(x) + \mu_0 O_{\text{lat}}^{01,3}(x) \right],$$

(26)

with untwisted quark mass $m_0 = M_0 \cos \theta_0$ and twisted quark mass $\mu_0 = M_0 \sin \theta_0$. 

8
The lattice operator $O_{\text{lat}}^{t,p,d}$ corresponds to a sum of continuum operators $O_{t_n p_n}^{t_n p_n, n}$ ($n$: non-negative integer) in the Symanzik theory as

$$O_{\text{lat}}^{t,p,d} \leftrightarrow O_{\text{eff}}^{t,p,d} = \sum_{n=0}^{\infty} a^{n-d} \sum_{t_n p_n} c_{t_n p_n, n, i_n}^{t,p,d} O_{t_n p_n, n}^{t_n p_n, n},$$  \hspace{1cm} (27)$$

where $n$ is the canonical dimension of the continuum operator $O_{t_n p_n}^{t_n p_n, n}$ which consists of $\bar{\psi}, \psi, A_{\mu}$ and $D_{\mu}$ only without any mass parameters, and

$$T_1 : O_{t_n p_n}^{t_n p_n, n}({\{x\}}) \rightarrow (-1)^{t_n} O_{t_n p_n}^{t_n p_n, n}({\{x\}}),$$  \hspace{1cm} (28)$$

$$P : O_{t_n p_n}^{t_n p_n, n}({\{\vec{x}, t\}}) \rightarrow (-1)^{p_n} O_{t_n p_n}^{t_n p_n, n}({\{-\vec{x}, t\}}),$$  \hspace{1cm} (29)$$

with $t_n, p_n = 0, 1$. Here we distinguish different operators with the same $(t_n p_n, n)$ by an index $i_n$. To have a total dimension $d$ in the expansion in Eq. (27), the coefficients $c_{t_n p_n, n, i_n}^{t,p,d}$ must be dimensionless: $c_{t_n p_n, n, i_n}^{t,p,d} = c_{t_n p_n, n, i_n}^{t,p,d}(g^2, \log(\Lambda a), m_q a, \mu_0 a)$, where $g^2$ is the bare gauge coupling constant, $\log(\Lambda a)$ represents log-divergences of the lattice theory with some scale parameter $\Lambda$ introduced in the Symanzik theory, and $m_q = m_0 - m_{cr}$ is a subtracted quark mass with an additive mass counter term $m_{cr}$, which will be specified later. Note that we consider possible power divergences of lattice operators by including operators with $n = 0, 1, \ldots, d - 1$ in the expansion.

The following selection rules among these operators are crucial for our proof of automatic $O(a)$ improvement:

$$t + p + d = t_n + p_n + n \mod(2),$$  \hspace{1cm} (30)$$

$$p + \#\mu_0 = p_n + (\#\mu_0)_n \mod(2),$$  \hspace{1cm} (31)$$

where $\#\mu_0$ and $(\#\mu_0)_n$ denote the numbers of $\mu_0$'s in $O_{\text{lat}}^{t,p,d}$ and $c_{t_n p_n, n, i_n}^{t,p,d}$, respectively. The second equality can be easily proven by the invariance of the lattice action (3) under the $\tilde{P} = P \times [\mu_0 \rightarrow -\mu_0]$ transformation, Eq. (9). To prove the first equality (30), we introduce the following transformation:

$$D_d^t : \begin{cases} U_\mu(x) \rightarrow U^\dagger_\mu(-x - a\mu) \\ (A_\mu(x) \rightarrow -A_\mu(-x)) \\ \psi(x) \rightarrow (e^{i\pi r_1})^{3/2} \psi(-x) \\ \bar{\psi}(x) \rightarrow \bar{\psi}(-x) (e^{i\pi r_1})^{3/2} \end{cases},$$  \hspace{1cm} (32)$$
which is a modified version of the transformation $\mathcal{D}_d$ introduced in Ref.\cite{8}. Since it is easy
to show that the lattice action \cite{3} is invariant under $T_1 \times \mathcal{D}_d^1$, in addition to the invariance
under $P^1_{\Phi}$, the lattice action is invariant under $T_1 \times \mathcal{D}_d^1 \times P^1_{\Phi}$. On the other hand, combining
the transformation property

$$
\mathcal{D}_d^1: \begin{cases}
(\nabla^)_\mu + \nabla^-_\mu) \cdot f(x) \to -(\nabla^)_\mu + \nabla^-_\mu) \cdot f(-x) \\
(D_\mu \cdot f(x) \to -D_\mu \cdot f(-x)
\end{cases}
$$

(33)

for an arbitrary function $f(x)$ with eqs.\cite{3} and \cite{3}, we can easily see that $\mathcal{D}_d^1 \times P^1_{\Phi}$ counts
the canonical dimension times the parity of the operator as

$$
\mathcal{D}_d^1 \times P^1_{\Phi}: \mathcal{O}^{\nu,d}_{\text{lat}}(\tilde{x}, t) \to (-1)^{d+p} \mathcal{O}^{\nu,d}_{\text{lat}}(\tilde{x}, -t)
$$

(34)

$$
\mathcal{D}_d^1 \times P^1_{\Phi}: \mathcal{O}^{t,n}_{\text{lat}}(\tilde{x}, t) \to (-1)^{n+p} \mathcal{O}^{t,n}_{\text{lat}}(\tilde{x}, -t).
$$

(35)

Therefore, the invariance of the action under $T_1 \times \mathcal{D}_d^1 \times P^1_{\Phi}$ implies the first equality \cite{30}.

Let us show how these selection rules are used to determine the structure of operators
in the Symanzik theory. As an example we consider the operator $\mathcal{O}^{01,3}_{\text{lat}}(x)$ in eq.\cite{25}. Since
$t + p + d = 4$, the first selection rule gives $t_n + d_n + n = 0 \text{ mod}(2)$, which leads to

$$
\mathcal{O}_{\text{eff}}^{01,3} = \frac{c_{00,0}^{13}}{a^3} \mathcal{O}_{00,0}^{13} + c_{10,3}^{13} \mathcal{O}_{10,3}^{13} + a c_{00,4,A}^{13} \mathcal{O}_{00,4,A}^{13} + a c_{10,4,B}^{13} \mathcal{O}_{10,4,B}^{13} + a c_{11,4}^{13} \mathcal{O}_{11,4}^{13} + a^2 c_{01,5,A}^{13} \mathcal{O}_{01,5,A}^{13} + a^2 c_{10,5,B}^{13} \mathcal{O}_{10,5,B}^{13} + \cdots
$$

(36)

where

$$
\mathcal{O}_{00,0} = 1, \quad \mathcal{O}_{10,3}^{13} = \bar{\psi} i \gamma_5 \tau^3 \psi, \quad \mathcal{O}_{10,4}^{13} = \bar{\psi} \gamma_\mu D_\mu \psi, \\
\mathcal{O}_{11,4}^{13} = \bar{\psi} \gamma_\mu D_\mu \gamma_5 \tau^3 \psi, \\
\mathcal{O}_{01,5,A}^{13} = \bar{\psi} i \gamma_5 \tau^3 D^2 \psi, \quad \mathcal{O}_{01,5,B}^{13} = \bar{\psi} i \gamma_5 \tau^3 \sigma_{\mu\nu} F_{\mu\nu} \psi, \\
\mathcal{O}_{10,5,A}^{13} = \bar{\psi} \gamma_\mu D_\mu \psi, \quad \mathcal{O}_{10,5,B}^{13} = \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi.
$$

(37)

Applying the second selection rule that $p + \# \mu_0 = 1 = p_n + (\# \mu_0)_n \text{ mod}(2)$, we obtain

$$
c_{00,0}^{13}(\mu_0 a) = \mu_0 a c_{00,0}^{13}(\mu_0^2 a^2), \quad c_{10,3}^{13}(\mu_0 a) = \mu_0 a c_{10,3}^{13}(\mu_0^2 a^2), \\
c_{00,4,A(B)}^{13}(\mu_0 a) = \mu_0 a c_{00,4,A(B)}^{13}(\mu_0^2 a^2), \quad c_{10,5,A(B)}^{13}(\mu_0 a) = \mu_0 a c_{10,5,A(B)}^{13}(\mu_0^2 a^2),
$$

(38)

where only the $\mu_0 a$ dependence is explicitly written, and the other $c_{t,n}^{13}$’s are even functions
of $\mu_0 a$. We then finally have

$$
\mathcal{O}_{\text{eff}}^{01,3} = a^2 \mu_0 c_{10,4,A}^{13} \mathcal{O}_{10,4,A}^{13} + a^2 \mu_0 c_{10,5,B}^{13} \mathcal{O}_{10,5,B}^{13} + a^3 \mu_0 c_{11,4}^{13} \mathcal{O}_{11,4}^{13} + \cdots
$$

(39)
where all dimensionless functions are even in $\mu a$. It is important to observe that all operators with $t = 0$ contain only even powers of $a$, while those with $t = 1$ have only odd powers of $a$.

Repeating the analysis given above for all operators which appear in the lattice action and introducing renormalized quantities (see appendix A for more details), we obtain

\[
S_{\text{QCD}} \Leftrightarrow S_{\text{eff}} = S_0 + m_q S_m + \sum_{n=1}^{\infty} \left[ a^{2n} S_{2n}^0 + a^{2n-1} S_{2n-1}^1 \right],
\]

(40)

where

\[
S_0 = \int d^4 x \left\{ \bar{\psi}_R \left( \gamma_\mu D_\mu + i \mu_R \gamma_5 \tau^3 \right) \psi_R(x) - \frac{1}{4} F_{\mu\nu,R}^2(x) \right\},
\]

(41)

\[
m_q S_m = m_R S_{mR} \equiv m_R \int d^4 x \bar{\psi}_R \psi_R(x),
\]

(42)

\[
S_{2n}^0 = \int d^4 x \left[ \sum_i Z_{0i,2n+4}^i \cdot \mathcal{O}_{R,i}^{0i,2n+4}(x) + \sum_i Z_{0i,2n+3}^i \cdot \mu_R \cdot \mathcal{O}_{R,i}^{0i,2n+3}(x) \right],
\]

(43)

\[
S_{2n-1}^1 = \int d^4 x \left[ \sum_i Z_{1i,2n+3}^i \cdot \mathcal{O}_{R,i}^{1i,2n+3}(x) + \sum_i Z_{1i,2n+2}^i \cdot \mu_R \cdot \mathcal{O}_{R,i}^{1i,2n+2}(x) \right].
\]

(44)

Renormalized parameters are introduced as\(^6\)

\[
\begin{align*}
\mu_0 &= Z_{\mu}^{-1}(g_R, \log(\Lambda a), m_R a, \mu_R^2 a^2) \mu_R, \\
m_q &= Z_m^{-1}(g_R, \log(\Lambda a), m_R a, \mu_R^2 a^2) m_R, \\
g &= Z_G^{1/2}(g_R, \log(\Lambda a), m_R a, \mu_R^2 a^2) g_R,
\end{align*}
\]

(45)

where $g_R, m_R, \mu_R$ are kept constant and finite as $a \to 0$. We also define renormalized fields as

\[
\bar{\psi}_R = Z_{\bar{\psi}}^{1/2}(g_R, \log(\Lambda a), m_R a, \mu_R^2 a^2) \bar{\psi}, \quad A_{\mu R} = Z_{A_{\mu}}^{1/2}(g_R, \log(\Lambda a), m_R a, \mu_R^2 a^2) A_\mu.
\]

(46)

A subscript $R$ in $\mathcal{O}_{R,i}^{t,p,n}$ means that the operators are expressed in terms of renormalized fields, and therefore $Z_{t,p,n}^i = Z_{t,p,n}^i(g_R^2, \log(\Lambda a), m_R a, \mu_R^2 a^2)$.

Similarly, applying the selection rules to an arbitrary operator $\mathcal{O}_{\text{lat}}^{t,p,d}$ (again we give more details in appendix A), we obtain

\[
\mathcal{O}_{\text{lat}}^{t,p,d} \Leftrightarrow \mathcal{O}_{\text{eff}}^{t,p,d} = \sum_{l=-d}^{\infty} a^l \left[ \sum_i \mathcal{O}_{R,i}^{t+l,p,d+l} + \mu_R \sum_i \mathcal{O}_{R,i}^{t+l,p,d+l-1} \right].
\]

(47)

\(^6\) Note that the renormalization differs from the one usually employed in the Symanzik improvement program.
where \([t + l] = t + l \mod(2)\), \(\bar{p} = 1 - p\), and coefficients \(c_{t,n,p,n,i}^{\mu,R} d\) and \(\tilde{c}_{t,n,p,n,i}^{\mu,R} d\) are even functions of \(\mu_R a\). Note here that, even though we use the same notations as in eq. (27), these coefficients are functions of \(g^2_R, \log(\Lambda a), m_R a\) and \(\mu_R^2 a^2\), therefore the functional forms are different from the original ones. Formula (47) tells us that, if the lattice operator has \(t = 0\), operators with \(t_n = 0\) in the Symanzik expansion appear with even powers of \(a\) while those with \(t_n = 1\) are associated with odd powers of \(a\). This is reversed in the case that the lattice operator has \(t = 1\): operators with \(t_n = 0\) are multiplied by odd powers of \(a\) in the Symanzik expansion and those with \(t_n = 1\) by even powers of \(a\).

In order to obtain a finite result in the continuum limit, we have to remove possible power divergences in the expansion (47) by subtracting lower dimensional lattice operators from the original operator \(O_{\text{lat}}\), in addition to subtractions of \(\log(\Lambda a)\) divergences including a possible mixing among operators whose canonical dimension is same as the original operator. We denote such a renormalized and subtracted operator as \(O_{\text{lat, sub}}\), which corresponds to

\[
O_{\text{lat}, \text{sub}, \mu,R}^{l_p,d} \Leftrightarrow O_{\text{eff, R, sub}}^{l_p,d} = O_{R}^{l_p,d} + \sum_{l=1}^{\infty} a^l O_{R; tpd}^{[t+l], d+l},
\]

\[
O_{R; tpd}^{[t+l], d+l} = \sum_i c_{[t+l], p+d+l,i}^{l_p,d} O_{R,i}^{[t+l], p+d+l} + \mu_R \sum_i \tilde{c}_{[t+l], p+d+l-1,i}^{l_p,d} O_{R,i}^{[t+l], p+d+l-1},
\]

where \(d + l\) in the short-hand notation \(O_{R; tpd}^{[t+l], d+l}\) represents a canonical dimension of the operator and \([t + l]\) labels the transformation property under \(T_1\):

\[
T_1 : O_{R; tpd}^{[t+l], d+l} \rightarrow (-1)^{t+l} O_{R; tpd}^{[t+l], d+l}.
\]

We conclude that, in terms of this general description in the Symanzik theory, the maximal twist condition corresponds to the property that the continuum theory is invariant under the \(T_1\) transformation. This condition then entails \(m_R = 0\), which we call exact invariance condition. However, it can be relaxed to \(m_R = O(a)\), which we call weak invariance condition. Imposing either of these we find

\[
\langle O_{R}^{l_p,d} \rangle_{\sum_{0}^{m_R} S_{0} + m_R S_{m_R}} = \frac{1}{Z} \int D\psi_R D\bar{\psi}_R DA_{\mu,R} e^{S_0 + m_R S_{m_R}} O_{R}^{l_p,d} = \begin{cases} 0 & \text{exact} \\ O(a) & \text{weak} \end{cases}
\]

for an arbitrary continuum operator \(O_{R}^{l_p,d}\) which is odd under \(T_1\). (In the operator formalism, this condition expresses the fact that the vacuum \(|0\rangle\) of \(S_0 + m_R S_{m_R}\) is invariant under \(T_1\): \(T_1|0\rangle = 0\) or \(O(a)\).)
Assuming the maximal twist condition is satisfied, i.e. $m_R = O(a)$ at least, we now consider the following correlation function:

$$
\langle \mathcal{O}^{\text{lat},R,\text{sub}}(\{x\}) \rangle \equiv \frac{1}{Z_{\text{lat}}} \int \mathcal{D}\psi_L \mathcal{D}\bar{\psi}_L \mathcal{D}U \; e^{S_{\text{SMQCD}}} \mathcal{O}^{\text{lat},R,\text{sub}}(\{x\})
$$

(52)

where $Z_{\text{lat}}$ is the partition function defined by $\langle 1 \rangle = 1$. In terms of the Symanzik effective theory, this correlation function corresponds to

$$
\langle \mathcal{O}^{\text{eff},R,\text{sub}}(\{x\}) \rangle = \langle \mathcal{O}^{\text{eff},R,\text{sub}}(\{x\}) \rangle_{\text{eff}}
$$

(53)

where we define

$$
\langle \mathcal{O} \rangle_{\text{S}} = \frac{1}{Z} \int \mathcal{D}\psi_R \mathcal{D}\bar{\psi}_R \mathcal{D}A_{\mu,R} e^{S} \mathcal{O}.
$$

(54)

For simplicity, we first consider the $m_R = 0$ case. In this case we have

$$
e^{S_{\text{eff}}} = e^{S_0} \exp \left\{ \sum_{n=1}^{\infty} \left[ a^{2n} S_2^n + a^{2n-1} S_{2n-1}^1 \right] \right\} \equiv e^{S_0} \sum_{n=0}^{\infty} a^n S^{(n)}
$$

(55)

where we define $a^n S^{(n)}$ to be the sum of the $a^n$ terms in eq. (55). For example, the first few terms are given as

$$
S^{(0)} = 1, \quad S^{(1)} = S_1^1, \quad S^{(2)} = S_2^0 + \frac{(S_1^1)^2}{2!}.
$$

(56)

Under the $T_1$ transformation, they behave as

$$
T_1 : S^{(n)} \to (-1)^n S^{(n)}.
$$

(57)

By expanding both action and operator, we have

$$
\langle \mathcal{O}^{\text{eff},R,\text{sub}}(\{x\}) \rangle_{\text{eff}} = \langle \mathcal{O}_R^{\text{eff},R,\text{sub}}(\{x\}) + \sum_{l=1}^{\infty} a^l \mathcal{O}_{R^2,t pd}^{[l+1],d+l}(\{x\}) \rangle \sum_{n=0}^{\infty} a^n S^{(n)} \rangle_{S_0}.
$$

(58)

Since terms with $t + l + n = \text{odd}$ in the above expansion vanish from the maximal twist condition (51), terms with $t + l + n = 2s$ remain as

$$
\langle \mathcal{O}^{\text{eff},R,\text{sub}}(\{x\}) \rangle_{\text{eff}} = \delta_{t,0} \langle \mathcal{O}_R^{\text{eff},R,\text{sub}}(\{x\}) \rangle_{S_0} + \sum_{s=1}^{\infty} a^{2s-t} \sum_{l=0}^{2s-t} \langle \mathcal{O}_{R^2,t pd}^{[l+1],d+l}(\{x\}) \rangle S^{(2s-t-1)} \rangle_{S_0}.
$$

(59)
where we define

\[ F_d^{2s-t}(\{x\}, g_R^2, \log(\Lambda a), \mu_R; \mu_R^2 a^2) = \sum_{l=0}^{2s-t} \langle O_R^{l+1, d+l}(\{x\}) \rangle \mathcal{S}^{(2s-t-l)} S_0, \]  

which is an analytic function for small \( \mu_R^2 a^2 \) (the last argument). This expression tells us that

\[ \langle O_{tp,d}^{\text{eff}, R, \text{sub}}(\{x\}) \rangle_{\text{eff}} = \begin{cases} 
\langle O_R^{l, d}(\{x\}) \rangle_{S_0} + a^2 F_d^2 + a^4 F_d^4 + \cdots, & t = 0 \\
F_d^1 + a^3 F_d^3 + \cdots, & t = 1 
\end{cases}. \]  

(61)

This proves automatic O(\( a \)) improvement at maximal twist that scaling violations of \( T_1 \) invariant quantities are even functions of \( a \): \( a^{2n+1} \) contributions are completely absent, while \( T_1 \) non-invariant quantities have only contributions odd in \( a \) and vanish in the continuum limit. This completes our proof of automatic O(\( a \)) improvement at maximal twist. (Here O(\( a^n \)) (\( n \geq 1 \)) represents contributions of the form \( a^{n+s}[\log(\Lambda a)]^k \) with \( s, k = 0, 1, 2, \cdots \)).

Notice that this proof for automatic O(\( a \)) improvement is not restricted to on-shell quantities, and the equation of motion is not required at all for the proof. It is also noted that the proof does not require \( \mu_R = 0 \): Automatic O(\( a \)) improvement is realized also for the massive theory.

If \( m_R = O(a) \) (weak invariance), the proof goes through with just a little modification (see appendix A). In the special case that \( m_R \) is odd in \( a \) (\( m_R = a f(a^2) \)), we obtain eq. (61) with a little modification in \( F_d^n \), while in more general cases with \( m_R = O(a) \) the result becomes

\[ \langle O_{\text{eff}, R, \text{sub}}^{l, d}(\{x\}) \rangle_{\text{eff}} = \begin{cases} 
\langle O_R^{l, d}(\{x\}) \rangle_{S_0} + O(a^2), & t = 0 \\
O(a), & t = 1 
\end{cases}. \]  

(62)

C. Ambiguity of the maximal twist condition in the lattice theory

In this subsection we consider the maximal twist condition in the lattice theory and discuss the possible ambiguities of it.

In the Symanzik theory, maximal twist is uniquely defined by the condition that an arbitrary \( T_1 \) non-invariant operator \( O_{t=1}^{l, p, d} \) has a vanishing expectation value,

\[ \langle O_{t=1}^{l, p, d} \rangle_{S_0} = 0. \]  

(63)
Provided this condition is fulfilled, the expectation values of all $T_1$-odd operators vanish. Hence the particular choice for $O^{lp,d}$ is irrelevant, and in that sense the condition is unique. In the lattice theory, however, the maximal twist condition, which may be defined by

$$\langle O^{lp,d}_{\text{lat},R,\text{sub}} \rangle = 0,$$

(64)

depends on the choice of the operator $O^{lp,d}_{\text{lat},R,\text{sub}}$, and is therefore not unique. In order to discuss this we make the Symanzik expansion of (64), which gives (see appendix A for unexplained notation and the derivation)

$$0 = \langle O^{lp,d}_{\text{eff},R,\text{sub}} \rangle = aH^0_d(\mu_R; a^2, m_R^2, m_R a, \mu_R^2 a^2) + m_R H^1_d(\mu_R; a^2, m_R^2, m_R a, \mu_R^2 a^2).$$  

(65)

The solution $m^{\text{maximal}}_R$ to eq. (65), provided it is unique, is of the form $m^{\text{maximal}}_R = af(a^2)$, due to the symmetry of eq. (65) under the transformation $m_R \rightarrow -m_R$ and $a \rightarrow -a$. Therefore, according to the analysis in the previous subsection, scaling violations in $T_1$-invariant quantities are even in $a$.

A different choice for the lattice operator in (64) leads to a different solution $\tilde{m}^{\text{maximal}}_R = a\tilde{f}(a^2)$, so that the difference between the two definitions is of $O(a)$: $\Delta m^{\text{maximal}}_R = a\{f(a^2) - \tilde{f}(a^2)\}$. Note that a solution $m^{\text{maximal}}_R$ in general depends on $\mu_R$, inherited from the $\mu_R$ dependence of $H^0_d$.

Let us consider some examples for maximal twist in the lattice theory. A simple one is given by

$$\langle (\bar{\psi}\psi)_{\text{lat},R,\text{sub}} \rangle = 0.$$  

(66)

Unfortunately, this definition is not very useful in practice, since the subtraction of power divergences necessary for $\langle \bar{\psi}\psi \rangle$ prevents a reliable determination of this VEV in the lattice theory. Instead one may take $O_{\text{lat}}(x,y) = A^0_\mu(x)P^a(y)$ or $O_{\text{lat}}(x,y) = \partial_\mu A^a_\mu(x)P^a(y)$ ($a = 1,2$), as was done in Refs. [3, 4, 14]:

$$\langle A^a_\mu(x)P^a(y) \rangle = 0 \quad \text{or} \quad \langle \partial_\mu A^a_\mu(x)P^a(y) \rangle = 0,$$  

(67)

where $A^a_\mu$ and $P^a$ denote the axial vector current and pseudo scalar density, respectively. Yet another choice is [30]

$$\langle A^3_\mu(x)P^3(y) \rangle = 0.$$  

(68)

This seems plausible at small enough $a$ and $\mu_R$, since the solution is unique in the Symanzik theory.
Depending on the choice for the axial vector current, either the local or the conserved one, the conditions (67) lead to a different definition of maximal twist. However, the difference will be again of $O(a)$.

We close this subsection with a final comment. Any maximal twist condition in the lattice theory determines a value for the bare mass $m_0$ as a function of the bare twisted mass $\mu_0$. It has been suggested to tune the bare mass to its critical value $m_0 = m_{cr}$ where the pion mass vanishes in the untwisted theory. However, this condition is not related to $T_1$ invariance. For example, contributions from excited states violate eq. (67) even at $m_\pi = 0$. Consequently, the pion mass definition does not correspond to maximal twist according to the $T_1$ invariance condition.

III. WCHPT ANALYSIS FOR $O(a)$ IMPROVEMENT IN TMQCD

According to our analysis in the Symanzik effective theory, maximal twist is determined by requiring $T_1$ invariance of expectation values. For example, for maximal twist we could impose

$$\langle \bar{\psi} \psi \rangle = 0, \quad \langle \bar{\psi} i\gamma_5 \tau_3 \psi \rangle = v(M_R) \neq 0. \quad (69)$$

In this section we study this condition in Wilson Chiral Perturbation Theory (WChPT) [15, 16, 27, 28], and check explicitly whether $O(a)$ improvement is indeed realized. We also compare to some other definitions of maximal twist, which have already been used in numerical simulations.

Automatic $O(a)$ improvement has been studied before in WChPT for various definitions of the twist angle and also for different power countings, which are determined by the relative size between the quark masses and the lattice spacing [12, 29, 30, 31]. Our analysis follows closely the one in Ref. [12]. We work mainly in the regime where $m$ and $\mu$ are of $O(a^2)$ unless stated otherwise. It is in this regime where the phase structure of the theory is determined by the competition between the mass term and lattice spacing artifacts [18, 32], and where the differences of the various maximal twist definitions start to become relevant [12]. In contrast to Ref. [12], we work at higher order and include the terms of $O(ma, \mu a, a^3)$ in our

---

8 Since the parameters $m$ and $\mu$ in WChPT are renormalized parameters we drop the subscript “$R$” in this section.
These terms, which were also included in Refs. [31, 33], provide a nontrivial check for automatic $O(a)$ improvement, since they are odd in the lattice spacing and, according to our Symanzik analysis, should not contribute to observables.

A. Chiral Lagrangian and power counting

In terms of the $SU(2)$ matrix-valued field $\Sigma$, which transforms under chiral transformations as $\Sigma \rightarrow L \Sigma R^\dagger$, the chiral effective Lagrangian reads

$$
\mathcal{L}_\chi = \frac{f^2}{4} \langle \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \rangle - \frac{f^2}{4} \langle \hat{m}^\dagger \Sigma + \Sigma^\dagger \hat{m} \rangle - \frac{f^2}{4} \langle \hat{a}^\dagger \Sigma + \Sigma^\dagger \hat{a} \rangle 
+ (W_4 + W_5/2) \langle \partial_\mu \Sigma^\dagger \partial_\mu \Sigma \rangle \langle \hat{a}^\dagger \Sigma + \Sigma^\dagger \hat{a} \rangle 
- (W_6 + W_8/2) \langle \hat{m}^\dagger \Sigma + \Sigma^\dagger \hat{m} \rangle \langle \hat{a}^\dagger \Sigma + \Sigma^\dagger \hat{a} \rangle 
- (W_6' + W_8'/2) \langle \hat{a}^\dagger \Sigma + \Sigma^\dagger \hat{a} \rangle^2 
- W_{c_1} \langle \hat{a}^\dagger \Sigma + \Sigma^\dagger \hat{a} \rangle^3 - W_{c_2} \langle \hat{a}^\dagger \hat{a} \rangle \langle \hat{a}^\dagger \Sigma + \Sigma^\dagger \hat{a} \rangle - W_X \langle \hat{a}^\dagger \hat{m} + \hat{m}^\dagger \hat{a} \rangle.
$$

The terms through $O(a^2)$ have been previously constructed [18, 34]. Two terms of $O(a^3)$ in the last line, which were also included in Refs. [31, 33], are easily derived with the spurion fields in Ref. [35]. Note that the $O(ma)$ term proportional to $W_X$ does not depend on $\Sigma$. This term is usually neglected since it does not contribute to the pseudo scalar masses and decay constant. Here, however, we will need it since it gives a contribution to the condensates.

The coefficients $f, B$ are familiar low energy coefficients of continuum chiral perturbation theory [36, 37], while all the $W$’s are additional low-energy parameters associated with the nonzero lattice spacing contributions [16, 35]. As usual, angled brackets denote traces over the flavor indices and the short-hand notation

$$
\hat{m} = 2B(m + i\mu \tau_3) \equiv 2Bm' e^{i\omega L \tau_3}, \quad \hat{a} = 2W_0 a, \quad (71)
$$

is used [38]. The mass parameters $m$ and $\mu$ denote the renormalized untwisted and twisted mass [2], which are defined according to

$$
m = Z_m (m_0 - m_{c_1}), \quad \mu = Z_\mu \mu_0. \quad (72)
$$

$^9$ The renormalization constants $Z_m, Z_\mu$ are related to the renormalization constant $Z_A$ of the axial vector, $Z_A = Z_m / Z_\mu$, which follows from the vector and axial vector Ward identities [2].
Even though the critical mass $m_{cr}$ includes the additive shift proportional to $1/a$, it does not include certain contributions coming from the $O(a, a^2)$ terms in the chiral Lagrangian \[15\]. For example, the third term in the first line of (70) gives rise to an $O(a)$ shift in the critical mass.\[10\]

Our power counting is based on the assumption that $m \approx a^2$ \[12, 28, 39\], where $m$ stands for both the untwisted and the twisted mass and for $p^2$ (proper powers of $\Lambda_{QCD}$ are, as usual in this type of argument, understood). Since $m$ and $a$ are smaller than one we have the inequalities

$$m \approx a^2 > ma \approx a^3 > m^2 \approx ma^2 \approx a^4.$$  (73)

According to this power counting the terms of $O(m, a^2)$ in the chiral Lagrangian are of leading order (LO), while the $O(ma, a^3)$ contributions are of next to leading order (NLO). Note that the size of the $O(a)$ term does not matter for the power counting, since it only contributes to the critical quark mass.

### B. Gap equation

Starting from the chiral Lagrangian a gap equation for the ground state of the chiral effective theory can be derived. From the NLO expression of the chiral Lagrangian we find the potential

$$V_\chi = \frac{f^2}{4} 2Bm'(P^\dagger \Sigma + \Sigma^\dagger P) + \frac{f^2}{4} 2W_0a(1 + \tilde{c}_3a^2)(\Sigma + \Sigma^\dagger) - \frac{f^2}{16}c_2a^2(\Sigma + \Sigma^\dagger)^2$$

$$+ \frac{f^2}{16} \tilde{c}_2am'(\Sigma + \Sigma^\dagger)(P^\dagger \Sigma + \Sigma^\dagger P) + \frac{f^2}{64}c_3a^3(\Sigma + \Sigma^\dagger)^3 + \frac{2Bf^2m'}{4}c_Xa(P^\dagger + P).$$  (74)

Here we introduced $P = \exp i\omega_L \tau_3$ with $\tan \omega_L = \mu/m$, and the following combinations of low energy parameters:

$$c_2 = -32 (2W_6' + W_8') \frac{W_0^2}{f^2}, \quad \tilde{c}_2 = 32 (2W_6 + W_8) \frac{W_0B}{f^2},$$

$$c_3 = 64W_{c1} \frac{(2W_0')^3}{f^2}, \quad \tilde{c}_3 = 32W_{c2} \frac{W_0^2}{f^2}, \quad c_X = 8W_X \frac{W_0}{f^2}. \quad (75)$$

These parameters are dimensionful and have $[c_2] = 4$, $[\tilde{c}_2] = [\tilde{c}_3] = 2$, $[c_3] = 5$ and $[c_X] = 1$.

\[10\] This term is often absorbed in the untwisted mass, giving rise to the so-called shifted mass \[15, 30, 31\].
Since a twisted mass term breaks flavor symmetry we make the ansatz

$$\Sigma_0 = e^{i\phi \gamma_3}$$  \hspace{1cm} (76)

for the ground state, and this ground state is determined by $dV_\chi/d\phi = 0$ with

$$V_\chi = 2Bf^2(mt + \mu \sqrt{1 - t^2}) + 2f^2W_0 a(1 + \tilde{c}_3 a^2)t - f^2c_2a^2t^2
+ f^2\tilde{c}_2 a(mt + \mu \sqrt{1 - t^2})t + f^2c_3 a^3 t^3 + 2Bf^2c_\chi ma.$$  \hspace{1cm} (77)

Taking the derivative with respect to $\phi$ in (77) we obtain a gap equation for

$$t = \cos \phi,$$  \hspace{1cm} (78)

which can be brought into the form

$$\sqrt{1 - t^2} \left[ \chi - t + 2\beta_m t + \gamma t^2 \right] = \alpha \left[ t - \beta_\mu (1 - 2t^2) \right],$$  \hspace{1cm} (79)

where we introduced the dimensionless parameters

$$\alpha = \frac{2B\mu}{2c_2 a^2}, \quad \chi = \frac{2Bm + 2W_0 a(1 + \tilde{c}_3 a^2)}{2c_2 a^2},$$

$$\beta_m = \frac{\tilde{c}_2 a m}{2c_2 a^2}, \quad \beta_\mu = \frac{\tilde{c}_2 a}{2B}, \quad \gamma = \frac{3c_3 a^3}{2c_2 a^2}.$$  \hspace{1cm} (80)

In the following we will assume

$$|\beta_\mu| < 1, \quad |\beta_m| < 1, \quad |\gamma| < 1,$$  \hspace{1cm} (81)

which can be justified by a naive dimensional analysis when all dimensionfull constants are assumed to be of $O(\Lambda_{QCD})$ together with the conditions $a\Lambda_{QCD} < 1$ and $m/\Lambda_{QCD} < 1$.

Note the sign convention for the coefficient $c_2$. A positive sign corresponds to the scenario with spontaneous parity-flavor breaking [15], which guarantees the existence a massless pion [21]. A negative coefficient $c_2$ results in a scenario with a first order phase transition [18, 32]. 11

The details of the discussion of $O(a)$ improvement differ depending on the scenario for the phase diagram. In the rest of this section we are mainly interested in the scenario with $c_2 > 0$, where spontaneous parity-flavor breaking causes some subtleties for automatic $O(a)$ improvement. These subtleties are absent for $c_2 < 0$ and we come back to this scenario at the end of this section.

11 See also Ref. [31] where it has been shown that the NLO terms in the chiral Lagrangian do not change the existence of two qualitatively different scenarios for the phase diagram.
C. Condition for $O(a)$ improvement in WChPT

Taking derivatives of $V_{\chi}$ with respect to $m$ and $\mu$, the two VEVs $\langle \bar{\psi} \psi \rangle$ and $\langle \bar{\psi} i \gamma_5 \tau_3 \psi \rangle$ are easily computed with the result

\[
\langle \bar{\psi} \psi \rangle \equiv \frac{dV_{\chi}}{dm} = 2 f^2 B [(1 + \beta_\mu t) t + c_X a] \\
\langle \bar{\psi} i \gamma_5 \tau_3 \psi \rangle \equiv \frac{dV_{\chi}}{d\mu} = 2 f^2 B (1 + \beta_\mu t) \sqrt{1 - t^2}. \tag{82}
\]

Therefore, the $T_1$ invariance condition (69) corresponds to $t = -c_X a + O(a^3)$ in WChPT. If general scalar and pseudoscalar operators are employed for $\bar{\psi} \psi$ and $\bar{\psi} i \gamma_5 \tau_3 \psi$, these results are modified by $O(a)$ stemming from the effective operators in the Symanzik effective theory \[40\]. This leads to

\[
\langle \bar{\psi} \psi \rangle = 2 f^2 B \left[ t (1 + c_S a t) + \tilde{c}_S a \right] \\
\langle \bar{\psi} i \gamma_5 \tau_3 \psi \rangle = \frac{2 f^2 B}{Z_P} (1 + c_P a t) \sqrt{1 - t^2}. \tag{83}
\]

Nevertheless, even in this case the condition (69) leads to a similar result: $t = -\tilde{c}_S a + O(a^3)$.

We would find a similar result using the alternative condition $\langle A^2_\mu P^2 \rangle = 0$, which is equivalent to $\cot \omega_{WT} = 0$ with

\[
\cot \omega_{WT} \equiv \frac{\langle A^2_\mu P^2 \rangle}{\langle V^1_\mu P^2 \rangle}. \tag{84}
\]

Note that $A^2_\mu$ is $T_1$-odd while $V^1_\mu$ and $P^2$ are $T_1$-even. Provided Noether currents are used for $A^2_\mu$ and $V^1_\mu$ one finds (see also appendix B)

\[
\langle 0|A^2_{\mu=0}\pi_2 \rangle = f m_\pi t (1 + c_0 a t), \quad \langle 0|V^1_{\mu=0}\pi_2 \rangle = f m_\pi \sqrt{1 - t^2} (1 + c_0 a t), \tag{85}
\]

where we defined the coefficient

\[
c_0 = 16 (2 W_4 + W_5) \frac{W_0}{f^2}, \tag{86}
\]

in analogy to the definitions in Eq. \[13\]. This leads to $\cot \omega_{WT} = \cot \phi$, hence the condition $\langle A^2_\mu P^2 \rangle = 0$ implies $t = 0$. The result differs if one uses general non-Noether currents. Additional contributions of $O(a)$ appear in the effective operators in the Symanzik expansion, which carry over to the chiral effective theory as well:

\[
\langle 0|A^2_{\mu=0}\pi_2 \rangle = \frac{f m_\pi}{Z_A} \left[ t (1 + c_A at) - \tilde{c}_A a \right], \quad \langle 0|V^1_{\mu=0}\pi_2 \rangle = \frac{f m_\pi}{Z_V} \sqrt{1 - t^2} [1 + c_V at]. \tag{87}
\]
Note that here the currents on the left hand side are bare currents, as one can infer from the explicit appearance of the renormalization constants $Z_A, Z_V$. The way we have written the expectation values correspond to what can be directly measured in a lattice simulation without the knowledge of $Z_A, Z_V$. For $\cot \omega_{WT}$ we find

$$\cot \omega_{WT} = \frac{t(1 + c_A at) - \tilde{c}_A a}{\sqrt{1 - t^2}} \times \frac{Z_V}{Z_A} \times \frac{1}{1 + c_V at},$$

(88)

and the maximal twist condition $\cot \omega_{WT} = 0$ gives $t = \tilde{c}_A a + O(a^3)$, which has the same form as in the case of the VEVs. Note here that imposing a non-vanishing value for $\cot \omega_{WT}$ is sensitive to the ratio $Z_V/Z_A$ as well as to $c_A, \tilde{c}_A$ and $c_V$. As a final example we consider the condition $\langle A_\mu^A P_3 \rangle = 0$ introduced in $[30]$. Since

$$\langle 0 | P_3 | \pi^3 \rangle = \frac{fB}{Z_P} \left[ t - (1 - 2t^2)c_P a \right]$$

(89)

we again find $t = c_P a + O(a^3)$.

To summarize, imposing $T_1$ invariance we find the condition $t = X a + O(a^3)$ with some constant $X$. This constant depends on the specific choice for the operator in the matrix element. Nevertheless, all definitions guarantee automatic $O(a)$ improvement, as we want to show next.

It is instructive to first consider the simpler condition $t = 0$ (which is equivalent to a vacuum angle $\phi = \pm \pi/2$). In this case the pseudo scalar mass and decay constant of charged pions, $m_\pi^2$ and $f_\pi$, are given by (see also appendix $[3]$)

$$m_\pi^2 = \frac{2B \mu}{\sqrt{1 - t^2}} \frac{1 + \beta_\mu t}{1 + c_0 at};$$

(90)

$$f_\pi = f \sqrt{1 - t^2} \left[ 1 + c_0 at \right].$$

(91)

These expressions are valid for arbitrary $t$, but for $t = 0$ they turn into the results familiar from leading order continuum ChPT,

$$m_\pi^2 = 2B\mu, \quad f_\pi = f.$$ 

(92)

Apparently there are no $O(a, a^3)$ corrections in these results. In addition, the $O(a^2)$ corrections are also absent, but this is not as surprising as one might first think. The charged pions are the Goldstone bosons associated with the spontaneous breaking of flavor and parity in the theory without a twisted mass term. Hence they must become massless when one enters the broken phase, i.e. when $\mu$ goes to zero. With the same argument one would also
conclude that no terms of order $O(a, a^3)$ terms are present. The same argument, however, does not apply to the $O(\mu a)$ terms, and their absence is indeed a non-trivial demonstration of automatic $O(a)$ improvement once $T_1$ invariance is imposed.

It is now simple to show that we can relax $t = 0$ to the weaker condition $t = O(a)$ without loosing automatic $O(a)$ improvement.\(^{12}\) Suppose that $t = Xa$ with some constant $X$. If we insert this into (90) and (91) we find (after expanding the denominator)

$$m_\pi^2 = 2B\mu \left(1 + \left[\frac{c_2}{2B} - c_0 + \frac{X}{2}\right] Xa^2\right) + O(\mu a^4),$$

$$f_\pi = f \left(1 + [c_0 - X/2] Xa^2\right) + O(a^4).$$

Again no $O(a, \mu a)$ corrections appear. This demonstrates, within WChPT and at least for the two observables we have chosen, that $t = O(a)$, which follows from imposing $T_1$ invariance, is a sufficient condition for automatic $O(a)$ improvement.

\section*{D. Other conditions for maximal twist and $O(a)$ improvement}

In the following we want to compare the condition of $T_1$ invariance to some other conditions for maximal twist which are proposed in the literature. In particular we are interested in definitions where the untwisted mass $m_0$ is set to a particular value and kept fixed as one varies the twisted mass $\mu_0$. Such definitions obviously have a practical advantage for numerical simulations. Finding the $\mu_0$ dependent value $m_0(\mu_0)$ such that a matrix element like the ones in (66) or (67) vanish is computationally quite demanding, in particular in dynamical simulations. One can save a substantial amount of computer time if one does not need to do this tuning for each twisted mass one wants to simulate, but rather stay at one fixed value of $m_0$. However, such definitions do violate $T_1$ invariance for most $\mu_0$ values and it is therefore not obvious how this affects automatic $O(a)$ improvement. This is the issue we want to study in this section.

The following two definitions keep the untwisted mass constant and both have already been employed in quenched numerical simulations \cite{3, 4, 5, 6}:

1. PCAC mass definition. For a given (bare) twisted mass $\mu_0$ the untwisted mass $m_0(\mu_0)$

\(^{12}\) A similar argument that the theory is $O(a)$ improved for $t = O(a)$ has also been given independently by S. Sharpe \cite{41}.
is first tuned such that the PCAC quark mass, defined by

$$2m_{\text{PCAC}} = \frac{\langle \partial_\mu A_\mu^2 P^2 \rangle}{\langle p^2 P^2 \rangle},$$  \hfill (95)

vanishes. Then $$m_0(0) = \lim_{\mu_0 \to 0} m_0(\mu_0)$$ is used as the choice for $$m_0$$ of the PCAC mass definition for all $$\mu_0$$. Therefore, this definition is independent of $$\mu_0$$.

2. Pion mass definition. The bare untwisted quark mass is set to its critical quark mass where the pion mass vanishes at $$\mu_0 = 0$$. In practice this value is usually obtained in the untwisted theory by performing an extrapolation of $$m_\pi^2$$ data to the massless point.

In order to study these two definitions we have to translate (“match”) them to the corresponding ones in WChPT:

1. PCAC definition: The denominator in Eq. (95) is found to be given by

$$\langle 0 | P^2 | \pi_2 \rangle = Bf Z_P (1 + \beta_\mu t)$$  \hfill (96)

so that the PCAC condition reads

$$m_{\text{PCAC}} = \frac{Z_P t(1 + c_A a t) - \tilde{c}_A a}{Z_A \sqrt{1 - t^2}(1 + c_0 a t)} = 0.$$  \hfill (97)

This leads to $$t = \tilde{c}_A a + O(a^3)$$ for any non-zero $$\mu$$. Keeping, for simplicity, only the leading term and setting $$t = \tilde{c}_A a$$ into the gap equation, one finds

$$\chi = \tilde{c}_A a [1 - 2\beta_m - \gamma \tilde{c}_A a]$$  \hfill (98)

in WChPT. In the following we will assume this $$\chi$$ to be smaller than one. This is in accordance with our previously made assumption that all dimensionful coefficients are of order $$\Lambda_{\text{QCD}}$$ and $$a\Lambda_{\text{QCD}} < 1$$.

2. Pion definition: We need the expression for the pion mass in the untwisted theory. We cannot simply take the $$\mu \to 0$$ limit of Eq. (90), since $$t$$ is equal to 1 in this limit and

---

13 Note that one can choose $$m_0(\mu_0)$$ at a fixed non-vanishing value $$\mu_0$$ as a (different) PCAC mass definition. Employing such a definition requires the determination of $$m_0(\mu_0)$$ at only one $$\mu_0$$ value. Taking the $$\mu_0 \to 0$$ limit, on the other hand, requires the determination of $$m_0(\mu_0)$$ for various twisted mass values and a subsequent extrapolation. Hence the latter is numerically more demanding.
the whole expression is ill-defined. Instead, we first use the gap equation and rewrite the pion mass as

\[ m_\pi^2 = \frac{2c_2a^2}{1 + c_0at} \left[ \frac{\chi}{t} - 1 + 2\beta_m + \gamma t + 2\beta_\mu\alpha \frac{\sqrt{1 - t^2}}{t} \right]. \] (99)

Here the limit \( \mu \to 0 \) is well-defined and the condition \( m_\pi^2 = 0 \) reads

\[ \chi = 1 - 2\beta_m - \gamma. \] (100)

In order to check whether \( O(a) \) improvement is realized we have to verify that \( t \) is at least of \( O(a) \). To do so we have to solve the gap equation (79) with the \( \chi \) values in (98) and (100), respectively. It is not necessary to solve the gap equation exactly, approximate solutions will be sufficient for our purposes.

Let us assume \( t \ll 1 \), since we are interested in the small \( t \) case. In this case we can neglect the \( t^2 \) terms in (79) and obtain the approximate solution

\[ t \simeq \frac{\alpha\beta_\mu + \chi}{\alpha + 1 - 2\beta_m}. \] (101)

For the PCAC mass condition we set \( \chi \) to the value in (98) and find

\[ t \simeq a \frac{\tilde{c}_2\mu + 2\tilde{c}_A (c_2 + \tilde{c}_2W_0/B) a^2}{2B\mu + 2 (c_2 + \tilde{c}_2W_0/B) a^2}. \] (102)

Here we rewrote (98) as

\[ am = -\frac{W_0}{B} a^2 + O(a^4), \] (103)

and dropped all but the leading term proportional to \( a^2 \). Taking into account that the denominator in eq. (102) is always of \( O(a^2) \) or larger for \( c_2 + \tilde{c}_2W_0/B > 0 \), together with our convention that \( B > 0 \) and \( \mu > 0 \), \( t \) is always of \( O(a) \) and our assumption that \( t \ll 1 \) is consistently satisfied.\(^{14}\) The solution in eq. (102) is of the form \( t = aX \) which we used at the end of the previous section (cf. eqs. (93) and (94)), with \( X \) representing the fraction in (102). However, here the value of \( X \) does depend on the relative size between \( a \) and \( \mu \). For

\(^{14}\) Recall that we here consider the case with \( c_2 > 0 \). If \( c_2 + \tilde{c}_2W_0/B < 0 \), the assumption \( t \ll 1 \) could be violated at some value of \( \mu \). Therefore, in the latter case, we exclude such values of \( \mu \) in the following consideration.
small $a$ and fixed $\mu$ such that $2B\mu \gg 2(c_2 + \tilde{c}_2 W_0/B) a^2$, we can expand the denominator and find

$$t \approx \frac{\tilde{c}_2}{2B}, \quad (104)$$

so $X = \tilde{c}_2/2B$ and $t = O(a)$. Hence our discussion in the last section can be applied and we find $O(a^2)$ scaling violations in physical observables. On the other hand, for larger $a$ such that $\mu = O(a^2)$ we expect a modification of the simple linear $a$ dependence of $t$, and this leads to distortions of the expected $O(a^2)$ scaling violations. In the extreme case of small fixed $\mu$ and large $a$ such that $2B\mu \ll 2(c_2 + \tilde{c}_2 W_0/B) a^2$ we find

$$t \approx a\tilde{c}_A, \quad (105)$$

as expected from the definition according to the PCAC definition. Even though we recover a constant $X$, it is different from (104). Since the sign of the low energy constants are a priori not known, it is even possible that the slope of $t$ changes sign, depending on the size of $a$. This is of potential danger when one analyzes numerical data assuming a simple $O(a^2)$ scaling violation. The non-trivial $a$ dependence of the r.h.s. in eq. (102) is likely to obscure automatic $O(a)$ improvement in the region where $\mu$ is of $O(a^2)$.\(^\text{15}\)

Let us now turn to the pion mass definition. Inserting (100) into the approximate solution (101) we obtain

$$t \approx \frac{a\tilde{c}_2}{2B} \mu + 2(c_2 + \tilde{c}_2 W_0/B) a^2 \quad (106)$$

In order to derive this result we rewrote (100) as in eq. (103) and used, for simplicity, only the leading term proportional to $a^2$. As before we find $t \approx a\tilde{c}_2/2B = O(a)$ for small values of $a$, and, since the denominator is the same as for the PCAC definition we expect the modifications to become visible once the lattice spacing is such that $\mu$ is of $O(a^2)$. The details of the modification will be different because the numerator differs compared to the PCAC mass definition.

However, the crucial difference between the PCAC and the pion mass definition is that the approximation (101) will eventually break down for the pion mass definition, since $t$ goes

\(^\text{15}\) We emphasize that the non-trivial behaviour in $t = aX(a^2)$ does not mean that there are terms linear in $a$ in physical observables.
to 1 for a vanishing $\mu$. In that case the $t^2$ terms can no longer be ignored. Interestingly, the approximate solution (106) gives the correct value $t = 1$ at $\mu = 0$ even though this approximation can not be justified. A more careful analysis finds 

$$t \simeq 1 - \delta, \quad \delta = \frac{1}{2} \left[ \frac{\mu(2B + \tilde{c}_2a)}{(c_2 + \tilde{c}_2W_0/B)a^2} \right]^{2/3} = O\left( \frac{\mu}{a^2} \right)^{2/3}. \quad (107)$$

Therefore, the condition $t = O(a)$ for automatic $O(a)$ improvement is satisfied only for small lattice spacings where $2B\mu \gg 2(c_2 + \tilde{c}_2W_0/B)a^2$. Even though this bound is asymptotically satisfied as $a \to 0$, at a given non-vanishing lattice spacing the scaling violation becomes sizable for small twisted quark masses. In particular in the region $2B\mu \ll 2(c_2 + \tilde{c}_2W_0/B)a^2$, where $t \to 1$ in the $\mu \to 0$ limit, automatic $O(a)$ improvement fails.

This failure is seen when one inserts (107) into expression (91) for the decay constant, for example. Ignoring the small correction coming $\delta^2$ and higher powers we find

$$f_\pi = f\sqrt{2\delta}(1 + c_0a - c_0a\delta), \quad (108)$$

which obviously has a term linear in $a$. We emphasize that the reason for the presence of terms linear in $a$ is the leading 1 in $t = 1 - \delta$, and not the correction $\delta$ with the peculiar dependence on fractional powers of $a$, even though the overall factor $\sqrt{2\delta}$ complicates the whole $a$ dependence. The leading constant term is the crucial difference to the PCAC mass definition, where $t = O(a)$, and this constant term spoils automatic $O(a)$ improvement for lattice spacings where $2B\mu \ll 2(c_2 + \tilde{c}_2W_0/B)a^2$.

We summarize the results in this section as follows. Although the PCAC mass and pion mass definitions lead to $O(a)$ improvement for small enough lattice spacings, the asymptotic $O(a^2)$ behaviour can only be seen at lattice spacings where the bound $\mu \gg a^2\Lambda^3_{\text{QCD}}$ is realized for a given $\mu$. If this bound is not satisfied, the naively expected scaling violation is compromised, in particular for the pion mass definition, but also for the PCAC mass definition, even though to a much lesser extent. Note that the bound $2B\mu \gg 2(c_2 + \tilde{c}_2W_0/B)a^2$ excludes automatic $O(a)$ improvement for the massless theory in the case of the pion mass definition, which is not unexpected since it is identical to the massless (untwisted) Wilson theory.
E. Automatic O(a) improvement for the $c_2 < 0$ case

Since the condition for automatic O(a) improvement discussed in the previous section does not depend on the details of the lattice QCD dynamics, it seems applicable quite generally. However, there are circumstances when conditions like $\langle A_\mu^2 P^2 \rangle = 0$ or $\cot \omega_{WT} = 0$ cannot be satisfied. This is the case when the 1st order phase transition scenario of Refs. [15, 42] is realized.

Let us consider this case in WChPT. For simplicity we work at LO only and set $\tilde{c}_2 = c_3 = 0$ in the following argument. In this case, if $c_2 < 0$, a first order phase transition appears at $\chi = 0$ [15, 32] and $t$ is given by [12]

$$
 t = \begin{cases} 
 \sqrt{1 - \alpha^2}, & \alpha^2 < 1, \chi \to 0^+ \\
 -\sqrt{1 - \alpha^2}, & \alpha^2 < 1, \chi \to 0^- , \quad \alpha = \frac{\mu}{\mu_{\text{min}}} . \\
 0, & \alpha^2 \geq 1, \chi \to 0 
\end{cases}
$$

(109)

Although the condition $t = 0$ can be realized for $\chi = 0$, the twisted mass $\mu$ must satisfy the bound $\mu^2 \geq \mu_{\text{min}}^2$, where

$$
\mu_{\text{min}}^2 = \left( \frac{2c_2 a^2}{2B} \right)^2 .
$$

(110)

Therefore, automatic O(a) improvement can only be realized for $\mu^2 \geq \mu_{\text{min}}^2$, in contrast to the parity conservation definition for the $c_2 > 0$ case, where no restriction on $\mu$ needs to be imposed. Note, however, that the same restriction on $\mu$ (at LO) is required for the pion mass definition in the $c_2 > 0$ case.

This argument does not change qualitatively when one includes the NLO terms, as has been done in Ref. [31]. The phase transition line is no longer a straight line in the $m_0 - \mu_0$ parameter plane. If the term with $\tilde{c}_2$ is included the maximal twist condition which gives $t = 0$ becomes $\mu$ dependent and reads $\chi = -\mu \tilde{c}_2 a/(2c_2 a^2)$. Nevertheless, the conclusion that one has to stay above the phase transition line in order to be able to satisfy the maximal twist condition remains unchanged.

IV. CONCLUSION

In this paper we gave an alternative proof for automatic O(a) improvement in twisted mass lattice QCD at maximal twist. Whereas previous proofs [8, 13] used symmetries of the
bare lattice theory such as $m_q \rightarrow -m_q$ and $r \rightarrow -r$, we have used only symmetries of the leading part of the Symanzik effective theory in our proof. A more important observation, however, is that a precise definition for the twist angle, and therefore a condition for maximal twist, is determined dynamically by the ratio of two vacuum expectation values in the Symanzik theory:

$$\cot \theta = \frac{\langle \bar{\psi} \psi \rangle}{\langle \psi i \gamma_5 \tau^3 \psi \rangle}.$$  \hspace{1cm} (111)

At $\theta = \pm \pi/2$, which is equivalent to $T_1$ invariance of the vacuum in the continuum theory, scaling violations for all quantities are shown to be even powers in $a$, as long as they are invariant under the $T_1$ transformation. Non-invariant quantities, on the other hand, vanish as odd powers in $a$. It is also shown that the ambiguity for the maximal twist condition in the lattice theory does not spoil automatic $O(a)$ improvement.

We also studied the $T_1$ invariance condition in WChPT. As expected, for the pseudo scalar mass and the decay constant we find automatic $O(a)$ improvement.

We finally compared the $T_1$ invariance condition to two other definitions for maximal twist, the PCAC mass and the pion mass definition. Both definitions have already been used in numerical simulations. These definitions have the practical advantage that the untwisted mass is tuned to a fixed value independent of the twisted mass $\mu$. Although both definitions give asymptotic $a^2$ scaling violations for $\mu \gg a^2 \Lambda^3_{\text{QCD}}$, we have shown that the expected $a^2$ scaling can be obscured once this bound is violated. Hence naive continuum extrapolations can be deceiving and may lead to wrong results for these definitions of maximal twist. Here a WChPT analysis seems to be indispensable for a controlled continuum extrapolation.

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APPENDIX A: SOME DETAILS FOR THE PROOF OF O(a) IMPROVEMENT

1. Derivation of Symanzik action

We apply the Symanzik expansion to all operators which appear in the lattice action, as was done to \( O^{01.3}_{\text{lat}} \) in the main text. After a little algebra we obtain the following expression for the effective action:

\[
S_{\text{tmQCD}} \leftrightarrow S_{\text{eff}} = S_0 + m_q S_m + \sum_{n=1}^{\infty} \left[ a^{2n} S^0_{2n} + a^{2n-1} S^1_{2n-1} \right],
\]

where

\[
S_0 = \int d^4x \left[ Z_F O_{A}^{00,4}(x) + Z_F Z_{\mu \mu} O^{01,3}(x) + Z_G O_B^{00,4} \right],
\]

\[
S_m = \int d^4x Z_F \cdot Z_m O^{10,3}(x),
\]

and

\[
S^0_{2n} = \int d^4x \sum_i C_{00,2n+4}^i O_{i}^{00,2n+4}(x) + \sum_i C_{01,2n+3}^i \mu O_{i}^{01,2n+3}(x),
\]

\[
S^1_{2n-1} = \int d^4x \sum_i C_{10,2n+3}^i O_{i}^{10,2n+3}(x) + \sum_i C_{11,2n+2}^i \mu O_{i}^{11,2n+2}(x).
\]

In the definitions of \( S_{tn} \), the superscripts \( t_n = 0, 1 \) represent the transformation property under \( T_1 \):

\[
T_1 : S_{tn}^t \rightarrow (-1)^{t_n} S_{tn}^t.
\]

All coefficients which appear in the expressions above, such as \( Z_{\{F,\mu,\nu,G\}} \) and \( C_{\mu,\nu}^i \), are dimensionless functions of \( g^2, \log(\Lambda a) \), \( m_q a \) and \( \mu^2 a^2 \). They are given in terms of \( c_{t_n,\mu,\nu, \alpha, i}^{p,d} \), but their explicit forms are unimportant except for \( m_{\alpha} \), which is given by

\[
Z_F Z_m m_{\alpha} = c_{10,3}^{10,5} - c_{10,3}^{00,4} - \mu^2 a^2 c_{10,3}^{01,3}
\]

where \( \mu a \ c_{10,3}^{01,3} \equiv c_{10,3}^{01,3} \). Using the selection rule \( [31] \) it is easy to show that \( c_{10,3}^{10,5}, c_{10,3}^{00,4} \) and \( c_{10,3}^{01,3} \) are even functions of \( \mu a \).

Using renormalized fields \( [16] \) and parameters \( [45] \), we finally obtain \( [40] - [44] \) in the main text.
2. Symanzik expansion of operators

Using the selection rules eqs. (30) and (31), we here determine the structure of the Symanzik expansion for the lattice operator, given by

\[ \mathcal{O}_{\text{lat}}^{t,p,d} \leftrightarrow \mathcal{O}_{\text{eff}}^{t,p,d} = \sum_{n=0}^{\infty} a^{n-d} \sum_{l_n,p_n} c_{l_n,p_n,n,i_n}^{t,p,d} \mathcal{O}_{l_n,p_n,n_i}^{t,n,p_i,n}. \]  

(A8)

In the case with \( d = 2s \), the selection rule (30) gives

\[ \mathcal{O}_{\text{eff}}^{t,p,2s} = \sum_{l=0}^{\infty} \sum_{i} \left[ a^{2(l-s)} \left\{ c_{l+p,2l,i}^{t,p,2s} \mathcal{O}_{l,i}^{t,p,2l} + c_{l+p,2l,i}^{t,p,2s} \mathcal{O}_{l,i}^{t,p,2l} \right\} 
+ a^{2(l-s)+1} \left\{ c_{l+p,2l+1,i}^{t,p,2s} \mathcal{O}_{l,i}^{t,p,2l+1} + c_{l+p,2l+1,i}^{t,p,2s} \mathcal{O}_{l,i}^{t,p,2l+1} \right\} \right]. \]  

(A9)

where \( \bar{t} = 1 - t \) and \( \bar{p} = 1 - p \). Furthermore, using the second selection rule (31), we have

\[ \mathcal{O}_{\text{eff}}^{t,p,2s+1} = \sum_{l=0}^{\infty} \sum_{i} \left[ a^{2(l-s)} \left\{ c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} + c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} \right\} 
+ a^{2(l-s)+1} \left\{ c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} + c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} \right\} \right]. \]  

(A10)

Similarly, for \( d = 2s + 1 \) we obtain

\[ \mathcal{O}_{\text{eff}}^{t,p,2s+1} = \sum_{l=0}^{\infty} \sum_{i} \left[ a^{2(l-s)} \left\{ c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} + c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} \right\} 
+ a^{2(l-s)+1} \left\{ c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} + c_{l+p,2l+1,i}^{t,p,2s+1} \mathcal{O}_{l,i}^{t,p,2l+1} \right\} \right]. \]  

(A11)

Combining the results and rewriting the operators in terms of renormalized fields we finally obtain eq. (37).

3. Expressions for \( m_q = O(a) \) case

In the case of \( m_R = O(a) \), the expansion of \( e^{S_{\text{eff}}} \) becomes

\[ e^{S_{\text{eff}}} = e^{S_0} \exp \left\{ m_R S_{m_R} + \sum_{n=1}^{\infty} \left[ a^{2n} S_{2n}^0 + a^{2n-1} S_{2n-1}^1 \right] \right\} \]
\[ = e^{S_0} \sum_{k,n=0}^{\infty} \frac{m_R^k}{k!} \sum_{m_R} S_{m_R}^k a^n S^{(n)}. \]  

(A12)

Under the \( T_1 \) transformation, it is easy to see that

\[ T_1 : S_{m_R}^k \rightarrow (-1)^k S_{m_R}^k, \quad S^{(n)} \rightarrow (-1)^n S^{(n)}. \]  

(A13)
Expanding both the action and the operator, and using the fact that terms with \( t + l + k + n = \) odd in the above expansion vanish by the maximal twist condition \((A11)\), we obtain

\[
\langle O_{\text{eff, R, sub}}^\text{p.d.} (\{x\}) \rangle_{\text{S eff}} = \delta_{t,0} \langle O_R^\text{p.d.} \rangle_{S_0} + \sum_{s=1}^{\infty} \sum_{k=0}^{2s-t} a^{2s-k-t} m_R^k F_d^{2s-t,k}(\{x\}, g_R^2, \log (\Lambda a), \mu_R, m_R a, \mu_R^2 a^2) (A14)
\]

where

\[
F_d^{2s-t,k}(\{x\}, g_R^2, \log (\Lambda a), \mu_R, m_R a, \mu_R^2 a^2) = \sum_{l=0}^{2s-t-k} \langle O_{R, t+k}^\text{p.d.} (\{x\}) \rangle_{S_0} \tilde{S}_{k,l}^{(2s-t-k)} (A15)
\]

is an analytic function for small \( m_R a \) and \( \mu_R^2 a^2 \). This expression tells us that

\[
\langle O_{\text{eff, R, sub}}^\text{p.d.} (\{x\}) \rangle_{\text{S eff}} = \begin{cases} \langle O_R^\text{p.d.} \rangle_{S_0} + O(a^2), & t = 0 \\ O(a), & t = 1 \end{cases} (A16)
\]

for \( m_R = O(a) \).

If we take \( m_R \) odd in \( a \) such that \( m_R = af(a^2) \), we have

\[
\langle O_{\text{eff, R, sub}}^\text{p.d.} (\{x\}) \rangle_{\text{S eff}} = \delta_{t,0} \langle O_R^\text{p.d.} \rangle_{S_0} + \sum_{s=1}^{\infty} a^{2s-t} F_d^{2s-t}(\{x\}, g_R^2, \log (\Lambda a), \mu_R; a^2, \mu_R^2 a^2)
\]

where

\[
F_d^{2s-t}(\{x\}, g_R^2, \log (\Lambda a), \mu_R; a^2, \mu_R^2 a^2) = \sum_{k=0}^{2s-t} \langle f(a^2)^k F_d^{2s-t,k}(\{x\}, g_R^2, \log (\Lambda a), \mu_R; a^2 f^2, \mu_R^2 a^2). (A17)\]

4. Maximal twist condition on the lattice

The maximal twist condition on the lattice leads to

\[
0 = \langle O_{\text{lat R, sub}}^\text{p.d.} \rangle = \langle O_{\text{eff, R, sub}}^\text{p.d.} \rangle + \sum_{s=1}^{\infty} \sum_{k=0}^{2s-1} a^{2s-k-1} m_R^k F_d^{2s-1,k}
\]

\[
= \sum_{k=0}^{\infty} \sum_{s=k+1}^{\infty} \left[ m_R^{2k} a^{2(s-k)-1} F_d^{2s-1,2k} + m_R^{2k+1} a^{2(s-k-1)} F_d^{2s-1,2k+1} \right]
\]

\[
= aH_d^0(\mu_R; a^2, m_R^2, m_R a, \mu_R^2 a^2) + m_R H_d^0(\mu_R; a^2, m_R^2, m_R a, \mu_R^2 a^2), (A18)\]
where
\[ H_d^\delta(\mu_R; a^2, m_R^2, m_Ra, \mu_R^2a^2) \equiv \sum_{k=0}^{\infty} m_R^{2k} \sum_{s=k+1}^{\infty} a^{2(s-k-1)} F_d^{2s-1,2k+\delta}(g_R^2, \log(\Lambda a), \mu_R; m_Ra, \mu_R^2a^2) \]

for \( \delta = 0, 1 \), and we keep the dependency on \( g_R^2 \) and \( \log(\Lambda a) \) implicit in \( H_d^\delta \).

**APPENDIX B: WARD-Takahashi Angle, Pion Mass and Decay Constant in WCHPT**

In this appendix we provide some details about the calculation of \( \cot \omega_{WT} \) and the pseudo scalar masses and decay constant. At leading order in our power counting scheme this has already be done in Ref. [12], and we refer also to this reference.

Our first observable is the twist angle \( \omega_{WT} \) defined in eq. (84). Instead of eq. (84) the twist angle can also be expressed as
\[ \cot \omega_{WT} = \frac{\langle \partial_\mu A_\mu^2 P^2 \rangle}{\langle \partial_\mu V_\mu^2 P^2 \rangle}. \]

The extra derivative gives rise to an additional factor of the pion mass in both the numerator and the denominator, which consequently cancels.

The Noether’s currents appearing in the correlators on the right hand side of eq. (B1) are given by \( (a = 1, 2) \)
\[ V_\mu^a = V_{0,\mu}^a \left[ 1 + \frac{c_0a}{4} \langle \Sigma + \Sigma^\dagger \rangle \right], \quad V_{0,\mu}^a = \frac{if^2B}{4} \langle \tau_a (\Sigma \partial_\mu \Sigma^\dagger + \Sigma^\dagger \partial_\mu \Sigma) \rangle, \]  
\[ A_\mu^a = A_{0,\mu}^a \left[ 1 + \frac{c_0a}{4} \langle \Sigma + \Sigma^\dagger \rangle \right], \quad A_{0,\mu}^a = \frac{if^2B}{4} \langle \tau_a (\Sigma \partial_\mu \Sigma^\dagger - \Sigma^\dagger \partial_\mu \Sigma) \rangle. \]

The factor involving \( c_0a \) stems from the wave function renormalization due to the \( O(p^2a) \) contribution in chiral Lagrangian, cf. (70). In Ref. [12] \( \cot \omega_{WT} \) was computed without the \( O(a\mu, a^3) \) contributions. Repeating the calculation including these terms we find
\[ \cot \omega_{WT} = \frac{t}{\sqrt{1-t^2}} = \cot \phi. \]

This is the same result as in Ref. [12]. The functional dependence of \( \cot \omega_{WT} \) is unchanged, and the \( O(a\mu, a^3) \) corrections contribute only indirectly through the gap equation.

Result eq. (B4) assumes that the currents in the correlators are Noether’s ones that stem from the vector and axial vector Ward-Takahashi identities [1]. This means that the point
split currents must be used in the lattice simulation. However, local currents are often used instead of there point split counter parts. This introduces additional contributions proportional to $a$. Taking into account the leading corrections of $O(a)$ only we obtain

$$Z_V V_\mu^{a,\text{local}} = V_0 a \left[ 1 + \frac{c_V}{4} a \langle \Sigma + \Sigma \dagger \rangle \right],$$

(B5)

$$Z_A A_\mu^{a,\text{local}} = A_0 a \left[ 1 + \frac{c_A}{4} a \langle \Sigma + \Sigma \dagger \rangle \right] + \frac{ij^2 B}{4} \tilde{c}_A \partial_\mu \langle \Sigma - \Sigma \dagger \rangle,$$

(B6)

where $c_{V,A}$ and $\tilde{c}_A$ are additional coefficients parameterizing the lattice artifacts stemming from the currents. Using these currents the expression (B4) changes to

$$\cot \omega_{\text{WT}} = \frac{Z_V}{Z_A} \frac{1}{1 + ac_V t} \left( 1 + ac_A t \right) - \tilde{c}_A a \sqrt{1 - t^2},$$

(B7)

which is the result in Eq. (88).

In order to calculate the pion masses we expand $\Sigma$ around the vacuum configuration $\Sigma_0$ defined in (76). We parametrize the field $\Sigma$ in terms of the pion fields according to

$$\Sigma(x) = \Sigma_0^{\frac{7}{2}} \exp \left( \sum_{i=1}^{3} i \pi_i(x) t_i / f \right) \Sigma_0^{\frac{7}{2}}.$$

(B8)

Using this form in expression (74) for the potential energy we expand in powers of the field $\pi$. The contribution quadratic in $\pi$ leads to the pion mass formulae

$$m_{\pi^\pm}^2 = 2Bm' \cos(\phi - \omega_L) + 2W_0 a \cos \phi - 2c_2 a^2 \cos^2 \phi$$

$$+ 3c_3 a^3 \cos^3 \phi + 2\tilde{c}_2 a m' \cos \phi \cos(\phi - \omega_L),$$

(B9)

$$m_{\pi^3}^2 = m_{\pi^\pm}^2 + 2c_2 a^2 \sin^2 \phi - 6c_3 a^3 \sin^2 \phi \cos \phi - 2\tilde{c}_2 a m' \sin \phi \sin(\phi - \omega_L).$$

(B10)

Expressing this in terms of $m$ and $\mu$ and taking into account the gap equation we can express the mass for the charged pion alternatively as

$$m_{\pi^\pm}^2 = \frac{2B\mu}{\sqrt{1 - t^2}} \frac{1 + \beta \mu t}{1 + c_0 at}.$$  

(B11)

Note that the expression (B11) is not singular for $t = 1$. From the gap equation one can infer that $t = 1$ can be a solution only if $\mu = 0$, and in that case the result (B11) is not well defined. For $t \neq 0$ one can, using the gap equation, rewrite the pion mass formula as in (99), which is well behaved for $t = 1$.

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16 This parameterization differs slightly from the one used in Ref. [12]. This difference does not affect any of the results in this reference.
The decay constant is conveniently computed with the so-called indirect method \cite{1, 43}, which is based on an exact PCVC relation and does not require the computation of any renormalization constants:

\[
    f_\pi = \frac{2\mu}{m_\pi^2} \langle 0 | P^\pm | \pi^\mp \rangle.
\]

(B12)

In order to calculate the decay constant according to Eq. (B12) we need the matrix element of the pseudo scalar between the vacuum and the one pion state, where the pseudo scalar in the effective theory is defined by \((\tau_\pm = \frac{\pi_1 \pm i \pi_2}{\sqrt{2}})\)

\[
P^\pm = \frac{f^2 B}{4i} \left[ 1 + \frac{\beta_\mu}{4} (\Sigma + \Sigma^\dagger) \right] \langle \tau_\pm (\Sigma - \Sigma^\dagger) \rangle
\]

\[
    \pi_\pm = \frac{\pi_1 \pm i \pi_2}{\sqrt{2}}
\]

(B13)

The matrix element in eq. (B12) is readily calculated at tree level with the result

\[
    \langle 0 | P^\pm | \pi^\mp \rangle = f B (1 + \beta_\mu t).
\]

(B14)

With the expression for the charged pion mass we obtain

\[
    f_\pi = f (1 + c_0 at) \sqrt{1 - t^2}
\]

(B15)

for the decay constant.

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