Twisted mass chiral perturbation theory at next-to-leading order

Stephen R. Sharpe

School of Physics and Astronomy, University of Southampton, Southampton, SO17 1BJ, UK

Jackson M. S. Wu

Physics Department, University of Washington, Seattle, WA 98195-1560, USA

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We study the properties of pions in twisted mass lattice QCD (with two degenerate flavors) using chiral perturbation theory ($\chi$PT). We work to next-to-leading order (NLO) in a power counting scheme in which $m_q \sim a \Lambda_{QCD}^2$, with $m_q$ the physical quark mass and $a$ the lattice spacing. We argue that automatic $O(a)$ improvement of physical quantities at maximal twist, which has been demonstrated in general if $m_q \gg a \Lambda_{QCD}^2$, holds even if $m_q \sim a \Lambda_{QCD}^2$, as long as one uses an appropriate non-perturbative definition of the twist angle, with the caveat that we have shown this only through NLO in our chiral expansion. We demonstrate this with explicit calculations, for arbitrary twist angle, of all pionic quantities that involve no more than a single pion in the initial and final states: masses, decay constants, form factors and condensates, as well as the differences between alternate definitions of twist angle. We also calculate the axial and pseudoscalar form factors of the pion, quantities which violate flavor and parity, and which vanish in the continuum limit. These are of interest because they are not automatically $O(a)$ improved at maximal twist. They allow a determination of the unknown low energy constants introduced by discretization errors, and provide tests of the accuracy of $\chi$PT at NLO. We extend our results into the regime where $m_q \sim a^2 \Lambda_{QCD}^3$, and argue in favor of a recent proposal that automatic $O(a)$ improvement at maximal twist remains valid in this regime.

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I. INTRODUCTION

Twisted mass lattice QCD (tmLQCD) \cite{1, 2} is an alternative regularization for lattice QCD that has recently received considerable attention.\footnote{For a recent review see Ref. \cite{3}.} It has the potential to match the attractive features of improved staggered fermions (efficient simulations \cite{4}, absence of “exceptional configurations” \cite{1}, $O(a)$ improvement at maximal twist \cite{2}, operator mixing as in the continuum \cite{2, 6, 7}) while not sharing the disadvantage of needing to take roots of the determinant to remove unwanted degrees of freedom. Initial numerical investigations of the unquenched theory \cite{5, 6} have, however, found surprisingly large discretization errors, which manifest themselves as a non-trivial phase structure.\footnote{Indications of surprisingly large discretization errors have also been found in quenched tmLQCD at maximal twist \cite{10}. On the other hand, use of an improved gauge action reduces the discretization errors \cite{11}.} While these errors do not pose a fundamental problem, and, indeed, appear to conform to the expectations of chiral perturbation theory applied to the lattice theory \cite{12, 13, 14, 15}, they do suggest that a thorough investigation of the impact of discretization errors on the theory is called for.

Such an investigation is possible by applying the methods of chiral perturbation theory to tmLQCD at non-zero lattice spacing. The discretization errors are included systematically in a joint expansion in the lattice spacing, $a$, and the quark mass, $m_q$. The resulting “twisted mass chiral perturbation theory” (tm$\chi$PT) has been formulated previously \cite{14, 15, 16}, building on earlier work for the untwisted Wilson theory \cite{12, 17, 18}. It has been used to study pion masses and decay constants in the regime where $m_q \gg a \Lambda_{QCD}^2$ \cite{14}, and to study the phase structure of tmLQCD when $m_q \sim a^2 \Lambda_{QCD}^3$ \cite{13, 14, 15, 19, 20, 21}. Here we build upon our previous work \cite{14}, in which we determined the chiral Lagrangian at next-to-leading order (NLO) in a power counting scheme in which we treat $m_q \sim a \Lambda_{QCD}^2$, and use this to study all the quantities involving pions that do not involve final state interactions and are thus straightforward to calculate in simulations: masses (previously calculated in this regime in Ref. \cite{14}), condensates, vacuum to pion matrix elements, and matrix elements between single pion states (i.e. form factors). The operators we use are the vector and axial currents and the scalar and pseudoscalar densities.
Calculating these quantities allows us to address some of the issues that are of concern when using tmLQCD. In particular, what is the impact of the breaking of flavor and parity symmetries at non-zero lattice spacing? What are good quantities to use to determine the typical size of discretization errors? How does the automatic $O(a)$ improvement at maximal twist manifest itself in tmLQCD? How do different definitions of the twist angle, all of which are equivalent in the continuum limit, differ at non-zero lattice spacing? How can we test the reliability of tmLQCD applied at a given order? We return to these questions in the concluding section.

Another issue, which is of particular importance for practical simulations, is the condition on the quark mass that must be enforced in order that physical quantities are automatically $O(a)$ improved at maximal twist. Does one need to enforce (A) $m_q \gg a^2 \Lambda_{\text{QCD}}$, (B) $m_q \ll a^2 \Lambda_{\text{QCD}}$, or (C) $m_q \gtrsim c a^2 \Lambda_{\text{QCD}}$, with $c$ a determinable constant of $O(1)$? If one takes $a^{-1} = 2$ GeV and $\Lambda_{\text{QCD}} = 0.3$ GeV, these conditions become (A) $m_q \gg 45$ MeV, (B) $m_q \ll 7$ MeV, and (C) $m_q \gtrsim 7$ MeV, respectively. Since the average light quark mass is $\sim 3$ MeV (at a renormalization scale of 2 GeV—for a recent review see Ref. [22]), we need to be able to use condition (B) if lattice masses are to allow extrapolation to physical values, or condition (C) if they are to approach them. Condition (A) is very restrictive.

On the theoretical side, Refs. [3, 5] argue that, in general, one must use the strongest condition, (A), although it is possible that the intermediate condition, (B), can be used if one is dealing with $O(a)$ improved quantities, e.g. if using an $O(a)$ improved quark action. By contrast, it has been recently proposed in Ref. [21] that there is no lower limit on $m_q$ in order for automatic $O(a)$ improvement to apply, as long as one uses an appropriate definition of twist angle.

We will argue here in favor of the weakest condition, (C), with the constant $c$ either of $O(1)$, or vanishing, depending on the sign of an unknown constant in the chiral Lagrangian. Our arguments are based on tmLQCD applied in the regimes where conditions (B) and (C) hold. The former we call the "generic small mass" (GSM) regime, the latter the "Aoki" regime (since it is in this region that non-trivial phase structure due to discretization effects appears [23]). For most of the paper we consider the GSM regime, in which we expect the bulk of future simulations to be done. We give a general argument for automatic $O(a)$ improvement in this regime (which requires the use of an appropriate non-perturbative definition of twist angle), and support it with results for the physical quantities listed above. We then extend the results to the Aoki regime, where, working to leading order (LO) in an expansion in which $m_q \sim a^2 \Lambda_{\text{QCD}}$, we argue that condition (B) can be relaxed to (C).

We stress that our discussion of $O(a)$ improvement is within the context of chiral perturbation theory up to a given order (NLO in the GSM regime, LO in the Aoki regime). This means that we only control those $O(a)$ corrections that are expected to be dominant in the regimes under study. For example, in both regimes we control corrections to the pion decay constant, $f_\pi$, which are of relative size $a \Lambda_{\text{QCD}}$, but do not control those of relative size $a m_q$. The latter corrections arise from terms in the chiral Lagrangian of $O(a^3)$ and $O(a^4)$ in the GSM and Aoki regimes, respectively, which are, in both cases, of higher order than we work.

The remainder of this article is organized as follows. In the next section, we recall the definition of tmLQCD and the construction of the corresponding NLO chiral Lagrangian, and use this to discuss the condition on the quark mass needed to obtain automatic $O(a)$ improvement at maximal twist. In Sec. III we use the Lagrangian, including sources for currents and densities, to determine the twist angle non-perturbatively, and to calculate the physical quantities listed above. In the final subsection, we give a summary of our results and a suggestion for how to use them in practice. In Sec. IV we show how our results extend into the Aoki regime, and comment on the considerations of Ref. [21]. We conclude in Sec. V and suggest various avenues for future work.

Some preliminary results from this paper have been presented in Ref. [17].

II. THE EFFECTIVE CHIRAL LAGRANGIAN

The theory we consider is tmLQCD with a degenerate doublet of quarks. The fermionic part of the Euclidean lattice action of the theory in the so-called "twisted basis" is [2, 3]:

$$S_F^L = \sum_x \bar{\psi}_l(x) \left[ \frac{1}{2} \sum_\mu \Gamma_\mu (\nabla_\mu + \nabla_\mu) - \frac{r}{2} \sum_\mu \nabla_\mu^* \nabla_\mu + m_0 + i \gamma_5 \tau_3 \mu_0 \right] \psi_l(x),$$

(1)

where $\psi_l$ and $\bar{\psi}_l$ are the dimensionless bare lattice fields (with "$l$" standing for lattice and not indicating left-handed), and $\nabla_\mu$ and $\nabla_\mu^*$ are the usual covariant forward and backward dimensionless lattice derivatives, respectively. The field $\psi_l$ is a flavor doublet, and $\tau_3$ acts in flavor space and is normalized so that $\tau_3^2 = 1$. The bare normal mass, $m_0$, and the bare twisted mass, $\mu_0$, both of which are dimensionless, are taken to be proportional to the identity matrix in flavor space.

The effective continuum chiral theory is derived using the two-step procedure of Ref. [12]. In Ref. [17], we have carried this procedure out to NLO in an expansion in which we treat quark masses and the leading discretization
errors as symmetry breaking parameters of the same size. Here we recall only the essential
details.

Following the program of Symanzik [24], we first write down an effective continuum
Lagrangian at the quark level which describes the long distance physics of the underlying lattice theory. Its form is constrained by the symmetries of the lattice theory to be

\begin{equation}
\mathcal{L}_{\text{eff}} = \mathcal{L}_g + \bar{\psi}(i\slashed{D} + m + i\gamma_5 \tau_3 \mu)\psi + b_1 a \bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi + O(a^2) .
\end{equation}

Here \( \mathcal{L}_g \) is the continuum gluon Lagrangian, \( m \) is the physical quark mass, defined in the usual way by

\begin{equation}
m = Z_m(m_0 - \bar{m}_c)/a ,
\end{equation}

and \( \mu \) is the physical twisted mass

\begin{equation}
\mu = Z_\mu \mu_0/a = Z^{-1}_\mu \mu_0/a ,
\end{equation}

with \( Z_\mu \) the matching factor for the pseudoscalar density. The quantity \( \bar{m}_c \) is the critical mass, aside from an \( O(a) \) shift. This shift, and methods for determining the critical mass after its inclusion, are discussed below. Note that the lattice symmetries forbid additive renormalization of \( \mu_0 \) [2]. Although the \( O(a^2) \) terms in Eq. (2) are of an appropriate size to be included at NLO, they do not break the continuum symmetries any further than the terms explicitly shown, and thus do not lead to any additional operators in the effective chiral theory [15]. Thus we do not need their explicit form.

We reiterate here that we have dropped from \( \mathcal{L}_{\text{eff}} \) terms proportional to \( a\mu^2 \bar{\psi}\psi \), \( am^2 \bar{\psi}\psi \) and \( a\lambda\bar{\psi}\gamma_5 \tau_3 \psi \). These terms are allowed by the lattice symmetries [25], and do lead to corrections linear in \( a \), but are of next-to-next-to-leading order (NNLO) in our power counting.

In the continuum limit [where the \( b_1 \) and higher order terms in (2) vanish] the apparent flavor-parity breaking due to \( \mu \) is misleading, since it can be rotated away by a non-anomalous axial rotation. Thus tmLQCD is, in this limit, equivalent to QCD with two degenerate quarks of mass \( \sqrt{m^2 + \mu^2} \). This has been established in detail in Ref. [2]. In this paper, we work away from the continuum limit, taking \( m \sim \mu \sim p^2 \sim aL_{QCD}^2 \). Thus the symmetry breaking induced by the \( b_1 \) term will play a crucial role.

The next step is to match the continuum effective Lagrangian [24] onto a generalized chiral Lagrangian. Working at NLO in our power counting, we found [15] (after simplifying using the properties of \( SU(2) \) matrices)

\begin{equation}
\begin{aligned}
\mathcal{L}_\chi &= \frac{f^2}{4} \text{Tr}(D_\mu \Sigma D^\dagger_\mu \Sigma) - \frac{f^2}{4} \text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) - \frac{f^2}{4} \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \\
&\quad - L_1 \text{Tr}(D_\mu \Sigma D^\dagger_\mu \Sigma^\dagger)^2 - L_2 \text{Tr}(D_\mu \Sigma D^\dagger_\nu \Sigma)\text{Tr}(D_\mu \Sigma D^\dagger_\nu \Sigma^\dagger) \\
&\quad + L_3 \text{Tr}(D_\mu \Sigma D^\dagger_\nu \Sigma)\text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) \\
&\quad + L_4 \text{Tr}(D_\mu \Sigma^\dagger D^\dagger_\nu \Sigma)\text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) \\
&\quad - L_5 \text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi)^2 \\
&\quad - L_6 \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A})^2 \\
&\quad + (L_5 - L_4) \text{Tr}(D_\mu \Sigma D^\dagger_\nu \Sigma^\dagger + R_{\mu\nu} D_\Sigma D^\dagger_\mu D^\dagger_\nu \Sigma) + L_7 \text{Tr}(L_{\mu\nu} \Sigma R_{\mu\nu} \Sigma) \\
&\quad + (L_4 - L_3) \text{Tr}(D_\mu \Sigma^\dagger D^\dagger_\nu \Sigma^\dagger + R_{\mu\nu} D_\Sigma^\dagger D^\dagger_\mu D^\dagger_\nu \Sigma) + L_8 \text{Tr}(L_{\mu\nu} \Sigma R_{\mu\nu} \Sigma) \\
&\quad + W_{68} \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A})^2 + W_{69} \text{Tr}(D_\mu \hat{A}^\dagger D^\dagger_\mu \Sigma + D_\mu \Sigma^\dagger D^\dagger_\mu \hat{A}) \\
&\quad + H_1 \text{Tr}(L_{\mu\nu} L_{\mu\nu} + R_{\mu\nu} R_{\mu\nu}) - H_2 \text{Tr}(\chi^\dagger \chi) - H_3 \text{Tr}(\hat{A}^\dagger \chi + \chi^\dagger \hat{A}) - H_4 \text{Tr}(\hat{A}^\dagger \hat{A}) .
\end{aligned}
\end{equation}

As usual, the field \( \Sigma \) is \( SU(2) \) matrix-valued, and transforms under the chiral group \( SU(2)_L \times SU(2)_R \) as

\begin{equation}
\Sigma \rightarrow L \Sigma R^\dagger , \quad L \in SU(2)_L , \quad R \in SU(2)_R .
\end{equation}

The quantities \( \chi \) and \( \hat{A} \) are spurions for the quark masses and discretization errors, respectively. At the end of the analysis they are set to the constant values

\begin{equation}
\chi \rightarrow 2B_0 (m + i\tau^3 \mu) \equiv \bar{m} + i\tau^3 \mu , \quad \hat{A} \rightarrow 2W_0 a \equiv \hat{a} ,
\end{equation}

where \( B_0 \) and \( W_0 \) are unknown dimensionful constants, and we have defined the quantities \( \bar{m} , \hat{a} \) and \( \hat{a} \). We have included sources for left- and right-handed currents in the standard way using covariant derivatives and associated field strengths, e.g.

\begin{equation}
D_\mu \Sigma = \partial_\mu \Sigma - i\ell_\mu \Sigma + i\Sigma \ell_\mu , \quad L_{\mu\nu} = \partial_\mu \ell_\nu - \partial_\nu \ell_\mu + i[\ell_\mu , \ell_\nu] .
\end{equation}
Sources for the scalar and pseudoscalar densities are similarly included by writing $\chi = 2B_0(s + ip)$. Note that $\ell_\mu$, $r_\mu$, $s$ and $p$ are all hermitian matrix fields. Finally, we note that at NLO we should also include the Wess-Zumino-Witten term $W_4$. We do not, however, consider here any processes to which it contributes (e.g. $\pi^0 \to \gamma\gamma$), and so do not write it out explicitly.

The chiral Lagrangian contains a number of parameters which are not determined by symmetries—the low energy constants (LECs). At leading order there are the usual $f$ (normalized so that $f_\pi = 93$ MeV) and $B_0$, supplemented by the additional constant $W_0$ introduced by discretization errors [12]. At NLO there are significantly more LECs. The $L_i$ are the usual Gasser-Leutwyler constants of continuum $\chi_{\text{PT}}$ [27]. We have introduced the combinations $L_{45} = L_4 + L_5/2$ and $L_{68} = L_6 + L_8/2$, which are useful for two flavors. The $W_i$ are introduced by discretization errors at linear order in the lattice spacing [17], while the $W'_i$ appear at quadratic order [15]. Again, certain combinations are useful: $W_{45} = W_4 + W_5/2$, $W_{68} = W_6 + W_8/2$ and $W_{48} = W_4 + W_8/2$. Finally, the $H_i$ involve sources alone, and give rise to contact terms in correlation functions of currents and densities, as well as contributing to their vacuum expectation values. The $H'_i$ are the extra such terms introduced by discretization errors (which we did not include explicitly in Ref. [15], but will need here).

It is useful to understand the relation of our result for $L_\chi$ to that in Ref. [16]. In that work, the authors used a different power-counting, namely $a\Lambda_{\text{QCD}} \sim (m^2 + \mu^2)/\Lambda_{\text{QCD}}$. They worked to linear order in $a$, and without sources. Our results agree with theirs to the order they worked. They also changed variables using an axial rotation so that $\chi$ was diagonal. This has the advantage of moving the twist entirely into the term caused by discretization errors, $A \to \hat{a}(m - i\mu\tau_3)/\sqrt{m^2 + \mu^2}$. It was then straightforward to see that discretization errors in $m_\pi$ and $f_\pi$ are proportional to $\hat{a}m/\sqrt{m^2 + \mu^2}$ and thus vanish under mass averaging ($m \leftrightarrow -m$) and at maximal twist ($m = 0$).

In our power counting, where discretization errors are superficially as large as quark mass effects, we must follow a different strategy to see automatic $O(a)$ improvement. The key point, first noted in Ref. [12], is that the leading discretization effect [the third term in $L_\chi$ in (6) has the same form as the leading mass term [the second term in $L_\chi$]. This follows directly from the fact that the $b_1$ term in the quark-level effective Lagrangian (2) has the same chiral transformation properties as the quark mass term. Thus the LO chiral Lagrangian is unchanged from its continuum form if one uses the shifted spurion

$$\chi' \equiv \chi + \hat{A}.$$  

This corresponds at the quark level to a redefinition of the untwisted component of the quark mass from $m$ to

$$m' \equiv m + aW_0/B_0 = (\hat{m} + \hat{a})/(2B_0).$$  

This shift corresponds to an $O(a)$ correction to the critical mass, so that it becomes

$$m_c = \bar{m}_c - aW_0/B_0.$$  

In practice one automatically determines $m_c$ (and thus automatically uses $m'$ rather than $m$) if one uses an appropriate non-perturbative definition of twist angle. This is discussed in detail in the following section and summarized in the last subsection of Sec. III.

Since the LO Lagrangian takes the continuum form, the vacuum expectation value of $\Sigma$ at this order is that which cancels out the twist in the shifted mass matrix:

$$\langle 0 | \Sigma | 0 \rangle_{\text{LO}} \equiv \Sigma_0 \equiv \frac{\hat{m} + \hat{a} + i\mu\tau_3}{M'} \equiv \exp(i\omega_0\tau_3),$$

where

$$M' = |\chi'| = \sqrt{(\hat{m} + \hat{a})^2 + \mu^2}$$

is the LO result for the pion mass-squared. If we define the physical quark mass by

$$m_q = \sqrt{m'^2 + \mu^2},$$

then it follows from (12) that

$$c_0 \equiv \cos\omega_0 = m'/m_q, \quad s_0 \equiv \sin\omega_0 = \mu/m_q.$$  

3 Strictly speaking the $H_i$ and $H'_i$ are not low-energy constants, since they absorb short-distance divergences. In fact, in Ref. [27] they are denoted “high-energy constants”. Nevertheless, for brevity, we refer to them also as LECs.
Equation (12) is one of the definitions of twist angle that we will use, although it is not the most simple to determine through simulations. It is important to realize that it differs by $O(1)$ from the naive definition $\tan \omega = \mu / m$ when $m \sim a \Lambda_{\text{QCD}}^2$. When working in this mass regime, it is thus crucial to use the shifted mass $m'$, or, equivalently at NLO, one of the definitions of twist angle discussed below. This point has also been emphasized in Ref. [21].

We can now present our argument for why automatic $O(a)$ improvement holds even when $m \sim \mu \sim a \Lambda_{\text{QCD}}^2$. This will be borne out later by our detailed results. We begin by expressing the chiral Lagrangian in terms of $\chi'$ instead of $\chi$:

$$\mathcal{L}_\chi = \frac{f^2}{4} \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f^2}{4} \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') - L_1 \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger)^2 - L_2 \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) + L_{45} \text{Tr}(D_\mu \Sigma D_\mu \Sigma) \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') - L_{68} \left[ \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') \right]^2 + L_5 \left\{ \text{Tr} \left( (D_\mu \Sigma^\dagger D_\mu \Sigma) (\chi'^\dagger \Sigma + \Sigma^\dagger \chi') - \text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') / 2 \right) \right\} - L_7 \left[ \text{Tr}(\chi'^\dagger \Sigma - \Sigma^\dagger \chi') \right]^2 - L_8 \left\{ \text{Tr}[\chi'^\dagger \Sigma + \Sigma^\dagger \chi')]^2 - \left[ \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') \right]^2 / 2 \right\} + i L_9 \text{Tr}(L_{\mu \nu} D_\mu \Sigma D_\nu \Sigma^\dagger + R_{\mu \nu} D_\mu \Sigma^\dagger D_\nu \Sigma) + \tilde{W} \text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) - W \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) - W' \left[ \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \right]^2 + W_{10} \text{Tr}(D_\mu \hat{A}^\dagger D_\mu \Sigma + D_\mu \Sigma^\dagger D_\mu \hat{A}) - H_2 \text{Tr}(\chi'^\dagger \chi' + \chi^\dagger \chi').$$

We have dropped the terms proportional to $L_{10}$, $H_3$ and $H_4$, since these lead only to contact terms in correlation functions, which we do not need below. We have also introduced the useful combinations

$$\tilde{W} = W_{45} - L_{45}, \quad W = W_{68} - 2 L_{68}, \quad W' = W'_{68} - W_{68} + L_{68}, \quad H' = H'_2 - H_2.$$

This Lagrangian has the same form as the NLO continuum chiral Lagrangian aside from the "$W$" and $H'$ terms.

We are interested in the terms which are linear in $a$. Setting aside the $H'$ term, since it contributes only to condensates, this leaves the terms multiplied by $\tilde{W}, W$ and $W_{10}$. The latter is in fact redundant, as we discuss below, so can be ignored. The key point is then that, in both the $W$ and $W$ terms, the lattice spacing appears in the combination

$$\text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}).$$

If we now expand $\Sigma$ about $\Sigma_0$ in the following way,

$$\Sigma = \exp(i \omega_0 \tau_3 / 2) \exp(i \vec{\pi} \cdot \vec{\tau} / f) \exp(i \omega_0 \tau_3 / 2),$$

then the quantity [18] with $\hat{A}$ set to its final value $\hat{a}$, is invariant under the spurionic symmetry

$$\pi(x) \mapsto -\pi(x), \quad \omega_0 \mapsto -\omega_0, \quad p \mapsto -p, \quad \ell_\mu \leftrightarrow r_\mu \Rightarrow \Sigma \leftrightarrow \Sigma^\dagger, \quad D_\mu \Sigma \leftrightarrow D_\mu \Sigma^\dagger, \quad \chi' \leftrightarrow \chi^\dagger.$$

It follows that terms even (odd) in pion fields must be even (odd) in $\omega_0$. Since the only functions of $\omega_0$ which can appear are $c_0$ and $s_0$, the former must be multiplied by an even function of pion fields, the latter by an odd. Thus at maximal twist ($c_0 = 0$) the quantity [18] produces only odd powers of pion fields, and, in particular, has no vacuum expectation value. We also need to consider the combinations

$$\text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \quad \text{and} \quad \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi'),$$

which appear in the $\tilde{W}$ and $W$ terms. These are also invariant under the spurionic symmetry, but are independent of $\omega_0$, and thus must be even in pion fields. Now, when determining the consequences of the NLO terms, it is sufficient to expand about the LO vacuum, as we have done in [19]. It then follows that the $\tilde{W}$ and $W$ terms only give rise, at maximal twist, to vertices involving odd numbers of pions. The physical vertices, which involve even numbers of pions, do not receive any corrections proportional to $a$ and are thus automatically improved. Of course, the contribution linear in the pion field coming from the $W$ term leads to an $O(a)$ tadpole, which can convert LO into NLO vertices with one less pion. However, since the LO vertices only have even numbers of pions, the resulting vertices with $O(a)$ corrections all contain an odd number of pions. Again, the physical vertices are not corrected until $O(a^2)$. 

These arguments can also be extended to external sources, with the conclusion that physical matrix elements are automatically improved. Conversely, parity violating matrix elements are maximal at maximal twist. According to the general considerations of Ref. [2], these results are expected for \( m_q \gg a\Lambda_{QCD}^2 \). Our argument here shows that they hold also in the GSM regime in which \( m_q \sim a\Lambda_{QCD}^2 \). This does not require the use of an improved quark action, but it is essential to use a definition of maximal twist that sets \( m' \), rather than \( m \), to zero.

A possible concern is how these considerations generalize to extensions of the chiral Lagrangian incorporating other particles, e.g. baryons and heavy-light mesons. The point is that, although the Pauli and mass terms in the effective continuum Lagrangian have the same chiral transformation properties, they are not proportional as operators. Thus, although they will always enter any extension of the chiral Lagrangian with the same form, their relative strength (\( B_0/W_0 \) in the pionic sector discussed above) will depend on the quantity being considered. For example, the coefficient of a baryon mass term of the form \( \text{Tr}(\mathcal{B}_A B) \) and that of the corresponding term caused by discretization errors, \( \text{Tr}(\mathcal{B}_A B) \), will not be in the ratio \( B_0/W_0 \). Thus using the shifted mass \( m' \) will not, in general, remove the \( \hat{A} \) term. It seems, then, that we should be concerned, when \( m \sim a\Lambda_{QCD}^2 \), that the mass and discretization contributions are of the same size in general. The resolution of this concern is simply that the term linear in \( a \) is removed by working at maximal twist. In fact, we can see this in our calculations, because quantities such as \( f_\pi \), which do not vanish in the chiral limit, have a similar status in the chiral expansion as does the nucleon mass (although the details of the expansion differ).

We conclude this section by addressing a few technical points. First, we discuss the \( W_{10} \) term. As noted above, this term is redundant: it can be transformed into a combination of the \( W, \tilde{W} \) and \( H' \) terms by the change of variables

\[
\delta \Sigma = \frac{2W_{10}}{f^2} (\Sigma \hat{A} \Sigma - \hat{A}).
\]

(22)

The shifted coefficients of the remaining three terms are \( W + W_{10}/4, \tilde{W} + W_{10}/2 \) and \( H' - W_{10} \). All physical quantities must depend on these combinations and not on \( W_{10}, W, \tilde{W} \) and \( H' \) separately. For this reason, we refer to them as “physical combinations” of LECs, despite the fact that they are introduced by discretization errors. Although we could remove \( W_{10} \) by this change of variables, we have kept it, both because we have found it to provide a useful diagnostic in the computations of matrix elements, and because it helps in understanding the impact of improving the underlying lattice theory, as we now discuss.

We next consider how the effective Lagrangian changes if the underlying Wilson action, currents and densities are \( O(a) \) improved, as this illuminates the nature of the LECs introduced by discretization errors.\(^4\) The required improvement coefficients have been presented in Ref. [2]. As already noted, mass dependent \( O(a) \) corrections are of higher order than we consider here. Thus the only improvement coefficients that are needed are \( c_{SW} \), i.e. the coefficient of the lattice Pauli term in the quark action, and the standard improvement terms for the vector and axial currents proportional to \( c_V \) and \( c_A \), respectively. We refer to Refs. [2, 28] for details of these terms and discussion of how they can be determined non-perturbatively. If \( c_{SW} \) is set to its non-perturbative value, then the coefficient \( b_1 \) in Eq. (2) vanishes, so that corrections to the quark effective action are of \( O(a^2) \). It follows that \( W_0 = 0 \), and the \( O(a) \) shift in \( \tilde{m}_c \) is absent, so that \( \chi' = \chi \). The chiral effective Lagrangian then takes the same form as in Eq. (10), except that the factor of \( W_0 \) in \( \hat{A} \) should be dropped (with concomitant changes in the dimensions of various LECs), and, most importantly, \( \tilde{W} = W = 0 \). These latter two terms, which are proportional to \( a\chi \) and \( ap^2 \) respectively, are absent because there is no term linear in \( a \) in the underlying quark Lagrangian. The coefficient \( W_{10} \) does not, however, vanish since it corresponds to \( O(a) \) corrections to currents, and these have not yet been improved. Similarly, \( H' \) is non-zero. Finally, \( W' \) is non vanishing since it is proportional to \( a^2 \). If the axial current is also non-perturbatively improved, then one has in addition that \( W_{10} = 0 \) (as can be seen from the result below for \( f_A \)). Improving the vector current by adding the \( c_V \) term has no further impact on the LECs, since it turns out that \( c_V \) does not contribute to the quantities we consider at NLO, as we discuss further below. In summary, if one non-perturbatively improves the action and currents, then the only remaining discretization errors are those of \( O(a^2) \) proportional to \( W' \), as well as the \( H' \) term which contributes terms of \( O(a) \) only to the condensate. Our subsequent results show that, in this case, while all physical quantities are then \( O(a) \) improved, the unphysical parity-flavor violating matrix elements do have contributions at NLO which are proportional to \( a^2/m_q \) (see sec. III I below).

Finally, we recall that the currents and densities can be obtained by taking appropriate functional derivatives of

\(^4\) We thank the referee for suggesting that we consider the impact of improvement.
the action $S = \int d^4x L_\chi$: 

\[ V^k_\mu = \frac{i}{2} \left( \frac{\delta}{\delta \chi^k_\mu} + \frac{\delta}{\delta \ell^k_\mu} \right) S, \quad (23) \]

\[ A^k_\mu = \frac{i}{2} \left( \frac{\delta}{\delta \chi^k_\mu} - \frac{\delta}{\delta \ell^k_\mu} \right) S, \quad (24) \]

\[ S^k = \frac{1}{2} \frac{\delta}{\delta \ell^k} S, \quad S^0 = \frac{\delta}{\delta \psi} S, \quad (25) \]

\[ P^k = \frac{i}{2} \frac{\delta}{\delta \psi} S, \quad P^0 = -\frac{i}{2} \frac{\delta}{\delta \bar{\psi}} S, \quad (26) \]

where $s = s^0 + \sum_{k=1}^3 s^k \tau_k$, and similarly for $p, \ell_\mu$, and $r_\mu$, although for the latter two we use only the flavor non-singlet parts. Note that these equations give the currents and densities in the twisted basis, which is that usually used in simulations. Our normalizations are such that the corresponding currents and densities at the quark level are obtained by taking the same functional derivatives as defined above of

\[ S_{\text{eff}} = \int d^4x L_{\text{eff}} - i\bar{\psi} \gamma_\mu (\{r_\mu + \ell_\mu\}/2 + \gamma_5[r_\mu - \ell_\mu]/2) \psi + \bar{\psi}(s + i\gamma_5 p)\psi \quad (27) \]

Note that the factors of $1/2$ in eqs. (23-26) imply that we are using $\tau_k/2$ in flavor non-singlet operators, while for the singlet we do not include the factor of one half. Thus, for example, $P^k = \bar{\psi}\gamma_5\tau_k/2\psi$ and $S^0 = \bar{\psi}\psi$ at the quark level.

An important issue is the normalization of the currents. This can be determined, in the continuum and chiral limits, by enforcing appropriate Ward identities [24]. The currents we use at the quark level automatically satisfy these identities. This carries over to the currents in the chiral theory, since the matching maintains normalizations. The ratio of the scalar to pseudoscalar densities is also correctly normalized. The overall normalization of these densities, however, is a scheme dependent quantity, and this ambiguity is reflected in the chiral theory in the presence of the parameter $B_0$ in $\chi$. Because of these considerations, the results we give below for matrix elements of these operators in the effective theory apply directly to lattice matrix elements, as long as the lattice operators include their matching factors.

Away from the continuum limit, the explicit breaking of symmetries implies that one cannot, in general, normalize the currents and the ratio of densities in a universal way. Different choices of normalization condition will lead to results differing by $O(a)$, in general. We stress that this is true both on the lattice and in the effective chiral theory, as must be the case since the latter is supposed to represent the former. This is not, however, an impediment to our calculations. Since the effective chiral Lagrangian includes all terms that are allowed by the reduced symmetries of the lattice theory, our results contain, explicitly, all possible non-universal terms at the order we work. Thus in particular our results for matrix elements of currents and densities should hold for any choice of lattice operators which are correctly normalized in the continuum limit.\footnote{This argument fails, however, if one determines the normalization of currents and densities using the Schrödinger functional, as discussed in the case of tmLQCD in Ref. [24]. In that case there are additional $O(a)$ contributions related to the boundary fields which are not accounted for by our analysis. It seems likely that our analysis could be generalized to include such boundary terms, but we have not worked this out. Thus we are assuming that the normalization constants are determined without the use of boundary fields, e.g. for $Z_V$ and $Z_A$ using the method proposed in Ref. [8]. We thank the referee for pointing out this issue.}

### III. CHIRAL PERTURBATION THEORY FOR GENERIC SMALL MASSES

In this section we work out in detail the consequences of the effective chiral Lagrangian in the GSM regime. In fact, we are now in a position to state precisely how we define this regime. What we require is that

\[ \Lambda_\chi^2 \gg M' \gtrsim \hat{a}, \quad (28) \]

where $M'$ is defined in Eq. (13) and $\Lambda_\chi = 4\pi f$. This ensures that the LO terms in the chiral Lagrangian (10) dominate over the NLO terms. This condition can also be written using quark masses:

\[ 1 \gg \frac{m_q}{\Lambda_{\text{QCD}}} \gtrsim a \Lambda_{\text{QCD}} \quad (29) \]
Note that our results for the GSM regime remain valid if \( \hat{a} \) is smaller than \( M' \). The converse does not, however, hold. In particular, if \( M' \) becomes as small as \( \hat{a}^2/\Lambda^2 \), then one enters the Aoki regime where NLO and LO contributions are comparable.

A. The vacuum and Feynman rules

The NLO terms cause a small realignment of the vacuum expectation value of \( \Sigma \) away from \( \Sigma_0 \). In fact, we know from continuum chiral perturbation theory that the \( L_i \) terms in the potential do not realign the condensate. While this is possible in principle, given the physical values of the \( L_i \), it does not occur for quark masses in the range of interest to simulations. Thus the only realignment of the condensate is due to the \( W \) and \( \tilde{W} \) terms.

We define the full NLO condensate to be

\[
\langle 0 | \Sigma | 0 \rangle_{NLO} \equiv \Sigma_0 \equiv \exp(i\omega_m \tau_3) = \exp(i(\omega_0 + \epsilon) \tau_3),
\]

so that \( \epsilon = \omega_m - \omega_0 \). Minimizing the potential, we find

\[
\epsilon = -\frac{16}{f^2} \hat{a} s_0 (W + 2W' \hat{a} c_0 / M') ,
\]

The \( \hat{a}^2/M' \) term is not singular in the GSM regime, since \( M' \) is not allowed to become smaller than \( \hat{a} \). We note that, to the order we are working, we could make the replacements \( s_0 \rightarrow s_0 \equiv \sin \omega_m \) and \( c_0 \rightarrow c_0 \equiv \cos \omega_m \) in the expression for \( \epsilon \).

Later on we will further replace \( s_0 \) and \( c_0 \), respectively, with the sine, \( s \), and cosine, \( c \), of a non-perturbatively defined twist angle \( \omega \) which differs from both \( \omega_0 \) and \( \omega_m \) by \( O(a) \). This is allowed as long as we make the replacement only in NLO terms. Because of this, from now on we will use \( s \) and \( c \) without subscripts in NLO terms, and point out explicitly where the choice of twist angle is important.

We now expand about the vacuum expectation value, defining physical pion fields by

\[
\Sigma = \xi_m \Sigma_{ph} \xi_m , \quad \xi_m = \exp(i\omega_m \tau_3/2) , \quad \Sigma_{ph} = \exp(i\vec{\pi} \cdot \vec{\tau} / f) .
\]

We use an axial rotation, which has the symmetric form, since this is the rotation needed at the quark level in the continuum limit to undo the twist. It gives rise to pion fields that are in the physical basis, as we will see below.

Inserting this expansion into the chiral Lagrangian \[10\] we find

\[
\mathcal{L}_\chi = \frac{\pi^2}{2} (M' + \Delta M') - \frac{\pi^3}{2} \frac{32}{f^2} \hat{a}^2 s^2 W' + \frac{1}{2} \partial \mu \vec{\tau} \cdot \partial \mu \vec{\tau} \left( 1 + \frac{16}{f^2} M' L_{45} + \frac{16}{f^2} \hat{a} c \tilde{W} \right)
\]

\[
- \frac{\pi^3}{2} \partial \mu \vec{\tau} \cdot \partial \mu \vec{\tau} \frac{16}{f^2} \hat{a} s \tilde{W} + \frac{\pi^3}{2} \frac{\pi^2}{2} \epsilon M' f
\]

\[
- (\pi^2)^2 \frac{24 f^2}{f^2} \left( M' + 4\Delta M' \right) + \pi^2 \frac{\pi^2}{3 f^2} \hat{a}^2 s^2 W' + \ldots
\]

where \( \pi^2 = \vec{\tau} \cdot \vec{\tau} \), and

\[
\Delta M' = \frac{32}{f^2} \left( M'^2 L_{68} + \hat{a} c M' W + \hat{a}^2 c^2 W' \right) .
\]

We stress again that \( s \) and \( c \) could equally well be \( s_0 \) and \( c_0 \), or \( s_m \) and \( c_m \), at NLO accuracy. With one exception, we show explicitly in \[33\] only terms which we need for our calculations below. In particular, we have not included vertices proportional to \( L_1 \) and \( L_2 \), nor four pion vertices with two derivatives. These are unchanged from continuum chiral perturbation theory [the rotation in Eq. \[32\] cancelling in these terms], and so lead to NLO contributions of the same form as in the continuum. The exception are the vertices involving four pions, which we do not need explicitly below, but which we included to show the type of flavor breaking which occurs.

These results illustrate the generic features discussed in the previous section. First, parity and flavor conserving terms of \( O(a) \) are also proportional to \( c \) and thus vanish at maximal twist. Second, the \( O(a) \) terms which do not vanish at maximal twist (i.e. the three pion vertices proportional to \( \hat{a} s \)) violate parity and flavor. The factor of \( s \) ensures that they vanish when \( \mu \rightarrow 0 \) (when the flavor symmetry is restored). Finally, flavor breaking, but parity conserving contributions (i.e. the additional mass-term for \( \pi_3 \) and the \( \pi^2 \pi^2 \) vertex) are proportional to \( a^2 \) and to \( s^2 \propto \mu^2 \). All these results are expected on general grounds for \( M' \gg \hat{a} \), but also hold, as we see here, for \( M' \sim \hat{a} \).
B. Currents and densities in the twisted basis

At LO, the currents and densities take the usual form (although other authors use different normalizations):

\[ V_{\mu,LO}^k = \frac{f^2}{4} \text{Tr} \left[ \tau_k [\Sigma^\dagger \partial_\mu \Sigma + \Sigma \partial_\mu \Sigma^\dagger] \right], \]  
\[ A_{\mu,LO}^k = \frac{f^2}{4} \text{Tr} \left[ \tau_k [\Sigma^\dagger \partial_\mu \Sigma - \Sigma \partial_\mu \Sigma^\dagger] \right], \]  
\[ S_{LO}^k = -\frac{f^2 B_0}{4} \text{Tr} \left( \tau_k [\Sigma + \Sigma^\dagger] \right) = 0, \]  
\[ S_0^0 = -\frac{f^2 B_0}{4} \text{Tr} \left( \Sigma + \Sigma^\dagger \right), \]  
\[ P_{LO}^k = \frac{f^2 B_0}{4} \text{Tr} \left( \tau_k [\Sigma - \Sigma^\dagger] \right), \]  
\[ P_0^0 = \frac{f^2 B_0}{4} \text{Tr} \left( [\Sigma - \Sigma^\dagger] \right) = 0, \]  

where \( k = 1, 2, 3 \). The vanishing of the isovector scalar and isoscalar pseudoscalar densities is a property of \( SU(2) \), and holds also at NLO, so we do not consider these quantities further.

At NLO, the vector and axial currents become

\[ V_\mu^k = V_{\mu,LO}^k (1 + C) + L_1, L_2, L_3 \text{ terms}, \]  
\[ A_\mu^k = A_{\mu,LO}^k (1 + C) + \frac{4\hat{W}_{10}}{B_0 f^2} j_\mu P_{LO}^k + L_1, L_2, L_3 \text{ terms}, \]

where \( k = 1, 2, 3 \) and

\[ C = \frac{4L_{45}}{f^2} \text{Tr}[\chi^\dagger \Sigma + \Sigma^\dagger \chi] - \frac{16\hat{W}}{2B_0 f^4} S_{LO}^0. \]

We do not give the form of the \( L_1, L_2 \) and \( L_3 \) terms since these are unchanged from the continuum.

For the scalar and pseudoscalar densities at NLO, if we drop contributions proportional to the sources \( s \) or \( p \), which give rise only to contact terms in correlation functions, we find

\[ S^0 = S_{LO}^0 (1 + D) - 8B_0 (cM' H_2 + \hat{a} H') , \]  
\[ P^a = P_{LO}^a (1 + D), \]  
\[ P^3 = P_{LO}^3 (1 + D) + 4iB_0 sM' H_2, \]

where \( a = 1, 2, \) and

\[ D = -\frac{4L_{45}}{f^2} \text{Tr} [D_\mu \Sigma D_\mu \Sigma^\dagger] + \frac{8L_{68}}{f^2} \text{Tr} ([\chi^\dagger \Sigma + \Sigma^\dagger \chi] - \frac{16\hat{W}}{2B_0 f^4} S_{LO}^0). \]

Note that the terms in the chiral Lagrangian proportional to \( L_5, L_7 \) and \( L_8 \) give no contribution to these densities, due to the properties of \( SU(2) \) matrices. The constant terms proportional to \( M' \) and \( \hat{a} \) in \( S^0 \) and \( P^3 \) contribute only their vacuum expectation values.

We stress that all expressions in this subsection so far are written in terms of \( \Sigma \), whereas to use them we need to change variables to \( \Sigma_{ph} \). To do this we first need the results:

\[ V_{\mu,LO}^a = c_m \hat{V}_{\mu,LO}^a - c_m^{ab} s_m A_{\mu,LO}^b, \quad V_{\mu,LO}^3 = \hat{V}_{\mu,LO}^3, \]  
\[ A_{\mu,LO}^a = c_m \hat{A}_{\mu,LO}^a - c_m^{ab} s_m \hat{A}_{\mu,LO}^b, \quad A_{\mu,LO}^3 = \hat{A}_{\mu,LO}^3, \]  
\[ S_{LO}^0 = c_m S_{LO}^0 - is_m 2\hat{P}_{LO}^3, \quad P_{LO}^3 = c_m \hat{P}_{LO}^3 - is_m S_{LO}^0/2, \quad P_{LO}^0 = \hat{P}_{LO}^0, \]

where \( a, b = 1, 2, \) and the “hatted” currents and densities on the right hand sides of these relations take the same form as the LO currents and densities in eqs. \[ \text{[35-40]} \] but with \( \Sigma \) replaced by \( \Sigma_{ph} \). For example

\[ \hat{V}_{\mu,LO}^a = \frac{f^2}{4} \text{Tr} \left( \tau^2 [\Sigma_{ph} \partial_\mu \Sigma_{ph}^\dagger + \Sigma_{ph}^\dagger \partial_\mu \Sigma_{ph}] \right). \]
These are LO currents and densities of the chiral effective theory expressed in terms of physical pion fields. The transformations in (48) are identical to those at the quark level between the physical and twisted basis. We stress that to obtain these results it is essential to relate $\Sigma$ to $\Sigma_{ph}$ using the axial transformation of Eq. (32), and not, say, a left- or right-handed transformation.

Finally, we will also need the results

\[
\operatorname{Tr}[\chi'^{+}\Sigma + \Sigma^{+}\chi'] = M'\operatorname{Tr}[\Sigma_{ph} + \Sigma_{ph}^{+}] + O(M'\epsilon) = -\frac{4M'}{2B_{0}f^{2}}\hat{\xi}_{\text{LO}} + O(M'\epsilon)
\]

\[
\operatorname{Tr}[D_{\mu}\Sigma D_{\mu}\Sigma^{+}] = \operatorname{Tr}[D_{\mu}\Sigma_{ph} D_{\mu}\Sigma_{ph}^{+}],
\]

which allow us to express $\mathcal{C}$ and $\mathcal{D}$ in terms of physical pion fields (with the spurion $\chi'$ set to its final value). We can drop the $O(M'\epsilon)$ term in the first line as this contributes only at NNLO.

C. Defining the twist angle

Using the expressions for the currents and densities, we can determine the twist angle non-perturbatively. In the continuum limit, if the input twist angle is $\omega = \tan^{-1}(\mu/m)$, the physical currents and densities are given by

\[
\begin{align*}
\hat{V}_{\mu}^{a} &= cV_{\mu}^{a} + c^{ab}sA_{\mu}^{b}, \quad \hat{V}_{3}^{a} = V_{\mu}^{a}, \\
\hat{A}_{\mu}^{a} &= cA_{\mu}^{a} + c^{ab}sV_{\mu}^{b}, \quad \hat{A}_{3}^{a} = A_{\mu}^{a}, \\
\hat{S}^{0} &= cS^{0} + is2P^{3}, \quad \hat{P}^{3} = cP^{3} + isS^{0}/2, \quad \hat{P}^{a} = P^{a},
\end{align*}
\]

where $a, b = 1, 2, c = \cos \omega$ and $s = \sin \omega$. As already noted, these have the form of the inverse of the transformations of the LO operators, Eq. (48), except that here the twist angle is $\omega$ rather than $\omega_{m}$. Note that we can unambiguously create charged pions using $P^{a}$ and neutral pions using $A_{3}^{a}$, since these operators are invariant.

In the continuum, we can determine $\omega$ by the condition that there is no flavor or parity breaking in the physical basis. Different ways of enforcing this all lead to the same result for $\omega$. On the lattice, however, discretization errors imply that the different definitions will lead to results differing by $O(a)$. We will take as our canonical definition of $\omega$ that obtained by enforcing

\[
(V_{\mu}^{2}(x)\hat{P}^{1}(y)) = 0.
\]

The result for $\omega$ depends, at $O(a)$, on the distance $|x - y|$. We enforce the relation at long distances, where the single-pion contribution dominates. Using the definitions in (52), we can express the condition as

\[
\tan \omega = \frac{(V_{\mu}^{2}(x)P^{1}(y))}{(A_{\mu}^{a}(x)P^{1}(y))}.
\]

We stress that, at long distances, this gives the same result as that involving a divergence,

\[
\tan \omega = \frac{(\partial_{\mu}V_{\mu}^{2}(x)P^{1}(y))}{(\partial_{\mu}A_{\mu}^{a}(x)P^{1}(y))},
\]

since the factors of $\partial_{\mu}$ acting on the pion propagator cancel. Both definitions (54) and (55) have been used in simulations (see, e.g., Refs. [3, 4, 11]).

To evaluate (54) at LO we use the results in Eq. (48). At this order, only $\hat{A}_{\mu,LO}$ and $P^{1} = \hat{P}^{1}$ couple to the single pion state, and we find that $\omega = \omega_{m}$. Since $\omega_{m} = \omega_{0}$ at LO, we also have that $\omega = \omega_{0}$. This shows that the non-perturbative definition (54) automatically includes the shift from $m$ to $m'$ discussed above. In particular, if $\omega = \pi/2$, then $m' = 0$ up to corrections of $O(a^{2})$.

The NLO calculation of $\omega$ is simplified by the fact that most contributions cancel in the ratio (53) and do not change the LO result. This holds for the factors of $1 + C$ in eqs. (44) (evaluated with $\Sigma_{ph} = 1$), as well as one-loop wave-function renormalization, and the one-loop corrections to the coupling of $A_{\mu,LO}$ and $P^{1}$ to the pion. The $L_{1}$, $L_{2}$ and $L_{3}$ terms do not contribute at this order. The sole non-trivial contribution is that from the $W_{10}$ term in $A_{\mu}^{a}$, and we find

\[
\tan \omega = \frac{s_{m}}{c_{m} + \delta}, \quad \delta = \frac{4\alpha_{10}W_{10}}{f^{2}},
\]
This result can be rewritten at NLO in a number of useful ways:

\[ s = s_m - \delta s_m c_m, \quad c = c_m + \delta s_m^2, \quad \omega - \omega_m = -\delta s_m. \]  

(57)

Note that in each of these relations one can substitute \( s \) for \( s_m \), etc., in the sub-leading term on the right hand side.

As discussed earlier, \( W_{10} \) cannot appear alone in a physical quantity. This is not a concern here, however, since \( \omega_m \) is not physical, i.e. not directly accessible through a non-perturbative calculation. What must be physical is the difference between results from alternative non-perturbative definitions of \( \omega \). In particular, we expect \( \omega_0 \) to be physical since it contains the physical quark masses. Indeed, the difference

\[ \omega_0 - \omega = \frac{16\delta s}{f^2} (W + W_{10}/4 + 2\alpha cW'/M') \]  

(58)

is given by a physical combination of LECs.

Another non-perturbative definition of \( \omega \) can be obtained by enforcing the continuum relation

\[ \langle \hat{V}_\mu^2(x)\hat{A}_\mu^1(y) \rangle = 0. \]  

(59)

This leads to the result

\[ \tan(2\omega) = \frac{\langle \hat{A}_\mu^1(x)V_\mu^2(y) + \hat{V}_\mu^2(x)\hat{A}_\mu^1(y) \rangle}{\langle \hat{A}_\mu^1(x)\hat{A}_\mu^1(y) - V_\mu^2(x)V_\mu^2(y) \rangle}. \]  

(60)

In lattice simulations this relation has been used along with Eq. (54) in order to determine \( \omega \) without knowing the normalization of the vector and axial currents \( S^\mu \). Here we do know these normalizations, so this relation gives, in principle, an independent determination. We find, however, that the result for \( \omega \) is identical to that obtained from (55). In fact, this could have been seen in advance since, when using the single pion contributions, enforcing both (59) and (55) amounts to requiring that \( \langle 0|\hat{V}_\mu^2|\pi^1 \rangle = 0 \).

We do obtain a different non-perturbative result for the twist angle at non-zero lattice spacing if we enforce \( \langle \hat{S}^0(x)\hat{A}_\mu^3(y) \rangle = 0 \). This leads to

\[ \tan \omega_P = \frac{i\langle \hat{S}^0(x)\hat{A}_\mu^3(y) \rangle}{2\langle \hat{P}^3(x)\hat{A}_\mu^3(y) \rangle}, \]  

(61)

where we have denoted the new angle \( \omega_P \) (and will use \( c_P = \cos \omega_P \), etc.). A straightforward calculation leads to

\[ \omega_P - \omega = \frac{4\delta s(4W + W_{10})}{f^2} \]  

(62)

at NLO. The difference between \( \omega \) and \( \omega_P \) contains a physical combination of LECs, as it must since they both can be calculated non-perturbatively.

Another way of stating this result is to use \( \omega \) obtained from (61) and calculate the coupling of the physical scalar density to \( \pi_3 \). The mismatch of twist angles implies a non-zero result, which can be expressed as

\[ \frac{\langle \hat{S}^0(x)\hat{A}_\mu^3(y) \rangle}{\langle \hat{P}^3(x)\hat{A}_\mu^3(y) \rangle} = \frac{-8\delta s(4W + W_{10})}{f^2}, \]  

(63)

where again we take only the single-pion contribution. The result would, of course, have vanished if the physical scalar density had been constructed using \( \omega_P \) rather than \( \omega \). We note that (63) [or (61)] provides a method of calculating one combination of the LECs that are introduced by discretization errors. We return to this point in more detail below.

In summary, using the currents and densities we have obtained two non-perturbative definitions of the twist angle. These are equivalent in the continuum limit, but differ by \( O(a) \) away from this limit. This \( O(a) \) ambiguity in the twist angle is maximal at maximal twist. Nevertheless, as we show below, it affects masses and physical matrix elements only at \( O(a^2) \), and thus does not contradict automatic \( O(a) \) improvement. Only flavor-parity violating quantities are affected at \( O(a) \).
D. Constructing the physical currents and densities

Using the NLO result for $\omega$ defined by (53), which we take as canonical from now on, we can now explicitly construct the physical currents and densities, using the relations in Eq. (52). We find for the currents (with $a, b = 1, 2$):

$$\hat{V}_\mu^a = \hat{V}_{\mu,LO}^a (1 + C) - \frac{4\hat{a}sW_{10}}{f^2} \epsilon^{3ab} \hat{A}_{\mu,LO}^b + \frac{4\hat{a}sW_{10}}{B_0f^2} \epsilon^{3ab} \partial_\mu \hat{P}_{LO}^b + L_1, L_2, L_3 \text{ terms},$$

$$\hat{V}_3^a = \hat{V}_{\mu,LO}^3 (1 + C) + L_1, L_2, L_3 \text{ terms},$$

$$\hat{A}_\mu^a = \hat{A}_{\mu,LO}^a (1 + C) - \frac{4\hat{a}sW_{10}}{f^2} \epsilon^{3ab} \hat{V}_{\mu,LO}^b + \frac{4\hat{a}cW_{10}}{B_0f^2} \partial_\mu \hat{P}_{LO}^b + L_1, L_2, L_3 \text{ terms},$$

$$\hat{A}_3^a = \hat{A}_{\mu,LO}^3 (1 + C) + \frac{4\hat{a}W_{10}}{2B_0f^2} \partial_\mu \left(2\hat{c}P_{LO}^3 - i\hat{s}S_{LO}^0\right) + L_1, L_2, L_3 \text{ terms},$$

where $C$ is the same as above, but we now write it using physical fields:

$$C = \frac{16}{2B_0f^4} \left[-(M'L_{45} + \hat{a}\hat{c}W)\hat{S}_{LO}^0 + \hat{a}sW2i\hat{P}_{LO}^3\right].$$

The $L_1, L_2,$ and $L_3$ terms take exactly the same form as in continuum chiral perturbation theory, but now expressed in terms of $\Sigma_{ph}$. This is because they rotate exactly like the LO currents under the axial rotation. Since we are interested in flavor-parity breaking contributions we do not give these terms explicitly.

For the densities, the results are

$$\hat{S}^0 = \hat{S}_{LO}^0 (1 + D) - \frac{4\hat{a}sW_{10}}{f^2} 2i\hat{P}_{LO}^3 - 4iB_0\hat{a}sH',$$

$$\hat{P}^a = \hat{P}_{LO}^a (1 + D),$$

$$\hat{P}^3 = \hat{P}_{LO}^3 (1 + D) - \frac{4\hat{a}sW_{10}i\hat{S}_{LO}^0}{f^2} \frac{1}{2} - 8B_0(M'\hat{H}_2 + \hat{a}\hat{c}H'),$$

where we now express $D$ in terms of physical fields:

$$D = -\frac{4L_{45}}{f^2} \text{Tr} \left[D_\mu \Sigma_{ph} D_\mu \Sigma_{ph}^\dagger\right] + \frac{16}{2B_0f^4} \left[-(2M'\hat{L}_{68} + \hat{a}\hat{c}W)\hat{s}S_{LO}^0 + \hat{a}sW2i\hat{P}_{LO}^3\right].$$

For both currents and densities, the mismatch between $\omega$ and $\omega_m$ leads to contributions on the right hand sides proportional to $W_{10}$. Note that the currents and densities themselves need not be composed of physical combinations of LECs, since they are not directly measurable. It is their matrix elements, such as those we compute below, which are physical.

One test of the results given above is that the single pion matrix elements of $\hat{V}_{\mu}^a$ should vanish, i.e. the physical vector currents do not couple to single pions. There are contributions both from the $\hat{A}_{\mu,LO}^b$ and $\partial_\mu \hat{P}_{LO}^b$ terms and these do cancel. In effect, our condition for determining $\omega$ has enforced this result.

There is a subtlety concerning the choice of twist angle. The results above for the physical currents and densities hold as written for our canonical choice, $\omega$. If instead we had used $\omega_P$ to define the rotation between twisted and physical bases, then some of the explicitly parity-flavor breaking terms are changed. In particular, in the terms proportional to $\hat{A}_{\mu,LO}^b$ in Eq. (53), to $\hat{V}_{\mu}^b$ in Eq. (56), to $\hat{P}^3$ in Eq. (59), and to $\hat{S}^0$ in Eq. (71), $W_{10}$ would be replaced by $-4W$. The other terms proportional to $W_{10}$ are not, however, changed. In our subsequent results, these changes would only impact the flavor-parity violating matrix elements.

Finally, we note the same general features in these results as observed earlier in the Feynman rules. Discretization errors which do not violate flavor and parity come with factors of $c$, and thus vanish at maximal twist. Flavor-parity breaking terms, however, are proportional to $\hat{a}\hat{s}$.

E. Pion masses

With the Feynman rules, currents and densities in hand, we now turn to the predictions for masses and matrix elements. We begin with the charged pion mass, which we find at NLO to be given by

$$m_{\pi,1,2}^2 = M' + \frac{16}{f^2} \left(M'^2(2L_{68} - L_{45}) + M'\hat{a}\hat{c}(2W - \tilde{W}) + 2\hat{a}c^2W'\right) + \text{1-loop}.$$
Here the one-loop contribution is unchanged from that in the continuum as long as the result is expressed in terms of the LO pion mass-squared \( M' \). This is because it involves only LO vertices and masses, which themselves have the same form as in the continuum. To be completely clear on this point we quote the result in this case

\[
1\text{-loop} = \frac{M'^2}{2\Lambda_X^2} \ln \left( \frac{M'}{\Lambda_R^2} \right),
\]

where \( \Lambda_R \) is the renormalization scale. Since our emphasis is on discretization errors, however, we will not give explicit expressions for the 1-loop contributions to other quantities below. They can be found in the original work on two-flavor ChPT \cite{27}, as well as in more recent works including the extension to the partially quenched theory, e.g. Refs. \cite{16, 17}.

There are various checks on our result \cite{23}. When \( s \to 0 \), it agrees with that of Ref. \cite{18}, where \( m_2^2 \) was calculated to NLO in the untwisted Wilson theory. It goes over to that of Ref. \cite{16} if we take \( \hat{a} \sim M'^2 \). And, after considerable algebra, it can be shown to agree with the result of Ref. \cite{14}, where the same quantity was obtained.

Various features of the result are noteworthy. First, it depends only on physical combinations of LECs, as required. Second, it is automatically \( O(a) \) improved at maximal twist (\( c = 0 \)), or after mass averaging. Finally, the \( a^2 \) correction provides a further shift to the critical mass. This shift vanishes, however, at maximal twist. Thus we find the somewhat surprising result that, at maximal twist, the charged pion mass differs from the continuum only by terms of NNLO in our expansion. This is not to say that the result is surprising, because there are contributions proportional to \( M' a^2 \).

The flavor breaking in the pion masses at NLO is given solely by the analytic contribution, and we find (in agreement with Ref. \cite{14}) that

\[
m_{\pi_3}^2 - m_{\pi_1}^2 = -\frac{32}{f^2} \hat{a}^2 s^2 W' \]

\[= -W' \frac{32}{f^2} \frac{\hat{a}^2 \bar{\mu}^2}{(\bar{m} + \bar{\mu})^2 + \bar{\mu}^2}.\]  

To obtain the final form we have used the fact that we can replace \( s \) with \( s_0 \) at the order we are working. We know on general grounds that this splitting must vanish quadratically in \( a \mu \), because it does not violate parity. Naively, then, one might have expected the splitting to arise first at fourth order in our expansion (NNNLO). What our result shows is that, in fact, there is mass dependence in the numerator such that the effect is of NLO.

Calculating the pion mass splitting in practice is complicated by the fact that the neutral pion propagator includes disconnected quark contractions. It would nevertheless be an interesting quantity to determine. For one thing, it would give an indication of the size of discretization errors. Furthermore, as noted in Ref. \cite{14}, determining \( W' \) gives information about the phase diagram in Aoki region. In particular, if \( W' < 0 \) there is an Aoki phase on the untwisted Wilson axis, while if \( W' > 0 \) there is a first order transition on the Wilson axis extending out into the twisted plane \cite{13, 14, 15, 19}. It is perhaps surprising that a simulation in the GSM regime can give information about the Aoki regime. The reason for this result is that the same terms in the chiral Lagrangian are responsible both for the mass splitting and for determining the phase structure. In fact, the first form of the result, \cite{76}, holds also in the Aoki regime, although the final form, \cite{75}, does not. We discuss this further in the next section.

F. Decay constants and PCAC quark mass

Using the expressions for the axial current and pseudoscalar density in the physical basis, we can determine their one-pion matrix elements up to NLO:

\[
f_A = f \left\{ 1 + \frac{4}{f^2} [2M' L_{45} + \hat{a} \bar{c}(2\tilde{W} + W_{10})] \right\} + \text{1-loop}, \]  

\[
f_P = f B_0 \left\{ 1 + \frac{8}{f^2} \left[ M' (4L_{68} - L_{45}) + \hat{a} \bar{c}(2W - \tilde{W}) \right] \right\} + \text{1-loop}. \]

Here, as for the pion masses, the one-loop term is the same as in continuum chiral perturbation theory \cite{27} and we do not give it explicitly. At this order there is no flavor breaking—this enters first at \( O(a^2) \), which is NNLO for the decay constants. The result shows the expected automatic \( O(a) \) improvement at maximal twist or under mass averaging, and the appearance of a physical combination of LECs.
In fact, the quantities that we have discussed so far—\( \omega, m^2, f_A \) and \( f_P \)—are not independent. To see this we first consider the so-called “PCAC quark mass” defined through

\[
m_{\text{PCAC}} = \frac{(\partial_\mu A^a_\mu(x) P^a(y))}{2(P^a(x) P^a(y))},
\]

where \( a = 1, 2 \). Note that it is not the physical axial current which appears, but rather that in the twisted basis. This quantity is of interest because in the continuum limit it gives the untwisted component of the quark mass. We evaluate the correlators for \( x - y \to \infty \) so that the single pion contribution dominates. At LO we find

\[
m_{\text{PCAC}}^{\text{LO}} = m' = \frac{\mu}{\tan \omega_0},
\]

showing that this quantity automatically includes the \( O(a) \) offset in the untwisted mass. At NLO we find

\[
m_{\text{PCAC}} = \frac{c f_A^{\text{NLO}} (m^2_\omega)^{\text{NLO}}}{2 f_P^{\text{NLO}}},
\]

where the superscripts indicate that the full NLO expressions must be used. In this result, we cannot change the overall factor of \( c = \cos \omega \) into, say, \( c_m \) or \( c_0 \).

The result \(^{31}\) also shows that \( m_{\text{PCAC}} \) is not independent of the quantities considered so far. In particular, using the condition \( m_{\text{PCAC}} = 0 \) to determine maximal twist is equivalent to setting \( \tan \omega = \infty \) in \(^{31}\). Both rely on the vanishing of the coupling of the axial current in the twisted basis to the pion.

To proceed further we recall that the lattice symmetry has an exact “PCVC” relation

\[
\partial_\mu V^k_\mu(x) = -2\mu c^{3k} \tilde{P}^k(x), \quad k, l = 1, 2, 3, \ldots
\]

where \( \partial_\mu^* \) is the backward lattice derivative, \( \tilde{P}^k \) the local bare pseudoscalar density, and \( V \) the point-split current:

\[
\tilde{V}^k_\mu(x) = \frac{1}{2} \left\{ \bar{\psi}(x)(\gamma_\mu - 1) \frac{k}{2} U(x, \mu)\psi(x + a\hat{\mu}) + \bar{\psi}(x + a\hat{\mu})(\gamma_\mu + 1) \frac{k}{2} U(x, \mu)^{-1}\psi(x) \right\}.
\]

The same relation must hold in the effective quark and meson theories, to all orders in our expansion, if we normalize our operators to maintain continuum Ward identities. In particular, at the meson level, we have

\[
\partial_\mu V^k_\mu(x) = -2\mu c^{3k} P^k(x).
\]

Using this, and the definition of the twist angle \(^{31}\), we find

\[
m_{\text{PCAC}} = \frac{(\partial_\mu A^1_\mu(x) P^1(y))}{(\partial_\mu V^2_\mu(x) P^1(y))} \times \frac{(\partial_\mu V^2_\mu(x) P^1(y))}{2(P^1(x) P^1(y))} = \frac{\mu}{\tan \omega},
\]

This relation should hold to all orders in \( a^3 \Lambda \) PT, and we have checked that it is valid at NLO. Using Eq. \(^{31}\), we see that \( f_A, f_P, m^2, \) and \( \omega \) are related.

### G. Parity conserving matrix elements

We next consider other flavor-parity conserving matrix elements that can be calculated in numerical simulations. The first example is pion vector form factor, which can be obtained from the matrix elements

\[
\langle \pi_1(p_1)|\tilde{V}^k_\mu(x)|\pi_2(p_2)\rangle.
\]

We find that, at NLO, the result is unchanged from that in the continuum, which is given, for example, in Ref. \(^{27}\). This holds true at any twist angle. It follows because the contribution from the factor \( C \) in \(^{08}\) cancels that from wave-function renormalization.

It is perhaps surprising that there are no \( O(a) \) terms even for untwisted Wilson fermions. We know in this case that to remove \( O(a) \) terms in general we need to add to the current a term containing the tensor bilinear. One can show, however, that this contributes to the pion matrix element terms suppressed by \( O(aq^2) \) compared to the LO contribution. While of \( O(a) \), these are NNLO corrections in our power counting scheme.
Our next quantity is the scalar form factor of the pions. This is flavor conserving at NLO, and can be obtained from the matrix elements:

$$\langle \pi_k(p_1)|S^0|\pi_k(p_2)\rangle = 2B_0 \left\{ 1 + \frac{8}{f^2} \left[ -q^2L_{45} + 4M'(2L_{68} - L_{45}) + 2a^2(2W - \tilde{W}) \right] + \text{1-loop} \right\}. \quad (87)$$

As usual, the one-loop contribution is the same as in the continuum $^2\!7$. Unlike the vector form factor, here $O(a)$ improvement occurs only at maximal twist.

We consider here also vacuum expectation values of $2iP^3$ and $S^0$. The former is the most interesting since it is calculable on the lattice and, at maximal twist in the continuum limit, it gives the physical condensate $(0|\bar{u}u + \bar{d}d|0)$. It is calculable because $P^3$ does not mix with the identity operator in the chiral limit. Away from this limit, the mixing is proportional to $\mu/a^2$ and can, in principle, be extrapolated away. By contrast, $S^0$ mixes with the identity operator for all quark masses, and thus is very hard to calculate on the lattice. Nevertheless, we quote results for it as they illustrate an interesting theoretical point.

Our results for these condensates at NLO are:

$$\langle 2iP^3 \rangle = -2f^2B_0a \left\{ 1 + \frac{4}{f^2} \left[ M'(8L_{68} + H_2) + \hat{a}c(4W + W_{10}) \right] + \text{1-loop} \right\}, \quad (88)$$

$$\langle S^0 \rangle = -2f^2B_0c \left\{ 1 + \frac{4}{f^2} \left[ M'(8L_{68} + H_2) + \hat{a}c(4W + W_{10}) \right] + \text{1-loop} \right\} + 8B_0\hat{a}(W_{10} - H'). \quad (89)$$

Here the relative 1-loop correction is of the same form for both quantities and of the same as for the continuum condensate. We stress that the inclusion of the $H'$ term in the chiral Lagrangian is essential to make the result for $\langle S^0 \rangle$ physical. We note that $\langle P^3 \rangle$ is $O(a)$ improved at maximal twist, which is expected because it is proportional to the physical condensate (in the chiral limit). We also note that the $M'$ term in $\langle P^3 \rangle$, since it is multiplied by the overall factor of $s$, is indeed proportional to $\mu$. Thus $H_2$ is the constant which contains the quadratic divergence. On the other hand, $S^0$ is not a multiplicatively renormalizable operator, as it mixes with the identity operator, even in the chiral limit. Thus the general considerations of Ref. $^3\!$ do not require that it be automatically $O(a)$ improved, and indeed it is not, as shown by the last term.

**H. Parity violating matrix elements**

We finally consider simple examples of unphysical, parity violating quantities which vanish in the continuum due to flavor and parity symmetries, but are present in tmLQCD at $O(a)$ since they are not automatically improved. The first such quantities are axial form factors of the pions. These are obtained from the matrix elements

$$\langle \pi_\alpha(p_1)|\hat{A}_\mu^n|\pi_\beta(p_2)\rangle, \quad \langle \pi_\alpha|\hat{A}_\mu^n|\pi_\beta\rangle, \quad \langle \pi_\alpha|\hat{A}_\mu^3|\pi_\beta\rangle, \quad (90)$$

where $\alpha = 1, 2$. Calculating these in lattice simulations is straightforward in principle as they involve only single particle states. The main complication is that there are quark-disconnected contributions in addition to the usual quark-connected contributions.

At NLO, the contributions to these matrix elements are of two types, as shown in Fig. $^4\!$, the direct two pion terms in the axial current (both the $\hat{A}_\mu^n P^3_L$ and the $\hat{V}^b_L$ terms), and a pole term in which the axial current creates a single pion which then connects with the two external pions through the three pion vertices in $\mathcal{L}_\chi$. There is no contribution from the $L_1, L_2, L_9$ terms since these do not break flavor or parity at this order. We also do not need to include wavefunction renormalization since the leading contribution is of NLO. There are also no one-loop contributions. Our results are (with $\alpha = 1, 2$):

$$\langle \pi_\alpha(p_2)|\hat{A}_\mu^n|\pi_\beta(p_1)\rangle = \frac{16\hat{a}^2s}{f^2} \times \left\{ (p_1)_\mu \left[ \frac{W_{10}}{4} + W + \frac{2a^2cW'}{q^2 + M'} + \frac{(\tilde{W}/2 - W)q^2}{q^2 + M'} \right] - (p_2)_\mu \left[ \frac{W_{10}}{4} + W - \tilde{W} + \frac{2a^2cW'}{q^2 + M'} + \frac{(\tilde{W}/2 - W)q^2}{q^2 + M'} \right] \right\}, \quad (91)$$

$$\langle \pi_\alpha(p_2)|\hat{A}_\mu^3|\pi_\beta(p_1)\rangle = \frac{16\hat{a}^2s}{f^2} \langle p_1 - p_2 \rangle_\mu \left\{ \left[ -\frac{W_{10}}{4} + W - \tilde{W} + \frac{2a^2cW'}{q^2 + M'} + \frac{(\tilde{W}/2 - W)q^2}{q^2 + M'} \right] \right\}, \quad (92)$$

$$\langle \pi_3(p_2)|\hat{A}_\mu^3|\pi_3(p_1)\rangle = \frac{16\hat{a}^2s}{f^2} \langle p_1 - p_2 \rangle_\mu \left\{ -\frac{W_{10}}{4} + 3W - 2\tilde{W} + \frac{6a^2cW'}{q^2 + M'} + \frac{3(\tilde{W}/2 - W)q^2}{q^2 + M'} \right\}. \quad (93)$$
particular, this means that all the matrix elements of the physical pseudoscalar density do not depend on $\omega$ results above are for our canonical choice, These are very closely related to the corresponding axial matrix elements. Since the pseudoscalar density does not require improvement through NLO in our expansion, one would expect that this definition of twist angle. This explains a puzzle that appears when considering the application of our results way in which these results could be used in simulations. We do not discuss the technical problems that can arise

\begin{align}
\langle \pi_2(p_2)|\hat{P}^a|\pi_1(p_1)\rangle &= \frac{16\alpha_i B_0}{f^2} \left[ \frac{2\alpha c W^\prime}{q^2 + M^\prime} + \frac{(\tilde{W}/2 - W)q^2}{q^2 + M^\prime} \right] \\
\langle \pi_2(p_2)|\hat{P}^3|\pi_1(p_1)\rangle &= \frac{16\alpha_i B_0}{f^2} \left[ \frac{-W_{10} q}{4} + \tilde{W} + \frac{2\alpha c W^\prime}{q^2 + M^\prime} + \frac{(\tilde{W}/2 - W)q^2}{q^2 + M^\prime} \right] \\
\langle \pi_2(p_2)|\hat{P}^3|\pi_1(p_1)\rangle &= \frac{16\alpha_i B_0}{f^2} \left[ \frac{-W_{10} q}{4} + \tilde{W} + \frac{6\alpha c W^\prime}{q^2 + M^\prime} + \frac{3(\tilde{W}/2 - W)q^2}{q^2 + M^\prime} \right].
\end{align}

These are very closely related to the corresponding axial matrix elements.

The results for the parity-flavor violating form factors do depend on the choice of definition of twist angle. The results above are for our canonical choice, $\omega$. If instead we use $\omega_P$ to rotate to the physical basis, then we find that in Eqs. (91), (95) and (96) [though not in Eqs. (92) and (93)] the factors of $W_{10}/4$ are replaced by $-\tilde{W}$. In particular, this means that all the matrix elements of the physical pseudoscalar density do not depend on $W_{10}$ with this definition of twist angle. This explains a puzzle that appears when considering the application of our results to an underlying lattice theory in which the quark action is non-perturbatively improved, but the currents are not. Since the pseudoscalar density does not require improvement through NLO in our expansion, one would expect that its parity violating matrix elements would have no terms linear in $a$. As discussed above, however, improving the quark action implies setting $\tilde{W} = W = 0$ but leaving $W_{10}$ non-zero, and so the results of Eqs. (95) and (96) do not vanish. The puzzle is explained by noting that the twist angle is determined using the axial and vector currents, which are unimproved. If instead one uses the pseudoscalar and scalar densities, i.e. uses $\omega_P$, then, as just noted, the $W_{10}$ dependence is absent as expected.

The matrix elements of this subsection provide a way of determining the LECs associated with the discretization. Using the momentum dependence one can, in principle, separately determine the physical combinations $\tilde{W} - 2W, W'$ and $W + W_{10}/4$. Furthermore, since only two of the expressions in square brackets in (91) are independent, and similarly for (92) and (93), there are a number of predictions implicit in these results. We stress that these predictions hold only at NLO in tm$\chi$PT, and will be broken at higher orders.

\section{Summary of results in GSM regime}

In this final subsection we summarize what we have learnt about the GSM regime using tm$\chi$PT, and describe one way in which these results could be used in simulations. We do not discuss the technical problems that can arise
when calculating the quantities we have discussed using lattice methods (e.g. the difficulty in simulating disconnected contractions). We simply assume that these difficulties can be overcome.

We imagine that a simulation is done with particular values of \(\mu_0\) and \(m_0\), and that all the needed Z factors have been determined. Thus, given \(Z_P\), we know the renormalized twisted mass, \(\mu\). We do not, however, yet know the shifted untwisted mass \(m'\); for this we need to determine the (shifted) critical mass with \(O(a)\) accuracy. Our only assumption about \(m'\) is that it (and \(\mu\)) are such that we are in the GSM regime. Our aim is to determine as many as possible of the parameters in \(tm\chi PT\), to make predictions about physical quantities, and to provide consistency tests of \(tm\chi PT\).

One possible way of proceeding is as follows.

1. We determine \(\omega\) non-perturbatively using Eq. (53). This determines the untwisted quark mass including the \(O(a)\) shift using

\[
m' = \frac{\mu}{\tan \omega_0} = \frac{\mu}{\tan \omega} [1 + O(a)].
\]

The relative uncertainty of \(O(a)\) (which corresponds to an absolute uncertainty of \(O(a^2)\) in the GSM regime) means, however, that the Aoki region cannot be resolved—it collapses to a point at this accuracy.

2. To obtain \(m'\) to greater accuracy we next calculate \(\omega_P\) using Eq. (61). From the difference \(\omega_P - \omega\), or equivalently from the ratio given in Eq. (62), we can determine \(\delta(4W + W_0)/f^2\). This is interesting in its own right, as it not only gives an indication of the size of discretization errors, but it also allows us to partially “correct” for the difference between \(\omega\) and \(\omega_P\). In fact, for maximal twist (\(\omega = \pm \pi/2\)) we have, using Eqs. (63) and (62),

\[
\omega_0 = \omega_{P} [1 + O(a^2)] \quad \text{(Maximal twist)}.
\]

In this case we now know \(m'\) with a relative uncertainty of \(O(a^2)\), and an absolute uncertainty of \(O(a^3)\). We stress that this accuracy is to be understood within our power counting scheme, in which, for example, shifts in \(m'\) proportional to \(a\mu^2\), which are expected to be present, are of \(O(a^3)\) and so are too small to be included. Because of this result, one might argue that it makes more sense to use \(\omega_P\) as the canonical choice rather than \(\omega\). One reason not to do so is that the calculation of \(\omega_P\) is more difficult as it involves disconnected quark contractions.

3. To obtain \(\omega_0\) (and thus \(m'\)) at NLO accuracy for arbitrary twist angle we next calculate the pion mass splitting. This indicates the size of \(a^2\) corrections, and specifically determines the combination \(a^2 W'/f^2\). We can then obtain \(\omega_0\) using

\[
\omega_0 = \omega_P - \frac{m_{\pi}^2 - m_{\rho}^2}{m_{\pi}^2 \tan \omega}.
\]

Here \(a = 1, 2\), and the mass of any of the pions can be used for \(m_\pi\) in the denominator.

At this point, we know where our simulation lies in the \(m', \mu\) plane with an \(O(a^3)\) relative uncertainty. Thus we know the physical quark mass \(m_q = \mu/\zeta_0 = M'/(2B_0)\) with similar accuracy. This resolution is good enough to resolve the Aoki region (\(m' \sim \mu \sim a^2 \Lambda^3_{QCD}\)), so we know what parameters to use if we want to study that region. Indeed, as discussed above, knowing the sign of \(W'\) we can predict the phase structure in the Aoki region.

4. We now use one of the parity-violating matrix elements to determine the final, linearly independent, unknown combination of LECs associated with discretization errors, namely \(2W - \bar{W}\). For example, we could use

\[
\frac{2\langle \pi^a(p_1)|\hat{P}^k|\pi^a(p_1)\rangle}{\langle \pi^a(p_1)|\bar{S}^0|\pi^a(p_1)\rangle} = \frac{-16a\delta(2W - \bar{W})}{f^2} + (\omega_P - \omega) + (\omega_P - \omega_0).
\]

Here we have taken \(p_2 = p_1\) so that \(q^2 = 0\), and normalized with the scalar matrix element to remove the overall factor of \(B_0\).

Given this result, we can make absolutely normalized predictions for the ratios of all the other parity violating matrix elements of \(\bar{P}^k\) to the pion matrix element of \(\bar{S}^0\), including their \(q^2\) dependence. Similarly we can predict, including normalization, the parity violating axial form factors given in Eqs. (91-93). These predictions provide a test of the applicability of \(tm\chi PT\) at NLO, as well as an indication of the size of discretization errors.
5. Finally, we calculate the physical quantities \( m^2_{\pi_a}, f_A, f_F, \langle P_3 \rangle \) and \( \langle \pi|S,V|\pi \rangle \). Here we distinguish between maximal and non-maximal twist.

(a) **Maximal twist.** All these quantities are automatically \( O(a) \) improved, i.e. they have exactly the same dependence on \( m_q \) as in the continuum up to \( O(a^2) \) corrections, within our power counting scheme. Our results show that this automatic improvement holds even if one is working in a region where \( m_q \sim a\Lambda_{\text{QCD}}^2 \).

We stress that this automatic \( O(a) \) improvement holds irrespective of whether we use \( \omega \) or \( \omega_F \) or some other choice for the twist angle differing from \( \omega \) by \( O(a) \). This is because an \( O(a) \) uncertainty in \( \omega \) leads to an uncertainty in physical quantities of size \( a^2 \), so that they are still \( O(a) \) improved.

(b) **Non-maximal twist.** Here we find that, having determined the LECs, we can completely remove \( O(a) \) errors in the physical quantities that we have calculated. These errors can simply be subtracted or divided out. For example, the quantity

\[
(m^2_{\pi_a})^{1/2} = \frac{m^2_{\pi_a} - 32\hat{a}^2 W/f^2}{1 + 16a c(2W - W'/f^2)}
\]

is predicted to have the same dependence on \( m_q \) as does \( m^2_{\pi_a} \) in continuum \( \chi \)PT, up to \( O(a^2) \) errors.

This is an amusing, though perhaps academic result. In practice, when using \( tm\Lambda_{\text{QCD}} \), one should clearly work at maximal twist and avoid the need for such corrections. Nevertheless, it might be worthwhile using \( tm\Lambda_{\text{QCD}} \) to determine the LECs (which, for small enough quark masses, are mass independent, though they do depend on the lattice spacing and gauge action) and then try to correct results previously obtained with unimproved untwisted Wilson fermions.

### IV. THE AOKI REGIME

As noted in the introduction, it is of practical interest to study how the results obtained in the GSM regime change when one enters the Aoki regime. We recall that the latter is defined at the quark level as the region where \( m_q \sim a\Lambda_{\text{QCD}}^2 \), or in \( tm\chi \)PT by \( M' \sim \hat{a}^2 / \Lambda_{\chi}^2 \).

In the Aoki regime, competition between terms of size \( M' \) and \( \hat{a}^2 / \Lambda_{\chi}^2 \) leads to a non-trivial phase structure, with first order transition lines ending at second-order endpoints. This has been discussed extensively in Refs. \[13, 14, 15\] and we do not recapitulate the analysis here. We will present results which hold throughout the Aoki regime except on the phase transition lines themselves.

Before presenting results we would like to make a general comment on the concept of \( O(a) \) improvement in the Aoki regime. The improvement program is predicated on the assumption of small discretization errors. In particular the discretization effects are assumed not to cause large changes in the vacuum. This assumption clearly breaks down in the Aoki regime, where, in general, the direction of the quark condensate is determined by a competition between quark masses and discretization errors and the result differs by angles of \( O(1) \) from the continuum theory. Thus in taking the limit \( a \to 0 \), quantities do not change in a manner which is perturbative in \( a \), and the language of \( O(a) \) improvement cannot be applied. This point has been emphasized in Ref. [16].

A possible exception to this discussion has been raised in Ref. \[21\]. They argue that \( O(a) \) improvement at maximal twist remains valid in the Aoki regime, as long as an appropriate choice of twist angle is used. We return to this point at the end of this section.

Irrespective of this general question, one can simulate in the Aoki regime and it is useful to obtain the predictions of \( tm\chi \)PT. We stress that, even though the language of \( O(a) \) improvement may not apply, one can still use Symanzik’s continuum effective Lagrangian to study the theory in the Aoki regime.

Now we turn to the results. We will keep the discussion brief, minimizing technical details, since much of the work is a straightforward generalization of that in the GSM regime.

As explained in Ref. [16], we do not need to augment the chiral Lagrangian used in the GSM regime in order to study the Aoki regime. Instead, since the power counting is now \( p^2 \sim m_q \sim a\Lambda_{\text{QCD}}^2 \), and we work only at LO in this expansion, we can drop some of the NLO terms used above. In particular, to study the vacuum alignment and pion masses, we need only keep the \( W' \) term—those proportional to \( W, W' \) and the \( L_i \), can be dropped. When we consider the currents and densities, however, a new feature emerges. Since the functional derivatives defining these quantities effectively “eat up” one power of \( p^2 \) or \( M' \) terms which were of too high order for pion masses (such as the \( W' \) term of size \( aM' \sim a^3 \)) now need to be kept. Indeed, for each quantity that we consider, a careful study is necessary to determine which terms coming from the GSM regime can be consistently kept.
As already noted, the fundamental difference between the GSM and Aoki regimes is that the condensate is no longer closely aligned with the quark mass. In other words, \( \epsilon = \omega_m - \omega_0 \) is no longer of \( O(a) \), but instead is generically of \( O(1) \). An indication of this is that the \( W' \) contribution to \( \epsilon \) in Eq. (84) is proportional to \( \hat{a}^2/(f^2M') \) and thus of \( O(1) \) in the Aoki regime. The precise alignment of the condensate is determined by a quartic equation which has been given in various forms in Refs. [13, 14, 17, 21]. It can be written:

\[
M' \sin(\omega_m - \omega_0) = M' \sin \epsilon = -\frac{32\hat{a}^2s_mc_mW'}{f^2} + O(a^3). \tag{102}
\]

Note that one solution is \( \omega_m = \omega_0 = \pi/2 \), so that \( \epsilon = 0 \) at maximal twist. The corrections to this result are of \( O(a) \), but we do not control these since they include contributions from \( a^3 \) terms in the chiral Lagrangian.

We now work our way through the quantities considered in the previous section, concentrating on how they differ in the Aoki regime. The precise alignment of the condensate is determined by a quartic equation which has been given in various forms in Refs. [13, 14, 15, 21]. It can be written:

\[
\text{Tr}[\chi^i \Sigma + \Sigma^i \chi] = M' \epsilon \text{Tr}[\Sigma_{ph} + \Sigma_{ph}^i] + iM' \sin \epsilon \text{Tr}[\tau_3(\Sigma_{ph} - \Sigma_{ph}^i)]. \tag{103}
\]

In fact, this change only matters if this term contributes at LO, and thus only affects the pion masses, which are discussed below. For all other quantities the \( M' \) contributions are of higher order than we control in the Aoki regime.

Because of these considerations, the determination of the twist angles \( \omega \) and \( \omega_\rho \) goes through unchanged. They differ from each other, and from \( \omega_m \), by \( O(a) \), with the differences given in Eqs. (61) and (62). The expressions for the physical currents and densities, Eqs. (51, 52), thus remain valid, except that the terms proportional to \( M' \) or \( p^2 \) can be dropped. We do, however, control the \( O(a) \) corrections proportional to \( W, \bar{W} \) and \( W_{10} \). The change of variables in Eqs. (48) and (50) also goes through unchanged, but that in (51) is replaced by

\[
\text{Tr}[\chi^i \Sigma + \Sigma^i \chi] = M' \epsilon \text{Tr}[\Sigma_{ph} + \Sigma_{ph}^i] + iM' \sin \epsilon \text{Tr}[\tau_3(\Sigma_{ph} - \Sigma_{ph}^i)]. \tag{103}
\]

As in the GSM regime, we can replace \( s \) and \( c \) with \( s_P \) and \( c_P \), respectively, to the accuracy we work. The vector form factor, which we do not display, is simply given by the leading order term in continuum \( \chi \text{PT} \) with no \( O(a) \) correction.

The results for the pion masses are changed more substantially. These have already been calculated in Refs. [14, 15, 21] so we only comment on the relation to our results in the GSM regime. In the Aoki regime, we need only keep the LO mass term and the \( W' \) term from (10). For the former, Eq. (103) shows that the contribution to \( m_\pi^2 \) changes from \( M' \) to \( M' \cos \epsilon \) in the Aoki regime. Combining this with the \( W' \) contribution, which is unchanged from the GSM regime, we find (in agreement with Refs. [14, 15, 21])

\[
m_\pi^2 = M' \cos \epsilon + \frac{32\hat{a}^2s_mW'}{f^2} + O(a^3) = \frac{\hat{m}}{s_m} + O(a^3). \tag{108}
\]

We have used Eq. (102) to obtain the second form.

The mass-squared splitting comes only from \( W' \) term in the chiral Lagrangian. It is easy to see that its contribution takes the same form as in Eq. (98), with \( s \) being \( s_m \). But since \( s \) and \( s_m \) differ only by \( O(a) \), one can use either at our accuracy. Thus the result (75) from the GSM regime remains valid in the Aoki regime, in agreement with Refs. [14, 15, 21].

The other quantities which are substantially changed in the Aoki regime are the parity violating matrix elements. These are \( O(a) \) in the GSM regime, but become of \( O(1) \) in the Aoki regime. This is indicated by the factors of \( \hat{a}^2/M' \) in the \( W' \) contributions in Eqs. (51, 52). In fact, it is straightforward to see that we control these quantities only at \( O(1) \), and not at \( O(a) \). This simplifies the calculation since only the pole terms give \( O(1) \) contributions. The results
are (with $a = 1, 2$):

\begin{align}
\langle \pi_a(p_2)|\hat{A}^{q_2}_\mu|\pi_3(p_1)\rangle &= q_\mu \frac{M' \sin \epsilon}{q^2 + m^2_{\pi_a}} + O(a), \\
\langle \pi_a(p_2)|\hat{A}^{\bar{q}}_\mu|\pi_a(p_1)\rangle &= \frac{1}{3} \langle \pi_3(p_2)|\hat{A}^{\bar{q}}_\mu|\pi_3(p_1)\rangle = q_\mu \frac{M' \sin \epsilon}{q^2 + m^2_{\pi_3}} + O(a), \\
\langle \pi_a(p_2)|\hat{P}^a|\pi_3(p_1)\rangle &= -iB_0 \frac{M' \sin \epsilon}{q^2 + m^2_{\pi_3}} + O(a), \\
\langle \pi_a(p_2)|\hat{P}^3|\pi_a(p_1)\rangle &= \frac{1}{3} \langle \pi_3(p_2)|\hat{P}^3|\pi_3(p_1)\rangle = -iB_0 \frac{M' \sin \epsilon}{q^2 + m^2_{\pi_3}} + O(a).
\end{align}

We have used Eq. (102) to simplify the expressions. Note that the choice of pion mass in the denominators makes an $O(1)$ difference to these quantities.

The expressions in this section all simplify at maximal twist. As already noted, we would then have $\epsilon = 0$ in addition to $c = 0$ and $s = 1$. Thus the $O(a)$ corrections to the physical quantities in Eq. (103) vanish, so that all are given simply by their LO continuum $\chi PT$ results. The charged pion masses are similarly given by the LO continuum result, $m^2_{\pi_a} = M'$. The pion mass-squared splitting does differ from the continuum, but this difference is of $O(a^2)$. Finally, the parity violating matrix elements become of $O(a)$ again, as in the GSM regime, although we cannot predict them at the order we are working.

We now return to the issue raised in Ref. [21]. The authors argue that automatic $O(a)$ improvement at maximal twist does extend into the Aoki regime, but only if one uses a twist angle based on a critical mass which includes the $O(a)$ offset, $m' - m$. They point out that one of the definitions of twist angle that accomplishes this is what we call $\omega$ as defined by Eq. (65) (and which they call $\omega_{WPT}$). We fully agree on the need to use such a definition, not only in the Aoki regime, but also in the GSM regime, as we discussed in Sec. 1.

As for automatic $O(a)$ improvement, our results support the proposal of Ref. [21], although with one caveat. We argued that, in the Aoki regime, the condensate did not vary smoothly as the masses are varied. This is true in general, but not at maximal twist, where the condensate remains fixed, with $\omega_{\mu} = \pi/2$ within an uncertainty of $O(a)$. Indeed, as we have already noted, at maximal twist physical quantities are described in the Aoki phase by continuum $\chi PT$ up to $O(a^2)$. If we start in the Aoki regime at $\omega = \pi/2$, and remain on the $\mu$ axis as $a$ is reduced (so that we move into the GSM regime and ultimately to the continuum limit) we expect that physical quantities, at fixed quark masses, will extrapolate smoothly to the continuum with errors quadratic in $a$.

The caveat is that the argument will fail if, as $\mu$ is reduced, one encounters a phase boundary. This is expected to happen in one of the two possible scenarios for the phase diagram [13, 14, 15]. In this scenario, in which $W' > 0$, the end-point of the phase boundary occurs at $\hat{\mu} = 32\hat{\Lambda}^2 W'/f^2$, where $m_{\pi_3} = 0$. Values of $\hat{\mu}$ greater than this are allowed, but for smaller values the condensate changes rapidly (by an amount of $O(1)$) while the quark mass changes by $O(a^2)$, and continuum $\chi PT$ expressions fail. In the other scenario ($W' < 0$) we see no need to impose a lower limit on $\mu$—unless $|W'|$ is unnaturally small, yet higher order terms in the chiral potential will not change the phase structure.

It is worth noting the accuracy with which the critical mass must be determined to stay at $\omega = \pi/2$ within an error of $O(a)$. This is the accuracy that is required to automatically remove the $O(a)$ terms. In the GSM regime, where $\mu \sim a\Lambda_{\overline{\text{QCD}}}$, this requires knowing $m'$ to an absolute accuracy of $O(a^3)$. In the Aoki regime, however, the required absolute accuracy decreases to $O(a^3)$. This sounds like a difficult goal, but, in fact, as we discussed in the summary of the previous section, it is attainable even by doing simulations in the GSM regime.

V. CONCLUSION

In this paper we have used effective field theory methods to study the discretization errors in tmLQCD. We have presented results for a number of pionic quantities that can be calculated in lattice simulations, and studied different possible definitions of the twist angle. Perhaps the most interesting quantities to calculate are the difference $\omega - \omega_P$ (which indicates the size of the $O(a)$ uncertainty in the twist angle), the splitting $m^2_{\pi_3} - m^2_{\pi_a}$ (which indicates the size of $O(a^2)$ flavor breaking, but parity conserving, quantities) and the axial and pseudoscalar form factors of the pion (which are the simplest examples of unphysical quantities). To our knowledge, none of these quantities have been calculated to date, and we urge that they be considered in the future.

In the introduction, we raised a number of issues concerning tmLQCD; now we can comment on what we have learnt about these. Concerning the impact of flavor and parity breaking, we have seen how this contributes to unphysical
quantities at $O(a)$, and in one case, to physical quantities at $O(a^2)$. This case is the pion mass splitting, where we confirm the interesting result of Ref. [14] that knowledge of the sign of the splitting allows one to predict the nature of the phase structure in the Aoki region. Nevertheless, at NLO in $\chi$PT, the pions in the loops are degenerate, and there is no flavor breaking in decay constants or vector and scalar form factors. For staggered fermions, where the “taste” breaking between pions is also of $O(a^2)$, it has been found essential to include this breaking in loop contributions in order to make good fits to the chiral behavior [30]. If this turns out to be true also for tmLQCD (which depends on the size of the as yet unmeasured flavor breaking), then the $\chi$PT calculations will need to be extended beyond NLO. One possibility which we are investigating is to use a power counting like that in Ref. [31], so that a full NNLO calculation is not needed.

We also asked which quantities are good indicators of the size of discretization errors. One answer is that it may be easier to use the flavor-parity violating quantities (i.e. the difference between different definitions of twist angle, and the axial and pseudoscalar form factors), since these are of $O(a)$ (even at maximal twist) and thus easier to calculate. In more general terms, studying these quantities in simulations would allow a more thorough test of our understanding of tmLQCD.

Another interesting question is how we can test the reliability of tm$\chi$PT at the order we are working. Our results, in fact, contain a number of predictions that are valid at NLO but not at higher order. In particular, as we have outlined in the summary subsection of Sec. III most of the flavor-parity violating form factors can be predicted once the other quantities that we have discussed have been calculated. Such tests are important for establishing the credibility of the chiral and continuum extrapolations that must ultimately be done.

We have discussed extensively the issue of the smallest quark mass that can be used without invalidating automatic $O(a)$ improvement at maximal twist. We have argued that one can certainly work in the GSM regime ($m_q \sim a\Lambda_{\overline{\text{QCD}}}^2$) and also at least part-way into the Aoki regime ($m_q \sim a^2\Lambda_{\overline{\text{QCD}}}^3$). This is only true, however, if one uses the appropriate definition of twist angle. Allowable choices are that determined from the vanishing of the coupling of the bare axial current in the twisted basis to the charged pion, or from the vanishing of the coupling of the pseudoscalar density to the neutral pion. Alternatively one could fix the twisted mass $\mu$ and vary the untwisted mass until the pion masses (either charged or neutral) reach their minimum values [21]. What is potentially problematic is to determine the critical quark mass by extrapolating the squared pion mass to zero along the untwisted Wilson axis using only moderately small quark masses. In the GSM regime this may not, in practice, give the critical mass with the accuracy needed (errors of absolute size $O(a^2)$) to ensure $O(a)$ improvement at maximal twist. Furthermore, this method does not apply in the Aoki regime, where it gives a determination of the critical mass with an absolute error of $O(a^2)$, whereas the required accuracy is $O(a^3)$.

One spin-off from our calculation is a method for determining the new LECs that enter when one incorporates discretization errors. This both allows a direct measure of their size, and can be used a posteriori to correct results obtained with untwisted Wilson fermions. Furthermore, our calculations extend the results that are available from $\chi$PT applied to untwisted Wilson quarks [17, 18] to several new quantities.

Many of the quantities we have considered will be difficult to calculate in lattice simulations because they involve quark-disconnected contractions. An important practical question to consider is whether, by using partially quenched tmLQCD and its corresponding $\chi$PT [32], one can make predictions for the quark-connected and disconnected contributions separately. It will also be interesting to extend the calculations to the case of a non-degenerate doublet of quarks [33].

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6 This point may explain the “bending phenomenon” observed at masses below $m_q \sim a\Lambda_{\overline{\text{QCD}}}^2$ in Ref. [16]. Such bending is expected in most quantities if one approaches the untwisted Wilson axis along a line parallel to the twisted mass axis. It would be interesting to fit the results from this work under this hypothesis, using the formulae we have provided.
[1] R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz, Nucl. Phys. Proc. Suppl. 83, 941 (2000).
[2] R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz [Alpha collaboration], JHEP 0108, 058 (2001).
[3] R. Frezzotti, “Twisted mass lattice QCD”, plenary talk at Lattice 2004, hep-lat/0409138.
[4] A. D. Kennedy, “Algorithms for lattice QCD with dynamical fermions,” plenary talk at Lattice 2004, hep-lat/0409167.
[5] R. Frezzotti and G. C. Rossi, JHEP 0408, 007 (2004).
[6] C. Pena, S. Sint and A. Vladikas, JHEP 0409, 069 (2004).
[7] R. Frezzotti and G. C. Rossi, JHEP 0410, 070 (2004).
[8] P. Farchioni et al., hep-lat/0406039.
[9] F. Farchioni et al., hep-lat/0409098.
[10] W. Bietenholz et al., hep-lat/0411001.
[11] F. Farchioni et al., hep-lat/0410031.
[12] S. Sharpe and R. Singleton, Jr, Phys. Rev. D 58, 074501 (1998).
[13] G. Münster, JHEP 0409, 035 (2004).
[14] L. Scorzato, Eur. Phys. J. C 37, 445 (2004).
[15] S. R. Sharpe and J. M. S. Wu, Phys. Rev. D 70, 094029 (2004).
[16] G. Münster and C. Schmidt, Europhys. Lett. 66, 652 (2004).
[17] G. Rupak and N. Shoresh, Phys. Rev. D 66, 054503 (2002).
[18] O. Bär, G. Rupak and N. Shoresh, Phys. Rev. D 70, 034508 (2004).
[19] S. Sharpe and J. Wu, hep-lat/0407035.
[20] G. Münster, C. Schmidt and E. E. Scholz, hep-lat/0409066.
[21] S. Aoki and O. Bar, Phys. Rev. D 70, 116011 (2004).
[22] S. Hashimoto, hep-ph/0411126.
[23] S. Aoki, Phys. Rev. D 30, 2653 (1984); Phys. Rev. Lett. 57, 3136 (1986); Prog. Theor. Phys. 122, 179 (1996).
[24] K. Symanzik, Nucl. Phys. B226, 187 (1983a); B227, 205 (1983b).
[25] R. Frezzotti, S. Sint and P. Weisz [AlPHA collaboration], JHEP 0107, 048 (2001).
[26] J. Wess and B. Zumino, Phys. Lett. B 37, 95 (1971); E. Witten, Nucl. Phys. B 223, 422 (1983).
[27] J. Gasser and H. Leutwyler, Annals Phys. 158, 142 (1984).
[28] M. Lüscher, S. Sint, R. Sommer and P. Weisz, Nucl. Phys. B 478, 365 (1996).
[29] M. Bochicchio, L. Maiani, G. Martinelli, G. C. Rossi and M. Testa, Nucl. Phys. B 262, 331 (1985).
[30] C. Aubin et al. [MILC Collaboration], Phys. Rev. D 70, 114501 (2004).
[31] S. Aoki, Phys. Rev. D 68, 054508 (2003).
[32] G. Münster, C. Schmidt and E. E. Scholz, Europhys. Lett. 66, 639 (2004).
[33] R. Frezzotti and G. C. Rossi, Nucl. Phys. Proc. Suppl. 128, 193 (2004), hep-lat/0311008.