Twisted Mass Finite Volume Effects

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Abstract

We calculate finite volume effects on the pion masses and decay constant in twisted mass lattice QCD (tmLQCD) at finite lattice spacing. We show that the lighter neutral pion in tmLQCD gives rise to finite volume effects that are exponentially enhanced when compared to those arising from the heavier charged pions. We demonstrate that the recent two flavour twisted mass lattice data can be better fitted when twisted mass effects in finite volume corrections are taken into account.
I. INTRODUCTION

For large enough lattices, finite volume effects (FVEs) are only sensitive to the long distance physics of the underlying theory – for lattice QCD simulations they are well described by chiral perturbation theory (ChPT) \[1\], and can be analyzed systematically in a chiral expansion. In a series of papers \[2–4\], FVEs on pseudoscalar meson masses and decay constants in the continuum limit have been studied with the help of resummed Lüscher formulae used in conjunction with ChPT. In the original asymptotic formula by Lüscher \[5\], the exponentially dominating FVEs for the mass of a particle \(P\) is expressed as an integral over the forward scattering amplitude of the particle \(P\) off the lightest particle in the spectrum (pions for QCD). Since the scattering amplitude is needed only at low energy, it can be evaluated in ChPT. In Ref. \[4\], it has been shown that by resumming a series of such integrals (over the same scattering amplitude but with kernels increasingly exponentially suppressed), one can improve the reliability of such formulae in describing FVEs.

As shown in Ref. \[4\], if one inserts the tree-level scattering amplitude in the resummed Lüscher formula, one obtains exactly the one-loop ChPT calculation of the FVEs. In Ref \[6\], the pion mass has been calculated in ChPT to two loops and compared with the result obtained from the resummed Lüscher formula using the one-loop ChPT representation of the scattering amplitude. The difference is found to be very small, and one has thus confidence in the validity of the resummed Lüscher formulae in predicting the size of FVEs. This allows for a much simpler evaluation of the main effects at the two-loop level and beyond, and for one to check the convergence of the chiral expansion for FVEs. Nevertheless, it is still essential to test these predictions against actual data.

Recently, the European Twisted Mass Collaboration (ETMC) has provided one such test for the pion mass and decay constant \[7, 8\], and the outcome was not entirely positive. While FVEs on the decay constant are rather well described by the resummed formula at the next-to-leading order (NLO), the same does not hold for the pion mass. For the pion mass, FVEs are larger than what is predicted from the NLO and NNLO resummed formulae (see Table 2 in Ref. \[7\]), and the discrepancy appears to be much larger than the size of the error estimated in Ref. \[4\], which calls for an explanation.

Before discussing possible sources of such a deviation, we stress that the ETMC data are on the borderline of applicability of ChPT for calculating finite volume corrections. It has
been argued in Ref. [2] that for ChPT to be applicable, a box size of $L > 2$ fm is necessary. The comparison made in Table 2 of Ref. [7] uses the largest volumes as reference points, and FVEs are measured with respect to these. The data sets used to study FVEs thus have $L \sim 2.0$ fm (where ChPT may still marginally work) or less (where ChPT is not expected to be valid). This may be a possible reason for the discrepancy.

In this paper we study another possible source for deviation from the continuum formulae, i.e. discretization effects. As is well known, at finite lattice spacing, isospin- and parity-breaking effects are sizeable in twisted mass lattice QCD (tmLQCD). In particular, the neutral pion mass becomes smaller than the charged ones $^1$, and parity-breaking interactions among pions become possible. Both of these effects are well described in the framework of tmChPT $^9$–$^{12}$, and they have nontrivial influences on the finite volume corrections as they generate exponentially enhanced FVEs. Indeed, if one takes the continuum limit first without explicitly accounting for these effects and make finite volume corrections using the continuum formulae, one will not be able to fully disentangle in the final results FVEs from discretization effects.$^2$

The rest of the paper is organized as follows. In the next section, we briefly describe the formalism of tmChPT, highlighting aspects that are relevant for our calculations. In Sec. III we explain why and which discretization effects are exponentially enhanced at finite volume with the help of LO asymptotic formulae. In Sec. IV we give resummed asymptotic formulae at NLO applicable to the ETMC data, which we use to perform a new analysis on the ETMC data. Sec. V contains relevant results and discussion of our analysis, and Sec. VI our conclusion. We concentrate in this paper on the charged pions where high quality lattice data are available, but also provide formulae for FVE for the neutral pion mass for future use.

$^1$ For the range of masses and lattice spacings of the ETMC simulations, the neutral pion is typically about 15-20% lighter than the charged ones.

$^2$ The size of the twisted mass discretization effects can only be determined after a detailed analysis. Nevertheless, one can argue that if these were responsible for the discrepancy between the FVEs observed by ETMC and those calculated in the continuum, they are at the percent level.
II. TWISTED MASS CHIRAL EFFECTIVE THEORY

Consider tmLQCD with a degenerate doublet of quarks [13]. The low energy, long distance dynamics of the underlying lattice theory can be described by an effective continuum chiral theory constructed using the two-step procedure of Ref. [14], whereby effects of discretization errors are systematically incorporated in a joint expansion of the lattice spacing, $a$, the quark mass, $m$, and the twisted mass, $\mu$. This was carried out to NLO in Ref. [11], and the resulting tmChPT studied in detail in Ref. [12]. Using the power counting scheme, $m \sim \mu \sim p^2 \sim a \Lambda_{\text{QCD}}^2$, the twisted mass effective chiral Lagrangian reads [12]:

\[
L_Ch = \frac{F^2}{4} \langle D_\mu U D_\mu U^\dagger - (\chi^\dagger U + U^\dagger \chi) \rangle - \frac{\ell_1}{4} \langle D_\mu U D_\mu U^\dagger \rangle^2 - \frac{\ell_2}{4} \langle D_\mu U D_\mu U^\dagger \rangle^2 - \frac{\ell_3}{16} \langle \chi^\dagger U + U^\dagger \chi \rangle^2 + \frac{\ell_4}{4} \langle D_\mu \chi^\dagger D_\mu U + D_\mu U^\dagger D_\mu \chi \rangle
\]

\[- W \langle \chi^\dagger U + U^\dagger \chi \rangle \langle \hat{A}^\dagger U + U^\dagger \hat{A} \rangle - W' \langle \hat{A}^\dagger U + U^\dagger \hat{A} \rangle^2
\]

\[+ W_{10} \langle D_\mu \hat{A}^\dagger D_\mu U + D_\mu U^\dagger D_\mu \hat{A} \rangle + \tilde{W} \langle D_\mu U D_\mu U^\dagger \rangle \langle \hat{A}^\dagger U + U^\dagger \hat{A} \rangle
\]

\[- H' \langle \hat{A}^\dagger \chi' + \chi^\dagger \hat{A} \rangle ,
\]

where we have displayed only parts relevant for our discussion and our study of FVEs below. Here, $F$ is normalized so that $F_\pi = 92.4$ MeV, $U$ is the usual $SU(2)$ matrix-valued field, $\langle \ldots \rangle$ denotes the trace, $\ell_i$ the usual Gasser-Leutwyler Low Energy Constants (LECs), and the rest of coefficients LECs arising from discretization errors. The quantities $\chi'$ and $\hat{A}$ are spurions for quark masses and discretization errors that are set to constant values at the end of the analysis:

\[
\chi' \rightarrow 2B_0 (m + i\tau_3 \mu) + 2W_0 a \equiv \hat{m} + \hat{\mu} + i\tau_3 \hat{\mu} , \quad \hat{A} \rightarrow 2W_0 a \equiv \hat{a} ,
\]

where $\tau_3$ is normalized so that $\tau_3^2 = 1$, $B_0$ and $W_0$ are unknown dimensionful constants, and we have defined the quantities $\hat{m}$, $\hat{\mu}$, and $\hat{a}$.

As explained in Ref. [12], the $W_{10}$ term in the effective chiral Lagrangian is redundant, and can be transformed away into a combination of $W$, $\tilde{W}$, and $H'$ terms. However, the same redundancy can be used to eliminate the $\tilde{W}$ term in favour of the $W_{10}$ term instead, which has the advantage of simplifying the Feynman rules when studying FVEs in tmChPT, as we see below. In doing so, results derived in Ref. [12] would remain the same except with
all $\tilde{W}$ terms removed. In particular, the expansion about the NLO vacuum with external fields set to zero now reads:

$$L_\chi = \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial_\mu \vec{\pi} + \frac{\pi^2}{2} (M' + \Delta M') + \frac{\pi^2}{2} \frac{32}{F^2} \hat{a}^2 s^2 W' + \frac{\pi^2}{2} \frac{\epsilon M'}{F} - (\pi^2)^2 \frac{M'}{24 F^2} + \ldots ,$$  (3)

where $\pi^2 = \vec{\pi} \cdot \vec{\pi}$, and we have used the convenient parametrization $U = \sigma + i \vec{\pi} \cdot \vec{\tau}/F$, with $\sigma = \sqrt{1 - \pi^2/F^2}$. The quantities $s$ and $c$ denote the sine and cosine of a nonperturbatively defined vacuum (twist) angle $\omega$, and $\epsilon$ is the shift of the vacuum angle at NLO tmChPT from that at LO:

$$\epsilon \equiv \omega_m - \omega_0 = -\frac{16}{F^2} \hat{a} s_0 (W + 2 W' \hat{a} c_0/M') .$$  (4)

Note that $\omega$ differs from both $\omega_0$ and $\omega_m$ by $O(a)$ so that at NLO accuracy, $s$ and $c$ could equally well be $s_0 (s_m)$ and $c_0 (c_m)$. The mass parameters are given by

$$M' = |\chi'| = \sqrt{(\hat{m} + \hat{a})^2 + \hat{\nu}^2} , \quad \Delta M' = \frac{2}{F^2} \left[ M'^2 \ell_3 + 16 (\hat{a} \hat{c} M' W + \hat{a} \hat{a} c^2 W') \right] ,$$  (5)

and the charged and neutral pion masses at NLO read:

$$M^2_{\pi\pm} = M' \left[ 1 - \frac{M'}{32 \pi^2 F^2} \bar{\ell}_3 + \frac{32 M'}{F^2} \hat{a} \hat{c} (M' W + \hat{a} c W') \right] ,$$

$$M^2_{\pi 0} = M^2_{\pi\pm} - \frac{32}{F^2} \hat{a}^2 s^2 W' \equiv M^2_{\pi\pm} - a^2 K , \quad K = \frac{128}{F^2} s^2 W_0^2 W' ,$$  (6)

with

$$\bar{\ell}_i = \bar{\ell}^{\text{phys}}_i + 2 \log \frac{M^{\text{phys}}_\pi}{M_\pi} \equiv \log \frac{\Lambda^2_i}{M^2_\pi}$$  (8)

the standard scale-independent LECs of $SU(2)$ ChPT [15]. We have defined the dimensionful quantities $\Lambda_i$ for use in our numerical analysis below. The pion decay constant at NLO reads

$$F_\pi \equiv F_{\pi\pm} = F \left[ 1 + \frac{M'}{16 \pi^2 F^2} \bar{\ell}_4 + \frac{4 M'}{F^2} \hat{a} \hat{c} W_{10} \right] .$$  (9)

Note that at maximal twist, $\omega = \pi/2$, the charged pion masses and pion decay constant above take their continuum form with $O(a)$ effects automatically removed. At NLO, the effects of twisting reside only in the $O(a^2)$ charged-neutral pion mass splitting, which is maximal at maximal twist.
III. EXPONENTIALLY ENHANCED TWISTED MASS DISCRETIZATION EFFECTS AT FINITE VOLUME

Consider Lüscher’s formula for the pion mass \(^3\):

\[
\frac{M_\pi(L) - M_\pi}{M_\pi} = -\frac{3}{16\pi^2\lambda_\pi} \int_{-\infty}^{\infty} dy \mathcal{F}(iy) e^{-\sqrt{1+y^2}\lambda_\pi} + \ldots,
\]

\[\lambda_\pi \equiv M_\pi L, \quad (10)\]

where \(\mathcal{F}(iy)\) is the forward \(\pi\pi\)-scattering amplitude evaluated for a purely imaginary argument (given in units of pion mass), and \(y\) is real and dimensionless. This formula gives the exponentially dominant contribution under the assumption that the pion is the lightest particle in the spectrum. In the presence of a splitting between the charged and the neutral pions, as is the case in tmLQCD, this formula is modified to

\[
R_i \equiv \frac{M_{\pi^i}(L) - M_{\pi^i}}{M_{\pi^i}} = -\frac{3}{16\pi^2\lambda_i} \sum_{j=1}^{3} \frac{M_{\pi^j}}{M_{\pi^i}} \int_{-\infty}^{\infty} dy \mathcal{F}_{ij}(iy) e^{-\sqrt{1+y^2}\lambda_j} + \ldots,
\]

\[\lambda_j \equiv M_{\pi^j} L, \quad (11)\]

where \(\mathcal{F}_{ij}(iy)\) is now the forward scattering amplitude of pions with isospin index \(i\) off pions with isospin index \(j\). Note that \(y\) is still dimensionless but now normalized to \(M_{\pi^j}\), and we use the shorthand \(\lambda_j\) for \(\lambda_{\pi^j}\).

With its lighter mass, the neutral pion contribution is (exponentially) dominant with respect to the heavier charged pions. The weights of these contributions are given by the forward scattering amplitudes, and at LO in tmChPT they read:

\[\mathcal{F}_{11} = -\mathcal{F}_{12} = -\mathcal{F}_{13} = \frac{M'}{F^2}, \quad (12)\]

where \(M'\) and \(F\) are the LO pion mass-squared and decay constant. This shows that since pions with index 1 and 2 are degenerate, their contributions cancel. The relative finite-volume shift for the charged pion mass at LO in tmChPT is then given by

\[R_{\pm} = \frac{3}{8\pi^2\lambda_\pm} \frac{M_{\pi^0}}{M_{\pi^\pm}} \frac{M'}{F^2} K_1(\lambda_0) + \ldots, \quad (13)\]

where \(K_i\) denotes the modified Bessel function. As an illustration of the importance of this discretization effect, we evaluate \(R_{\pm}\) for the ETMC \(B_1\) ensemble in Ref. [7], for which

\[\text{For clarity in demonstrating the idea here, we do not write out the resummed version of this formula, but will defer to the next section where we give our final formulae in full.}\]
\[ M_{\pi^\pm} = 0.33 \text{ GeV and } M_{\pi^0} = 0.27 \text{ GeV:} \]

\[ R_\pm = 0.26\% \quad \text{(B1 ensemble).} \quad (14) \]

However, if we set \( M_{\pi^0} = M_{\pi^\pm} = 0.33 \text{ GeV}, \) i.e. turning off the twisted mass effects, we get

\[ R_\pm = 0.15\% \quad \text{(B1 ensemble).} \quad (15) \]

We note that if one here resums the whole series of exponentially subdominant LO contributions (corresponding to a LO ChPT evaluation of FVEs), 0.15\% goes up to 0.62\%; using the NNLO resummed asymptotic formula of Ref. [4] gives 1\%, whereas the ETMC measurement is 1.8(5)\%.

There is a second discretization effect arising from the parity-violating cubic interactions (see Eq. \(3\)), which could be potentially significant as well. The contributions to FVEs due to these in the pion mass formally come in at higher order: they are NNLO FVEs, or \( \mathcal{O}(p^8) \) corrections to the pion mass.\(^4\) But because of the different topology of the relevant loop diagrams, these contributions are exponentially enhanced with respect to the tadpole diagrams that contain virtual neutral pions. For these diagrams, the dominating exponential behavior goes as \( e^{\lambda_0 \sqrt{1-w^2}} \), where \( w \equiv M_{\pi^0}/(2M_{\pi^\pm}) \). From the parameters extracted from the \( B_1 \) ensemble, the enhancement of such a contribution with respect to the standard \( e^{-\lambda_\pm} \) behavior is more than 200\%, i.e. \( e^{-\lambda_0 \sqrt{1-w^2}}/e^{-\lambda_\pm} \simeq 2.4 \), which motivates us to investigate these effects in our analysis even when they are formally of higher order. Now these contributions to the FVEs are proportional to \( \epsilon^2 \), which involves unknown LECs \( W \) and \( W' \) that have to be determined if the size of these contributions are to be predicted. If one works at maximal twist, only \( W \) is required, which one can determine e.g. from the ratio of density matrix elements \([12]\).\(^5\) We remark here that if the exponentially enhanced parity-violating contributions are truly large or that FVEs can be measured precise enough, one can turn it around and use instead FVEs to get a measure of \( W \); one could even determine \( W_0 \), the additional unknown dimensionful constant in tmChPT, if \( W \) is already determined elsewhere.

\(^4\) In the tmChPT counting we use, these vertices are \( \mathcal{O}(p^4) \), and one needs at least two of them to contribute to the \( \pi\pi \)-scattering amplitude entering Lüscher’s formula given by Eq. \(10\). Equivalently, one needs at least two such vertices to make a self-energy correction to the pion propagator that yields FVEs.

\(^5\) The LEC \( W' \) can be determined from the mass splitting between the charged and neutral pion \([12]\). But this is difficult in practice as calculating the neutral pion mass on the lattice involves quark disconnected contributions.
IV. NLO FORMULAE FOR THE PION MASSES AND DECAY CONSTANT IN FINITE VOLUME

A. The standard contributions

We provide here the complete resummed asymptotic formulae at NLO for the relative finite volume shift of the charged pion mass and decay constant. We split the contributions to the NLO FVEs for the charged pion mass into contributions in decreasing exponential importance:

\[ R_{M_\pm} = R_{M_\pm}(\lambda_0) + R_{M_\pm}(\lambda_\pm), \]  

(16)

where \( R_{M_\pm}(\lambda_0) \) is the standard contribution due to neutral pions traveling around the whole volume (\( \sim e^{-\lambda_0} \)), and \( R_{M_\pm}(\lambda_\pm) \) that due to the charged pions (\( \sim e^{-\lambda_\pm} \)).

The standard contributions \( R_{M_\pm} \) start at \( O(p^2) \), and it is easy to obtain the next order correction by evaluating \( \pi\pi \)-scattering at NLO in tmChPT. Inserting this into the resummed Lüscher formula, we have:

\[ R_{M_\pm}(\lambda_i) = -\frac{\xi_\pm}{2\lambda_\pm} \sum_{n=1}^\infty \frac{m(n)}{\sqrt{n}} \left[ I_{M,i}^{(2)}(\sqrt{n}\lambda_i) + \xi_\pm I_{M,i}^{(4)}(\sqrt{n}\lambda_i) + O(\xi^2) \right], \quad \xi_\pm \equiv \frac{M_{\mp}^2}{16\pi^2 F_\pi^2}, \]  

(17)

where \( i \in \{\pm, 0\} \) is the isospin index, \( m(n) \) is the multiplicity of the integer vector \( \vec{n} \) of length \( n = |\vec{n}| \), and

\[ I_{M,0}^{(2)} = -B^0, \quad I_{M,\pm}^{(2)} = 0, \]  

(18)

\[ I_{M,\pm}^{(4)} = \left[ \frac{4}{3}\tilde{\ell}_1 - \frac{1}{2}\tilde{\ell}_3 - 2\tilde{\ell}_4 + \frac{13}{18} \right] B^0 + \left[ \frac{20}{9} - \frac{8}{3}\tilde{\ell}_2 \right] B^2 + \frac{2}{3}(R_0^0 + 2R_0^1 - 4R_0^2), \]  

\[ I_{M,\pm}^{(4)} = \left[ \frac{8}{3}(\tilde{\ell}_1 + \tilde{\ell}_2) - 2\tilde{\ell}_3 - \frac{34}{9} \right] B^0 + \left[ \frac{92}{9} - \frac{8}{3}\tilde{\ell}_1 - 8\tilde{\ell}_2 \right] B^2 + \frac{1}{3}(11R_0^0 - 20R_0^1 - 32R_0^2), \]  

with \( B^{2k} \equiv B^{2k}(\sqrt{n}\lambda_i) \) and \( R_0^{k(t)}(\sqrt{n}\lambda_i) \) integrals given by

\[ B^{2k}(\sqrt{n}\lambda_i) = r_i^{2k+1} \int_{-\infty}^\infty dy y^{2k} e^{-\sqrt{n}(1+y^2)\lambda_i} = r_i^{2k+1} \frac{\Gamma(k+1/2)}{\Gamma(3/2)} \left( \frac{2}{\sqrt{n}\lambda_i} \right)^k K_{k+1}(\sqrt{n}\lambda_i), \]  

(19)

\[ R_0^{k(t)}(\sqrt{n}\lambda_i) = \begin{cases} \text{Re} & \text{for } k \text{ even} \\ \text{Im} & \text{for } k \text{ odd} \end{cases} \int_{-\infty}^\infty dy y^k e^{-\sqrt{n}(1+y^2)\lambda_i} g^{(t)}(2 + 2iy), \]  

(20)

\[ R_0^{k(t)}(\sqrt{n}\lambda_i) = \begin{cases} \text{Re} & \text{for } k \text{ even} \\ \text{Im} & \text{for } k \text{ odd} \end{cases} \int_{-\infty}^\infty dy y^k e^{-\sqrt{n}(1+y^2)\lambda_i} g^{(t)}(2 + 2iy), \]  

(20)

For simplicity, we have set \( M_{\pi^0} = M_{\pi^\pm} \) in the NLO \( \pi\pi \)-scattering amplitude, as the effects of the charged-neutral pion mass splitting is higher order. The same goes for the amplitude entering the Lüscher formula for \( F_\pi \).
where \( r_i = M_{\pi^i}/M_{\pi^\pm} \) and \(^7\)

\[
g(x) = \sigma \log \frac{\sigma - 1}{\sigma + 1} + 2, \quad \sigma(x) = \sqrt{1 - 4/x}. \tag{21}
\]

For completeness we give here also the full NLO resummed asymptotic formula for FVEs in the neutral pion mass, although these will not be used in our numerical analysis. The formula reads:

\[
R_{M_0} = R_{M_0}^{(\lambda_0)} + R_{M_0}^{(\lambda_\pm)}, \tag{22}
\]

where

\[
R_{M_0}^{(\lambda_i)} = -\frac{\xi_\pm}{2\lambda_0} \sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}} \left[ I_{M_0,i}^{(2)}(\sqrt{n}\lambda_i) + \xi_\pm I_{M_0,i}^{(4)}(\sqrt{n}\lambda_i) + \mathcal{O}(\xi_\pm^2) \right]. \tag{23}
\]

The integrals \( I_{M_0,i}^{(n)} \) can be expressed in terms of the \( I_{M,i}^{(n)} \) integrals defined for the charged pion mass:

\[
I_{M_0,0}^{(n)}(\sqrt{n}\lambda_0) = I_{M,\pm}^{(n)}(\sqrt{n}\lambda_0) - I_{M_0,0}^{(n)}(\sqrt{n}\lambda_0)
\]

\[
I_{M_0,\pm}^{(n)}(\sqrt{n}\lambda_\pm) = 2I_{M,\pm}^{(n)}(\sqrt{n}\lambda_\pm). \tag{24}
\]

For the pion decay constants, the decomposition of the finite volume shifts is similar to that given for the pion mass. We have:

\[
R_{F_\pm} = R_{F_\pm}^{(\lambda_0)} + R_{F_\pm}^{(\lambda_\pm)}, \tag{25}
\]

where

\[
R_{F_\pm}^{(\lambda_i)} = \frac{\xi_\pm}{\lambda_\pm} \sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}} \left[ I_{F,i}^{(2)}(\sqrt{n}\lambda_i) + \xi_\pm I_{F,i}^{(4)}(\sqrt{n}\lambda_i) + \mathcal{O}(\xi_\pm^2) \right], \tag{26}
\]

and

\[
I_{F,0}^{(2)} = I_{F,\pm}^{(2)} = -B^0, \quad I_{F,0}^{(4)} = \left[ \frac{1}{9} + \frac{2}{3} \bar{\ell}_1 - \bar{\ell}_4 \right] B^0 + \left[ \frac{20}{9} - \frac{8}{3} \bar{\ell}_2 \right] B^2 + \frac{1}{3} \left( 2R_0^0 + 4R_0^1 - 8R_0^2 - R_0^0' - 2R_0^1' + 4R_0^2' \right),
\]

\[
I_{F,\pm}^{(4)} = \left[ -\frac{8}{9} + \frac{4}{3} \bar{\ell}_1 + \frac{4}{3} \bar{\ell}_2 - 2\bar{\ell}_4 \right] B^0 + \left[ \frac{92}{9} - \frac{8}{3} \bar{\ell}_1 - 8\bar{\ell}_2 \right] B^2
\]

\[
+ \frac{1}{3} \left[ 2R_0^0 + 8R_0^1 - 32R_0^2 - \frac{11}{2} R_0^0' + 10R_0^1' + 16R_0^2' \right]. \tag{27}
\]

\(^7\)The function \( g(x) \) is related to the standard \( J \) one-loop function through \( g(x) = 16\pi^2 J(xM_{\pi^\pm}^2) \).
B. The parity-violating cubic interaction contributions

As discussed above, because of the exponential enhancement, contributions due to parity-violating cubic interactions in tmChPT may have an effect at NLO in addition to the standard contributions to FVEs (arising from parity-conserving quartic interactions), despite being formally higher order. For the charged pion mass, they are given by

$$\Delta R_{M\pm} = -\epsilon^2 \frac{\xi_{\pm}}{\lambda_{\pm}} \sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}} \left[ \pi e^{-\lambda_0 \sqrt{n(1-w^2)}} - \frac{1}{4} \int_{-\infty}^{\infty} dy \frac{e^{-\lambda_0 \sqrt{n(1+y^2)}}}{y^2 + w^2} \right].$$  \hspace{1cm} (28)

Recall that $w \equiv M_{\pi^0}/(2M_{\pi^\pm}) < 1$. As explained above, the leading exponential contributions to pion mass in finite volume arises first at $O(p^8)$ in the chiral counting. Thus, contributions to the relative shift given here is $O(p^6)$. Note that the sign of $\Delta R_{M\pm}$ is fixed, and is opposite to the standard contributions given in Eq. (16), which tend to make the pion masses larger; $\Delta R_{M\pm}$ would hence reduce this enlargement.

For the pion decay constants, the exponentially enhanced contributions arise from the parity-violating interaction with the axial current. These have the same form as that for the charged pion mass except for a different prefactor involving the LEC $W_{10}$:

$$\Delta R_{F\pm} = -\frac{3s}{4\epsilon} \Delta R_{M\pm}, \quad \delta = \frac{4\delta W_{10}}{F^2}. \hspace{1cm} (29)$$

Note that $\Delta R_{F\pm}$ is actually proportional to $\epsilon$, and unlike the case for pion mass above, its sign is not fixed because $W_{10}$ is unknown. We also remark that this contribution to the FVEs depends on how exactly $F_\pi$ is calculated. If the pseudoscalar density is used instead of the axial current as is the case here, $\Delta R_{F\pm}$ would be proportional to $W$ instead of $W_{10}$. This is a consequence of the fact that the Ward identity

$$G_\pi m_q = F_\pi M^2_\pi \hspace{1cm} (30)$$

is violated by discretization effects in tmChPT.

V. NUMERICAL ANALYSIS

As a first illustration of the importance of the full NLO discretization effects in finite volume corrections, we evaluate them numerically using the formulae derived in the previous section for a box of size 2 fm and with pion masses close to those in the ETMC ensemble.
Relative shift LO NLO Cubic interactions

| (%) | ChPT | tmChPT | ChPT | tmChPT |
|-----|------|--------|------|--------|
| $M_\pi$ | 0.38 | 0.71 | 0.74 | 1.24 |
| $F_\pi$ | -1.5 | -2.2 | -2.1 | -3.0 |

TABLE I: Relative finite volume corrections in percentage for a $L = 2$ fm box. The ChPT columns denote the case of degenerate pion with $M_{\pi^\pm} = M_{\pi^0} = 0.33$ GeV, while the tmChPT columns that where charged and neutral pions are split with $M_{\pi^\pm} = 0.33$ GeV and $M_{\pi^0} = 0.27$ GeV. At these mass values, $F_\pi$ is about and so taken to be 0.11 GeV [2]. The $3\pi$-vertex contributions are obtained by setting $\epsilon = \xi$ and $s\delta/\epsilon = 1$.

Overall, Table I shows that the corrections to the continuum formulae are substantial, especially for the pion masses, and this argues for a more detailed analysis of the ETMC data. Using the most recent ETMC data [8], we performed a new analysis to evaluate the impact on the finite volume corrections when effects due to the lighter neutral pion are included. A global $\chi^2$ fit to the ensembles $B_1 - B_4, B_6, B_7, C_1 - C_3$ and $D_1$ is performed, which all have a charged pion mass below 500 MeV and a box size of at least 2 fm (so that ChPT can be safely applied). Our fit is purely statistical and does not include systematic errors, which have not been released. We recall that ensembles in the B (D) set have a

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8 Ensembles $C_5$ and $D_2$ have $L \simeq 1.6$ fm, and thus too small a volume to have the FVEs reliably described by our formulae. Nevertheless, we have checked that including them in our fits does not deteriorate the quality of the fits, nor changes any of our conclusions.
coarser (finer) lattice than the \( C \) set.

The forms we use to fit the ETMC data on the charged pion masses and decay constants at maximal twist read:

\[
M_{\pi \pm}(a, L) = \sqrt{M'} \left[ 1 - \frac{M'}{32\pi^2 F^2} \bar{\ell}_3 + a^2 D_m \right]^{1/2} \left( 1 + R_{M_{\pi \pm}} \right),
\]

\( 31 \)

\[
F_{\pi}(a, L) = F \left[ 1 + \frac{M'}{16\pi^2 F^2} \bar{\ell}_4 + a^2 D_f \right] \left( 1 + R_{F_{\pi \pm}} \right).
\]

\( 32 \)

Notice that we have not included \( \Delta R_{M_{\pi \pm}} \) and \( \Delta R_{F_{\pi \pm}} \) in our fitting forms: we have checked that the data at their current precision, have no sensitivity to these higher order parity-violating effects.\(^9\) We have however included parameters \( D_m \) and \( D_f \) in our fit, which account for the relative \( \mathcal{O}(a^2) \) effects in \( M_\pi \) and \( F_\pi \) respectively. Although such effects are formally higher order (NNLO) in the counting we use, they may appear spuriously if the maximal twist condition, \( \omega = \pi/2 \), is only determined to \( \mathcal{O}(a) \) accuracy. They are therefore included to provide useful diagnostics.

In all, our fitting parameters at maximal twist thus consist of the tmChPT parameters (in lattice units) \( a_C F \), \( 2a_C B_0 \), \( a_C A_3 \), \( a_C A_4 \) and \( a_C^4 K \), the ratios of lattice spacings \( a_B/a_C \) and \( a_D/a_C \), and additional lattice discretization parameters \( a_C^2 D_m \) and \( a_C^2 D_f \). The notation \( a_X \) here denotes the lattice spacing for the ensemble set \( X \), and we have chosen \( a_C \) to be the reference lattice unit. The scale setting is accomplished by fixing \( F_\pi = 92.4 \text{ MeV} \) at the point where the ratio \( M_\pi/F_\pi \) assumes its physical value. Note that the \( r_0/a_X \) data provide constraints on the ratios of lattice spacings. In our fitting the values of \( r_0/a_X \) are taken in the chiral limit as provided in Ref. [8]. We do not fit the LECs \( \bar{\ell}_{1,2} \), which appear at NLO (or \( \mathcal{O}(p^4) \)) in the finite volume corrections. They are fixed as in Ref. [15], with their mass independent parts set to

\[
\bar{\ell}_1^{phys} = -0.4 \pm 0.6, \quad \bar{\ell}_2^{phys} = 4.3 \pm 0.1.
\]

\( 33 \)

We have investigated in our fitting, the effects of turning on the pion mass splitting (\( K \)) and higher order \( \mathcal{O}(a^2) \) discretization effects (\( D_m \) and \( D_f \)) in various combinations. We

\(^9\) When fitting with \( \Delta R_{M_{\pi \pm}} \) and \( \Delta R_{F_{\pi \pm}} \) included, we find that \( \epsilon \) is driven to be vanishingly small, as the data do not favour a reduction of FVEs in the charged pion masses that \( \Delta R_{M_{\pi \pm}} \) necessarily brings about. Because of this, fluctuations in the pion decay constant data tend to drive \( \delta \) into a run-away increase, as it has to compensate for the smallness of \( \epsilon \) (see Eq. (29)), and this is seen in the fitting. As a result, no firm conclusions can be drawn about the presence of these parity-violating contributions from the data.
| Fit     | I       | II      | III     | IV      | V*      |
|---------|---------|---------|---------|---------|---------|
| $\tilde{\ell}_3$ | 3.44(14) | 3.31(16) | 3.45(13) | 3.35(15) | 3.38(11) |
| $\tilde{\ell}_4$ | 4.69(3)  | 4.63(4)  | 4.75(5)  | 4.70(6)  | 4.71(6)  |
| $F_\pi/F$ | 1.0748(7) | 1.0736(9) | 1.0760(10) | 1.0749(11) | 1.0752(11) |
| $2B_0\mu_q/M_\pi^2$ | 1.0281(12) | 1.0269(14) | 1.0283(12) | 1.0273(14) | 1.0276(10) |
| $a_C$ (fm) | 0.0665(6) | 0.0676(7) | 0.0644(22) | 0.0649(28) | 0.0647(24) |
| $a_B$ (fm) | 0.0856(6) | 0.0871(9) | 0.0811(40) | 0.0815(48) | 0.0813(43) |
| $a_D$ (fm) | 0.0528(5) | 0.0536(6) | 0.0519(12) | 0.0523(15) | 0.0521(14) |
| $a_C^4K$ | -       | 0.0030(4) | -       | 0.0032(11) | 0.0028(4) |
| $a_C^2D_m$ | -       | -       | 0.055(28) | 0.055(38) | 0.057(35) |
| $a_C^2D_f$ | -       | -       | 0.038(32) | 0.045(44) | 0.044(39) |
| $\chi^2/n_{\text{dof}}$ | 37.5/16 | 32.6/15 | 20.6/14 | 16.1/13 | 21.8/19 |
| $p$-value | 0.00    | 0.01    | 0.11    | 0.24    | 0.29    |

TABLE II: Results of all our fits of the ETMC data from ensembles $B_1 - B_4, B_6, B_7, C_1 - C_3$ and $D_1$ [8]. The asterisk besides the fit number indicates the inclusion of the $M_{\pi^0}$ data. The quantities $M_\pi$ and $F_\pi$ are physical pion mass and decay constant, and $\mu_q$ is the value of the quark mass corresponding to the physical pion mass.

have also investigated the impact of including the $M_{\pi^0}$ data on our fit. We do not include the $M_{\pi^0}$ data à priori because it is of a much lower quality compared to the $M_{\pi^\pm}$ data (the uncertainty associated with it is at least an order of magnitude larger), and it has rather different systematics. Since the finite volume corrections are expected to be $O(1\%)$, which would be easily subsumed by the $O(10\%)$ error in $M_{\pi^0}$, we do not apply them to the $M_{\pi^0}$ data when including them in our fitting. Nevertheless, this should be done when the neutral pion mass can be calculated more reliably in the future, and we have provided the full NLO resummed formula for FVEs associated with $M_{\pi^0}$ in Sec IV.

The results of our fits are shown in Table III To establish a baseline, we performed Fit I with pure ChPT fitting forms that included neither twisted mass nor NNLO discretization

\[^{10}\] We have checked explicitly that applying finite volume corrections to the $M_{\pi^0}$ data do not alter our fit in any way.
effects, and we see it gives the worst description of the data. Turning on just the pion mass
splitting in Fit II induced only a marginal improvement, as the $\chi^2$ decreased by 2.4% with
the number of degrees of freedom, $n_{\text{dof}}$, reduced by one. However, turning on instead $D_m$ and
$D_f$ in Fit III produced a dramatic improvement with a 45% reduction in the $\chi^2$ compared to
Fit I as $n_{\text{dof}}$ reduced by two. A further improvement is gained when all parameters associated
with discretization effects, $K$, $D_m$ and $D_f$, are simultaneously turned on in Fit IV, as the $\chi^2$
decreased another 22% compared to Fit III with $n_{\text{dof}}$ reduced by one. Finally the best fit is
Fit V* when $M_{\pi^0}$ data are also included (indicated by the asterisk beside the fit number).

For each fit, we have also calculated the $p$-value, namely the probability of obtaining a
normalized $\chi^2$ greater than that actually found from the fit. It is particularly illuminating
to compare the $p$-values in Table III, as it shows that despite the substantial improvement in
$\chi^2$, Fit III is not yet fully convincing in terms of its $p$-value. Only after including the twisted
mass effects as in Fit IV does the $p$-value rise to a much more acceptable level. Finally, the
inclusion of the $M_{\pi^0}$ data gives a further increase in the $p$-value in Fit V*.

We remark here that for the pion mass-squared splitting, $a^2K = M_{\pi^+}^2 - M_{\pi^0}^2 \equiv \Delta M_{\pi}^2$,
itst fitted value changes little whether $M_{\pi^0}$ data are included in the fit or not. Incidentally,
including $M_{\pi^0}$ data seems to reduce the uncertainty in $a^2K$ substantially, and leads to a
result which is (statistically) different from zero by about $7\sigma$ compared to a bit under $3\sigma$
when $M_{\pi^0}$ data are not included. By combining the analysis of the FVEs of the charged
pion masses and the $M_{\pi^0}$ data, one can see unambiguously the mass splitting predicted
in tmChPT, and that $\Delta M_{\pi}^2 > 0$. This represents the first determination of the tmChPT
quantity $W_0^2 W'$ from tmLQCD simulations. We emphasize here that $\Delta M_{\pi}^2$, and hence $M_{\pi^0}$,
can already be determined from the FVEs alone. Although large uncertainties are associated
with the determination of $M_{\pi^0}$ either through analyzing FVEs or by direct lattice calculation,
it is reassuring to see that both provide compatible results.

To provide further insight into exactly where improvements arise by taking into account
twisted mass effects, we give a breakdown of the individual contributions to the total $\chi^2$
from each ensemble for Fit III and IV in Table III. We would like to see the individual
contribution from each $M_\pi$ and $F_\pi$ data, and this is given by $\chi^2_{M_\pi}$ and $\chi^2_{F_\pi}$ in Table III. Note
that since $M_\pi$ and $F_\pi$ are correlated non-trivially in any given ensemble, $\chi^2_{M_\pi}$ and $\chi^2_{F_\pi}$ do
not sum up to the full contribution from that particular ensemble, $\chi^2_{\text{pair}}$, which takes into
account the correlation between the pair: they are $\chi^2$ values calculated for each $M_\pi$ and $F_\pi$.
| Ensemble data | Fit III |         |         | Fit IV |         |         |
|---------------|---------|---------|---------|--------|---------|---------|
| Ensemble      | $L/a$   | $a\mu_q$| $\chi^2_{M_\pi}$ | $\chi^2_{F_\pi}$ | $\chi^2_{\text{pair}}$ | $\chi^2_{M_\pi}$ | $\chi^2_{F_\pi}$ | $\chi^2_{\text{pair}}$ |
| $B_1$         | 24      | 0.0040  | 3.16    | 0.51   | 3.24    | 0.63    | 0.42    | 2.23    |
| $B_2$         | 24      | 0.0064  | 1.84    | 0.00   | 3.74    | 1.91    | 0.00    | 3.68    |
| $B_3$         | 24      | 0.0085  | 0.03    | 0.39   | 0.40    | 0.00    | 0.20    | 0.23    |
| $B_4$         | 24      | 0.0100  | 1.61    | 0.40   | 1.87    | 1.52    | 0.37    | 1.76    |
| $B_6$         | 32      | 0.0040  | 1.37    | 0.53   | 1.37    | 0.19    | 0.03    | 0.50    |
| $B_7$         | 32      | 0.0030  | 0.02    | 0.57   | 1.64    | 0.74    | 0.01    | 1.87    |
| $C_1$         | 32      | 0.003   | 4.85    | 1.04   | 4.88    | 3.76    | 0.61    | 3.76    |
| $C_2$         | 32      | 0.006   | 0.16    | 0.06   | 0.38    | 0.18    | 0.02    | 0.30    |
| $C_3$         | 32      | 0.008   | 0.00    | 1.25   | 1.46    | 0.07    | 0.66    | 0.99    |
| $D_1$         | 48      | 0.0020  | 1.20    | 0.96   | 1.51    | 0.58    | 0.49    | 0.75    |

TABLE III: The contribution of each individual ensemble to the total $\chi^2$ for Fit III and IV. The quantities $\chi^2_{M_\pi}$ and $\chi^2_{F_\pi}$ denote the contribution each $M_\pi$ and $F_\pi$ data makes separately to the total $\chi^2$ neglecting the correlation between them. The full contribution from the correlated pair is denoted by $\chi^2_{\text{pair}}$.

data separately neglecting the correlation

A comparison of Fit III and IV shows very clearly for which ensemble and for which quantity is the improvement from taking into account twisted mass effects the most significant. The largest improvements are seen in $M_\pi$ for ensembles $B_1$ and $C_1$, which indeed have small volumes and small pion masses. For these two ensembles, the relative improvement in $F_\pi$ is also quite evident. In all, we see clear improvements across-the-board.

VI. CONCLUSIONS

In this paper we have analyzed the finite volume corrections to pion masses and decay constant in tmChPT. The presence of a lighter neutral pion gives exponentially enhanced finite volume corrections, and we have calculated these to NLO accuracy. We have performed a detailed analysis of the ETMC data and found out that they are better fitted by the
formulae derived here than by the continuum ones \[4\], particularly in regards to the finite volume dependence. We are able to extract the pion mass splitting predicted in tmChPT from analyzing FVEs on charged pions alone without having to calculate directly the neutral pion mass. An important benefit of this is, as far as we know, a first determination of the LEC $W'$ of tmChPT. This example shows that, though small, FVEs can be successfully used to determine interesting physical observables.

Other LECs of tmChPT appear in parity-violating cubic interactions, which give exponentially enhanced FVEs. Despite the fact that they are formally of higher order in the combined twisted mass chiral expansion, we have calculated their analytical form and investigated their effects in our fitting in the hope that the exponential enhancement may be large enough to allow them to be seen, and thus enable extraction of more LECs of tmChPT. Unfortunately, their contribution is found to be small, and below the precision of the present ETMC data.

As the precision of the lattice calculations increases and as the simulations move towards lighter pions, the corrections discussed here will become even more important and may have an impact also on the extracted physically relevant parameters. We suggest that future tmLQCD lattice studies perform analyses of FVEs taking full account of the twisted mass discretization effects, as was done in deriving our formulae in this paper.

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