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O(a^2) cutoff effects in lattice Wilson fermion simulations

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In this paper we propose to interpret the large discretization artifacts affecting the neutral pion mass in maximally twisted lattice QCD simulations as O(a^2) effects, whose magnitude is roughly proportional to the modulus square of the (continuum) matrix element of the pseudoscalar density operator between vacuum and one-pion state. The numerical size of this quantity is determined by the dynamical mechanism of spontaneous chiral symmetry breaking and turns out to be substantially larger than its natural magnitude set by the value of Λ_{QCD}.

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I. INTRODUCTION

In recent simulations of maximally twisted lattice QCD (Mtm-LQCD) [1] with $N_f = 2$ dynamical light quarks, numerical results [2,3] on the neutral pseudoscalar meson mass at different lattice spacings (in the range from 0.10 to 0.065 fm) and quark masses (corresponding to charged pseudoscalar meson masses ranging from 600 to 300 MeV) show large cutoff effects. The latter appear at fixed lattice spacing in the form of sizeable deviations from the expected continuum QCD chiral behavior.

This finding is in striking contrast with the smallness of cutoff effects observed not only in the mass of the charged pions (which is related through the Goldstone theorem to exactly conserved lattice currents [4]), but also in all of the other hadronic observables so far measured by the European Twisted Mass (ETM) Collaboration (see Sec. III and Refs. [3,5–10]). Quite remarkably small lattice artifacts are found even in matrix elements where the neutral pion is involved (see Table I below).

In Mtm-LQCD, the additive cutoff effect in the squared mass of the neutral pion is expected on general grounds [11] to be of the order $a^2\Lambda^4_{\mathrm{QCD}}$; whereas, the leading additive corrections to the squared mass of the charged pion are [4,12,13] only of order $a^4\Lambda^6_{\mathrm{QCD}}$ and $a^2\mu_q\Lambda^3_{\mathrm{QCD}}$ (μ_q denotes the bare quark mass). The neutral vs charged pion (squared) mass splitting, $\Delta m^2_\pi|^{\mathrm{Mtm}}_L = m^2_{\pi^3}|_L - m^2_{\pi^\pm}|_L$, in the small quark-mass region is then dominated by O($a^2\Lambda^4_{\mathrm{QCD}}$) terms. Numerical data (see Fig. 1 and Table I) at two different lattice spacings and for charged pion masses below 500 MeV are indeed consistent with the expected behavior of $\Delta m^2_\pi|^{\mathrm{Mtm}}_L$, but with a large coefficient in front of the O($a^2\Lambda^4_{\mathrm{QCD}}$) correction.[1] For instance, taking $\Lambda_{\mathrm{QCD}} = 250$ MeV, one finds $\Delta m^2_\pi|^{\mathrm{Mtm}}_L \sim -50a^2\Lambda^4_{\mathrm{QCD}}$.

[1]The issue of the N_f dependence of this coefficient is beyond the scope of this paper and will be discussed elsewhere.

On a more general ground, the question of the numerical size of the neutral vs charged pion mass splitting is an important issue to assess the viability of the Mtm-LQCD approach. This is so mainly because of the established relation [12,14] between the magnitude of the pion mass splitting and the strength of the metastabilities detected in the theory at coarse lattice spacings [15–18].

One may suspect that the size of $\Delta m^2_\pi|^{\mathrm{Mtm}}_L$ represents the generic magnitude of the isospin breaking effects inherent in the twisted form of the action. This is not so, however. Numerical data in several other observables indicate, in fact, that in general isospin breaking artifacts are pretty small, with a relative magnitude in line with their naive order of magnitude estimate.

The main purpose of this paper is to provide an explanation for this peculiar pattern of isospin breaking effects, and, in particular, for the fact that only the neutral vs charged lattice pion mass splitting among all the other O(a^2) effects is large.

Relying on arguments based on the Symanzik analysis [19,20] of lattice artifacts, we are able to identify the form of the leading O(a^2) corrections that, in Mtm-LQCD, affect the value of the squared mass of the neutral pseudoscalar meson. Interestingly, one can give an approximate evaluation of these effects finding that they are proportional to the modulus square of the continuum matrix element of the isotriplet pseudoscalar density operator between the vacuum and one-pion state. The latter is a dynamically large number determined by the mechanism of spontaneous chiral symmetry breaking. This fact, together with the vanishing of the pion mass in the zero quark mass limit of continuum QCD, explains the large relative size of the cutoff effects observed in the neutral pion mass.

Lattice artifacts, of course, also depend on the many unknown coefficients multiplying the operators occurring in the Symanzik expansion. However, the numerical evidence provided in this paper (see Sec. III) and in Refs. [3,6] about the fact that all of the other so far measured observ-

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ables exhibit only small lattice artifacts should be taken as a strong indication that the coefficients multiplying the (quark mass independent) operators of the Symanzik effective Lagrangian of relevance here (operators of dimension 5 and 6) are not unnaturally large, at least in the gauge coupling regime explored up to now in ETMC simulations. Indeed, if this was not the case, one would have seen large cutoff effects in some other physical observables besides the neutral pion mass.

A preliminary version of this investigation was presented some time ago in [21]. Ideas and a few results along the line of reasoning developed in this paper have been already put forward in [12,13,22] and in [23].

Plan of the paper

The plan of the paper is as follows. In Sec. II, we illustrate the nature and the structure of O(a^2) artifacts in Mtm-LQCD and how they affect charged and neutral pion masses. In Sec. III, we give numerical evidence that among the many observables recently measured by the ETM Collaboration only the pion mass splitting seems to display large cutoff effects. Conclusions can be found in Sec. IV. More technical issues are discussed in the Appendices. In Appendix A, we review the notion and the properties of the Symanzik expansion for the description of the cutoff effects of LQCD with Wilson fermions (either maximally twisted or untwisted) and how, depending on the value of the twisting angle, its form is affected by the way the critical mass is determined. In Appendix B, we give the structure of the Symanzik expansion of the two-point pseudoscalar correlator from which the formula for the O(a^2) discretization errors affecting the pion masses can be derived. Finally, in the (long) Appendix C, we give details on the theoretical analysis and numerical estimate of the matrix elements controlling the magnitude of certain cutoff corrections affecting neutral and charged pion masses.

II. NEUTRAL AND CHARGED PION MASS IN MTM-LQCD

In this section, we want to describe and compare the structure of the lattice artifacts affecting the neutral and the charged pion mass in Mtm-LQCD. The key formulas yielding the O(a^2) corrections to the charged and neutral squared pion mass are immediately derived by writing down the leading correction to the pion (rest) energy induced by the O(a^2) terms of the Symanzik expansion. In Mtm-LQCD, one gets ($b = \pm, 3$)

$$m^2_{\pi^b}|_L = m^2_\pi + a^2\Big[\langle \pi^b(\vec{0})|\mathcal{L}_6^{\rm Mtm}(0)|\pi^b(\vec{0})\rangle|_{\rm cont} - \frac{1}{2}\langle \pi^b(\vec{0})|\int d^4x\,\mathcal{L}_5^{\rm Mtm}(x)\mathcal{L}_5^{\rm Mtm}(0)|\pi^b(\vec{0})\rangle|_{\rm cont}\Big] + \mathrm{O}(a^2m^2_\pi, a^4), \tag{2.1}$$

where the form of $\mathcal{L}_5^{\rm Mtm}$ and $\mathcal{L}_6^{\rm Mtm}$ is detailed in Appendix A. Equation (2.1) complies with elementary lowest order perturbation theory formulas and Lorentz covariance. For completeness in Appendix B, we give another derivation of Eq. (2.1) starting from the Symanzik expansion of the Fourier transform of the two-point pseudoscalar correlator (no sum over b),

$$\Gamma^b_L(p) = a^4\sum_x e^{ipx}\langle P^b(x)P^b(0)\rangle|_L, \tag{2.2}$$

where $P^b = \bar\psi i\gamma_5(\tau^b/2)\psi$ and τ^b, $b = 1, 2, 3$, are the Pauli matrices.

The main conclusions of this paper are derived from the following two observations concerning the structure of Eqs. (2.1).

(1) The pion matrix elements $\langle \pi^b(\vec{0})|\mathcal{L}_6^{\rm Mtm}(0)|\pi^b(\vec{0})\rangle|_{\rm cont}$ are O(1) for $b = 3$, but only O(m^2_π) for $b = \pm$ (see Appendix B), viz.

$$\langle \pi^\pm(\vec{0})|\mathcal{L}_6^{\rm Mtm}(0)|\pi^\pm(\vec{0})\rangle|_{\rm cont} = \mathrm{O}(m^2_\pi), \tag{2.3}$$

$$\zeta_\pi \equiv \langle \pi^3(\vec{0})|\mathcal{L}_6^{\rm Mtm}(0)|\pi^3(\vec{0})\rangle|_{\rm cont} = \mathrm{O}(1). \tag{2.4}$$

(2) Upon use of the optimal critical mass [4], one can show (see Appendix C) that the matrix element

$$\Delta^b_{55} = -\frac{1}{2}\langle \pi^b(\vec{0})|\int d^4x\,\mathcal{L}_5^{\rm Mtm}(x) \times \mathcal{L}_5^{\rm Mtm}(0)|\pi^b(\vec{0})\rangle|_{\rm cont} \tag{2.5}$$

is parametrically of O(m^2_π) close to the chiral limit for $b = \pm$, and numerically negligible (in modulus) compared to $|\zeta_\pi|$ in the case of $b = 3$.

The direct consequence of these statements is that close to the chiral limit, there are no additive O(a^2) terms affecting the value of the lattice charged squared pion mass. The neutral squared pion mass instead receives nonvanishing corrections at this order. In formulas, one gets

$$m^2_{\pi^\pm}|_L = m^2_\pi + a^2\Delta^\pm_{55} + \mathrm{O}(a^2m^2_\pi, a^4) = m^2_\pi + \mathrm{O}(a^2m^2_\pi, a^4), \tag{2.6}$$

$$m^2_{\pi^3}|_L = m^2_\pi + a^2[\zeta_\pi + \Delta^3_{55}] + \mathrm{O}(a^2m^2_\pi, a^4). \tag{2.7}$$

One can also show that in Δ^b_{55}, the numerically dominant O(m^2_π) terms, coming from the insertion of one-pion states in (2.5), are actually independent of the isospin index b. As a result, what is left in the difference $\Delta^3_{55} - \Delta^\pm_{55}$ is a tiny correction, so that for the pion squared mass difference, we can finally write down the simple formula

$$\Delta m^2_\pi|_L^{\rm Mtm} = m^2_{\pi^3}|_L - m^2_{\pi^\pm}|_L \simeq a^2\zeta_\pi + \mathrm{O}(a^2m^2_\pi, a^4), \tag{2.8}$$

where the symbol $\simeq$ is to remind us that the (negligibly small) $\Delta^3_{55} - \Delta^\pm_{55}$ correction has been dropped.

In the rest of the paper, we want to give a proof of the propositions (1) and (2) above and provide a numerical estimate of $\Delta_{55}^{3,\pm}$ and ζ_π. In this section, we shall see, in particular, that for dynamical reasons ζ_π is large compared to its natural value ($\sim \Lambda_{\rm QCD}^4$), providing in this way an explanation for the fairly big value of $\Delta m_\pi^2|_L^{\rm Mtm}$ measured in numerical simulations [2,3].

The arguments leading to the Eqs. (2.6) and (2.7) and the statements above are quite elaborate. To keep the line of reasoning as straight as possible, we have deferred them to Appendix B [derivation of Eqs. (2.6) and (2.7)] and Appendix C (expression and estimate of $\Delta_{55}^{3,\pm}$).

A. General computational strategy

For the reader's convenience, we summarize here the strategy we followed to numerically estimate the quantities entering Eqs. (2.6) and (2.7), and the approximations we had to rely on.

The key quantity we need to evaluate is ζ_π in the chiral limit. This is done in Sec. II B by first exploiting soft pion theorems (SPT's) [24,25] to simplify the structure of the continuum matrix elements of $\mathcal{L}_6^{\rm Mtm}$ we are interested in. Actual numbers are finally obtained making use of the vacuum saturation approximation (VSA). In this way, one obtains a theoretical expectation for the value of the pion mass splitting $\Delta m_\pi^2|_L^{\rm Mtm} = m_{\pi^3}^2|_L - m_{\pi^\pm}^2|_L$ at a very small quark mass, which in Sec. II C is directly compared with the measured values of $\Delta m_\pi^2|_L^{\rm Mtm}$ at pion masses ranging from 320 to 450 MeV (and with our numerical estimate of $\Delta_{55}^3 - \Delta_{55}^\pm$).

The results (2.3) and (2.4) follow from the symmetries of (the Symanzik effective Lagrangian for) Mtm-LQCD upon reducing one external pion with the help of SPT's. Concerning Eq. (2.5), the derivation of the results on the m_π^2 behavior of $\Delta_{55}^\pm$ and the evaluation of the magnitude of Δ_{55}^3 are rather involved problems because of the nonlocal nature of the operator $\int d^4x \mathcal{L}_5^{\rm Mtm}(x)\mathcal{L}_5^{\rm Mtm}(0)$ appearing in the definition of $\Delta_{55}^{3,\pm}$. A careful analysis of various tadpole and intermediate state contributions is required, as well as (approximate) chiral symmetry and/or phenomenological arguments applied to the matrix elements of the local operators appearing in individual contributions.

As discussed in Appendix C 1, the dominant contributions to $\Delta_{55}^{3,\pm}$ are proportional (and related via exactly or approximately known factors; see Appendix C 2) to the square of the matrix element ξ_π [Eq. (A16)], which in turn can be estimated starting from data on certain two-point lattice correlators, plus standard SPT-based approximations (Appendix C 3). Given the smallness of ξ_π (as a result of the optimal critical mass condition enforced in ETMC
simulations), and consequently of $\Delta_{55}^3 - \Delta_{55}^\pm$ compared to ζ_π, the uncertainties on the former quantity coming from statistical errors and the various approximations we employed, though entailing a large error (of about 100%), do not harm in any way the conclusions of this work.

B. Estimating O(a^2) lattice artifacts in $\Delta m_\pi^2|_L$

Relying on the results of Appendix C about the numerical irrelevance of Δ_{55}^b [either because parametrically of O(m_π^2), for $b = \pm$, or because numerically small, for $b = 3$], we only need to evaluate ζ_π in (the chiral limit of) continuum QCD in order to estimate the size of the O(a^2) artifacts in (2.7) and (2.8). This can be done under the assumption that a sufficiently accurate order of magnitude estimate of this hadronic parameter can be obtained in the VSA. Quenched LQCD studies support the assumption that VSA works well for matrix elements of four-fermion operators between pseudoscalar states [26,27]. It is very likely that this remains true also in the unquenched theory. Indications in this sense are actually born out by recent studies with two or three dynamical flavors [28,29].

1. The theoretical argument

The evaluation of ζ_π [see Eq. (2.4)] requires the estimate of the matrix elements of the operators in Eq. (A8) (rotated from the twisted to the physical quark basis) between zero three-momentum neutral pion states. This is done in two steps.

(I) By the use of classical SPT's [24,25], one recognizes that some operators have O(1) neutral pion matrix elements, while others vanish proportionally to m_π^2. The latter are those that are invariant under axial-τ^3 transformations. The former are

$$\begin{aligned}
&\tfrac{1}{4}(\bar\psi i\gamma_5\tau^3\psi)(\bar\psi i\gamma_5\tau^3\psi), && \tfrac{1}{4}(\bar\psi\psi)(\bar\psi\psi),\\
&\tfrac{1}{4}(\bar\psi\tau^3\psi)(\bar\psi\tau^3\psi), && \tfrac{1}{4}(\bar\psi i\gamma_5\psi)(\bar\psi i\gamma_5\psi),\\
&\tfrac{1}{4}(\bar\psi\sigma_{\mu\nu}\tau^3\psi)(\bar\psi\sigma_{\mu\nu}\tau^3\psi), && \tfrac{1}{4}(\bar\psi\sigma_{\mu\nu}i\gamma_5\psi)(\bar\psi\sigma_{\mu\nu}i\gamma_5\psi),\\
&\tfrac{1}{4}(\bar\psi\gamma_\mu\gamma_5\tau^1\psi)(\bar\psi\gamma_\mu\gamma_5\tau^1\psi), && \tfrac{1}{4}(\bar\psi\gamma_\mu\tau^2\psi)(\bar\psi\gamma_\mu\tau^2\psi),\\
&\tfrac{1}{4}(\bar\psi\gamma_\mu\gamma_5\tau^2\psi)(\bar\psi\gamma_\mu\gamma_5\tau^2\psi), && \tfrac{1}{4}(\bar\psi\gamma_\mu\tau^1\psi)(\bar\psi\gamma_\mu\tau^1\psi).
\end{aligned} \tag{2.9}$$

The operators (2.9) are obtained from those of Eq. (A9) after use of the chiral rotation (A2). We note that SPT's relate through the trivial numerical factor -1 the matrix elements between neutral single-pion states of the two operators in each line.[2] Not surprisingly, this remark implies that ζ_π would vanish if we were to deal with an exactly chiral invariant lattice formulation. In fact, such a formulation would be described by a Symanzik effective Lagrangian where the two operators in each line of the list (2.9), being related by a chiral transformation, would necessarily appear with identical coefficients.

(II) In VSA, one can give an estimate of the value of ζ_π [Eq. (2.4)] as follows. First of all, one has to rewrite the matrix elements of the operators (2.9) between zero-momentum neutral pion states in the form that is obtained reducing external pions by the use of SPT's.[3] In this way, one checks that only the pion matrix elements of the two operators in the first line of the list (2.9) are not vanishing in VSA. Their actual contribution to ζ_π depends of course on the magnitude of the Symanzik coefficients (dimensionless functions of the bare gauge coupling) by which the two operators are multiplied in the expression of $\mathcal{L}_6^{\rm Mtm}$. In the gauge coupling regime of interest for large volume simulations of Mtm-LQCD, these coefficients are expected to be O(1) quantities, but their value (and sign) is otherwise unknown. We must thus limit ourselves to an order of magnitude estimate of $|\zeta_\pi|$ for which, relying on the line of reasoning outlined above, we write

$$|\zeta_\pi| \overset{\rm VSA}{\sim} \frac{2\hat{\Sigma}^2}{f_\pi^2} \simeq 2\hat{G}_\pi^2, \qquad (2.10)$$

where $f_\pi \simeq 92.4$ MeV. The quantities $\hat{\Sigma}$ and $\hat{G}_\pi$ denote the continuum renormalized chiral condensate and the vacuum-to-pion matrix element of the pseudoscalar density, with

$$G_\pi = \langle\Omega|P^b|\pi^b(\vec{0})\rangle|_{\rm cont}, \qquad P^b = \bar{\psi}\frac{i}{2}\gamma_5\tau^b\psi, \qquad (2.11)$$

$$\Sigma = \langle\Omega|\tfrac{1}{2}S^0|\Omega\rangle|_{\rm cont}, \qquad S^0 = \bar{\psi}\psi. \qquad (2.12)$$

The first relation, as explicitly indicated, comes from a direct use of SPT's and vacuum insertion. The second holds up to $O(m_\pi^2)$ corrections and comes from combining the Gell-Mann-Oakes-Renner formula [31]

$$-2\hat{\mu}_q\hat{\Sigma} = f_\pi^2 m_\pi^2 + O(m_\pi^4) \qquad (2.13)$$

with the continuum Ward-Takahashi identity (WTI)

$$2\hat{\mu}_q\hat{G}_\pi = f_\pi m_\pi^2. \qquad (2.14)$$

We conclude this subsection by stressing that sign of ζ_π, which, as we said, depends on the operator coefficients in $\mathcal{L}_6^{\rm Mtm}$, is not predicted by our arguments and is to be learned from numerical simulation experience.

2. Numerics about Eq. (2.10)

A numerical evaluation of $\hat{G}_\pi$, or equivalently of $-\hat{\Sigma}/f_\pi$, can be obtained in various ways, i.e. either exploiting the direct lattice measurement of $\hat{G}_\pi$ or by using (at the physical pion point) the continuum WTI (2.14).

(I) The direct lattice measurements of $\hat{G}_\pi$ carried out in Refs. [2,3,9] at different lattice resolutions give in the continuum and chiral limit

$$\hat{G}_\pi(\overline{MS}, 2\ {\rm GeV}) \sim (490\ {\rm MeV})^2,$$
$$[-\hat{\Sigma}(\overline{MS}, 2\ {\rm GeV})]^{1/3} \sim 275\ {\rm MeV} \qquad (2.15)$$

with a total error on $\hat{G}_\pi$ not larger than 5%. In order to arrive at these numbers, the renormalization constant of the operator P^b, computed in the regularization independent momentum scheme [32] and converted to the $\overline{MS}$ scheme, was employed in [33].

(II) A second, independent determination of $\hat{G}_\pi$ can be obtained by making reference to only continuum quantities if Eq. (2.14) and the PDG [34] estimate $\hat{\mu}_q(\overline{MS}, 2\ {\rm GeV}) = [(\hat{m}_u + \hat{m}_d)/2](\overline{MS}, 2\ {\rm GeV}) \sim 3.8$ MeV are used. In this way one gets, at the physical pion mass,

$$\hat{G}_\pi(\overline{MS}, 2\ {\rm GeV}) \sim (470\ {\rm MeV})^2. \qquad (2.16)$$

Taking into account the small error in the extrapolation from the chiral point to the physical pion and the uncertainty on the light quark mass value, we see that the two estimates of $\hat{G}_\pi$ are in very good agreement with each other.

The conclusion of this analysis is that numerically the estimate (2.8) of the neutral to charged squared mass shift

[2] For the reader's convenience, we recall that SPT's amount to the relation $if_\pi\langle\alpha + \pi^b(\vec{0})|O^c|\beta\rangle = \langle\alpha|[Q_A^b, O^c]|\beta\rangle$, where Q_A^b is the axial charge with isospin index b. External states must carry isospin indices such that the two matrix elements are not trivially vanishing. We also note the crossing symmetry relation $\langle\alpha + \pi^b(\vec{0})|O^c|\beta\rangle = \langle\alpha|O^c|\beta + \pi^b(\vec{0})\rangle$. For an introduction to SPT's and a more detailed discussion (including limitations in their use if intermediate states with the quantum numbers of $O^c|\alpha\rangle$, or $O^c|\beta\rangle$ happen to be degenerate in energy with the states $|\alpha\rangle$ or $|\beta\rangle$), see e.g. [30], Sec. IV-5, and references therein.

[3] In doing so, we are enforcing consistency with SPT's in using VSA-based estimates of the matrix elements of the operators (2.9). This step is necessary, because it is not guaranteed that VSA estimates comply with SPT relations.

is substantially larger than its natural size, $a^2\Lambda^4_{\rm QCD}$, by a factor [see Eqs. (2.10), (2.15), and (2.16)] of the order of $2\hat{G}^2_\pi/\Lambda^4_{\rm QCD} \sim 25 \div 30$.

C. Numerical results for $\Delta m^2_\pi|_L$

In this section, we wish to summarize the simulation results for $\Delta m^2_\pi|_L$ that have been obtained from $N_f = 2$ ETMC ensembles at two different lattice resolutions, $a^{-1} \simeq 2.3$ GeV and $a^{-1} \simeq 2.8$ GeV (corresponding to $\beta = 3.9$ and $\beta = 4.05$, respectively; see Appendix C 3 b and Table II for details), and compare them with the number expected on the basis of Eq. (2.10) for ζ_π as well as with the estimate of $\Delta^3_{55} - \Delta^\pm_{55}$ derived in Appendix C [see Eq. (C26)].

In Fig. 1, we display the lattice results for $(r_0/a)^2 r_0^2 \Delta m^2_\pi|_L$ vs $r_0^2 m^2_{\pi^\pm}|_L$ for the six gauge configuration ensembles specified in Table II. The factor of $(r_0/a)^2$ in the vertical axis has been inserted[4] to be able to combine together data from $\beta = 3.9$ and $\beta = 4.05$, thus giving an impression of the quality of the scaling behavior of $\Delta m^2_\pi|_L$. In the same figure, we also report the value of $r_0^4\zeta_\pi$ (empty square), which from Eqs. (2.10), (2.15), and (2.16) and $r_0 \simeq 0.44$ fm is computed to be[5]

$$r_0^4\zeta_\pi = -(2.6 \pm 1.3) \quad @\mu_q = 0. \tag{2.17}$$

The error in (2.17) is dominated by the uncertainty inherent in the theoretical arguments given in Sec. II B 1, particularly the use of VSA [see Eq. (2.10)], which we conservatively estimate to be about 50%. Finally, the empty diamond symbol in Fig. 1 represents the result of the estimate (C26) we give of $\Delta^3_{55} - \Delta^\pm_{55}$ expressed in r_0 units, yielding

$$r_0^4(\Delta^3_{55} - \Delta^\pm_{55}) = -0.10 \pm 0.06 \pm 0.03, \tag{2.18}$$

where the first error is essentially statistical and stems from the evaluation of ξ_π in Eq. (C54), and the second is the systematic uncertainty reflecting the approximations involved in the way we parametrize (Appendix C 1) and evaluate (Appendix C 2) the quantity $\Delta^3_{55} - \Delta^\pm_{55}$.

We see from Fig. 1 that within statistical errors (mainly coming from the noisy quark-disconnected diagrams entering the calculation of m_{π^3}), the available data for $\Delta m^2_\pi|_L$ show the expected scaling behavior with the lattice spacing. The quark mass dependence of $(r_0/a)^2 r_0^2 \Delta m^2_\pi|_L$ turns out to be of reasonable magnitude and is not inconsistent with our theoretical estimate (2.17) within the large uncertainty affecting $(d\Delta m^2_\pi/d\hat{\mu}_q)|_L$ [from the plotted data one finds $(d\Delta m^2_\pi/d\hat{\mu}_q)|_L \sim 300 \div 900$ MeV at $\beta = 3.9$].

[4] According to Ref. [3], we use $r_0/a = 5.22(2)$ at $\beta = 3.9$ and $r_0/a = 6.61(3)$ at $\beta = 4.05$.

[5] The sign of ζ_π, which appears in Eq. (2.17) has been inferred from the numerical evidence that $m_{\pi^3} < m_{\pi^\pm}$.

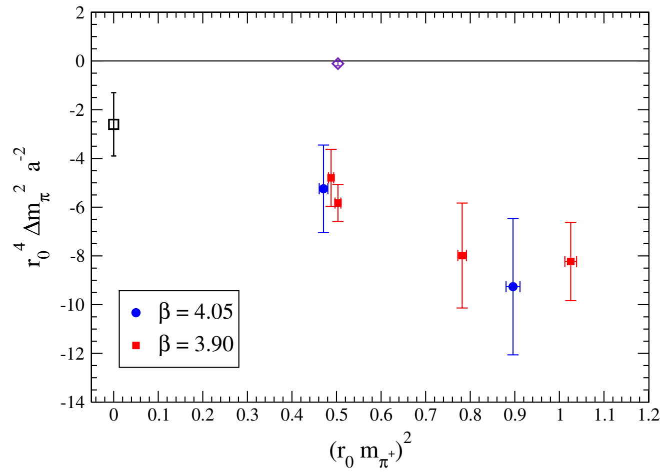

FIG. 1 (color online). Data for $(r_0/a)^2 r_0^2 \Delta m^2_\pi|_L$ vs $r_0^2 m^2_{\pi^\pm}|_L$ are compared with the estimate of $r_0^4\zeta_\pi$ (empty square) and $r_0^4(\Delta^3_{55} - \Delta^\pm_{55})$ (empty diamond).

The estimated value of $r_0^4(\Delta^3_{55} - \Delta^\pm_{55})$ with its error [see Eq. (2.18)] is (in modulus) much smaller than the observed pion (squared) mass splitting, and also about 20 times smaller than $r_0^4|\zeta_\pi|$. We thus conclude that the dominant contribution to $\Delta m^2_\pi|_L$ comes from the $a^2\zeta_\pi$ correction, as announced.

III. O(a^2) ISOSPIN VIOLATING EFFECTS IN MTM-LQCD

In this section, we want to provide numerical evidence of the fact that in Mtm-LQCD simulations, O(a^2) isospin breaking effects are negligible in all the physical quantities measured up to now by the ETM Collaboration, with the exception of the neutral pion mass.

In Table I, we report the relative difference of pseudoscalar meson squared masses and decay constants between neutral and charged particles for pseudoscalar and vector mesons, as well as the relative splitting between the masses of Δ^+ and Δ^{++} baryons. Most of these data already appeared in the conference contributions of Ref. [3] and in Ref. [6].

We refer to [7] for a detailed description of the techniques used to compute correlators, extract physical observables, and perform the necessary error analysis. The results presented in this paper are based on the configurations generated by the ETM Collaboration using the formulation of lattice QCD at maximal twist (with $c_{\rm SW} = 0$ [35]) and tree-level Symanzik improved gluon action. We show data coming from $\beta = 3.9$ [2] and $\beta = 4.05$ [3,6] simulations at two, roughly matched (in physical units) values of the twisted-mass parameter μ_q for each β. Again, we stress that the computation of the mass and decay constant of neutral (pseudoscalar and vector) mesons involves the evaluation of quark-disconnected diagrams, which is the reason for the relatively larger errors affecting these quantities. In the case of Δ-baryon masses (where no computation of quark-disconnected diagrams is required), we give results at four values of μ_q for $\beta = 3.9$ and $\beta = 4.05$.

We quote in Table I the relative isospin splitting, R_s, measured between the observables $\mathcal{O}$ and $\mathcal{O}'$, namely

$$R_s[\mathcal{O}] = \frac{\mathcal{O} - \mathcal{O}'}{\mathcal{O}}, \tag{3.1}$$

with $\mathcal{O}$ ($\mathcal{O}'$) denoting the quantity in the charged (neutral) sector in the case of meson data and the $\Delta^{+,0}$-mass ($\Delta^{++,-}$-mass) in the case of nucleons. We recall that, owing to the invariance of the Mtm-LQCD action under parity and $u \leftrightarrow d$ flavor exchange, Δ^+ and Δ^0 baryons, as well as Δ^{++} and the Δ^-, are exactly mass degenerate.

It should also be remarked that to calculate $R_s[\mathcal{O}]$ in the cases of the pseudoscalar and vector (isotriplet) meson decay constants, use has been made of the appropriate renormalization constants (Z_A and Z_V[6]) which were taken from Ref. [33]. The expressions of the pseudoscalar and vector meson decay constants in the physical quark basis read (no sum over b)

$$f_{\mathrm{PS}^b} = \frac{1}{m_{\mathrm{PS}^b}} \langle \Omega | \Big(\bar{\psi} \gamma_0 \gamma_5 \frac{1}{2} \tau^b \psi \Big)_R | \mathrm{PS}^b \rangle, \qquad b = \pm, 3, \tag{3.4}$$

$$f_{\mathrm{V}^b} \epsilon_k^\sigma = \frac{1}{m_{\mathrm{V}^b}} \langle \Omega | \Big(\bar{\psi} \gamma_k \frac{1}{2} \tau^b \psi \Big)_R | \mathrm{V}^{b,\sigma} \rangle, \qquad b = \pm, 3, \tag{3.5}$$

where the suffix R denotes renormalized operators, ϵ_k^σ is the polarization vector of the V state with third spin component σ, and k is a spatial Lorentz index.[7] Preliminary results on f_{V^b} have appeared in [29].

The striking conclusion which emerges looking at Table I is that among the many relative splittings reported there, we observe a large and statistically significant value of R_s *only* when pion masses are compared. For all other observables, the splitting is consistent with zero within the quoted errors.

TABLE I. The ratio $R_s[\mathcal{O}]$ of Eq. (3.1) for the observables $\mathcal{O}$ indicated in the first column at the simulation parameters specified in the second and third column (lattice size is about $L = 2.1$ fm). The large statistical error on R_s for mesonic observables at $\beta = 4.05$, $a\mu_q = 0.0030$ is due to limited statistics for the quark-disconnected contributions to the neutral meson correlators.

Obs. $\mathcal{O}$	β	$a\mu_q$	$R_s[\mathcal{O}]$
m_{PS}	3.90	0.0040	0.185(44)
m_{PS}	3.90	0.0085	0.139(51)
m_{PS}	4.05	0.0030	0.120(110)
m_{PS}	4.05	0.0060	0.120(42)
f_{PS}	3.90	0.0040	0.04(6)
f_{PS}	3.90	0.0085	−0.09(8)
f_{PS}	4.05	0.0030	−0.03(6)
f_{PS}	4.05	0.0060	0.01(5)
m_{V}	3.90	0.0040	0.022(68)
m_{V}	3.90	0.0085	0.021(44)
m_{V}	4.05	0.0030	−0.104(108)
m_{V}	4.05	0.0060	0.003(49)
$m_{\mathrm{V}} f_{\mathrm{V}}$	3.90	0.0040	−0.07(18)
$m_{\mathrm{V}} f_{\mathrm{V}}$	3.90	0.0085	−0.01(11)
$m_{\mathrm{V}} f_{\mathrm{V}}$	4.05	0.0030	−0.31(29)
$m_{\mathrm{V}} f_{\mathrm{V}}$	4.05	0.0060	−0.12(13)
m_{Δ}	3.90	0.0040	0.022(29)
m_{Δ}	3.90	0.0060	0.001(21)
m_{Δ}	3.90	0.0085	0.005(19)
m_{Δ}	3.90	0.0100	0.007(19)
m_{Δ}	4.05	0.0030	−0.004(45)
m_{Δ}	4.05	0.0060	0.004(17)
m_{Δ}	4.05	0.0080	0.000(18)
m_{Δ}	4.05	0.0120	0.007(16)

Concluding this section, we may observe that the detailed theoretical explanation of why, in quantities other than the pion mass O(a^2), lattice artifacts are small depends on the particular observable one is considering, and a case by case analysis is necessary. For completeness, let us briefly illustrate the situation in a few examples. We start by comparing $f_{\pi^\pm}$ with f_{π^3}. In this case, the smallness of $R_s[f_\pi]$ can be understood by noting that the large $\mathcal{L}_6$ matrix element represented by $a^2\zeta_\pi$ simply plays no role in the Symanzik description of the cutoff effects in both the neutral and the charged pion decay constant. This situation in turn implies that the (unknown) coefficients multiplying the dimension-6 Symanzik operators of Eq. (A9) [or (2.9)] are not exceptionally large; otherwise, all $\mathcal{L}_6$ matrix elements would generically have been large. In the case of the Δ mass, the fact that $R_s[m_\Delta]$ is small can be understood from the observation that the relevant matrix elements of $\mathcal{L}_6$ are just zero in the VSA. An even different situation

[6]We recall that Z_A and Z_V are the renormalization constants of the χ-basis bare operators $\bar{\chi}\gamma_\mu\gamma_5\tau^b\chi$ and $\bar{\chi}\gamma_\mu\tau^b\chi$, respectively. For the reader's convenience, we also report the renormalization rules for the currents in Mtm-LQCD [11,33] in the physical basis. For the charged ($b = \pm$) axial and vector currents, they read

$$\begin{aligned} (\bar{\psi}\gamma_\mu\gamma_5\tau^\pm\psi)_R &= Z_V \bar{\psi}\gamma_\mu\gamma_5\tau^\pm\psi, \\ (\bar{\psi}\gamma_\mu\tau^\pm\psi)_R &= Z_A \bar{\psi}\gamma_\mu\tau^\pm\psi, \end{aligned} \tag{3.2}$$

while for their neutral ($b = 3$) counterparts, one has

$$\begin{aligned} (\bar{\psi}\gamma_\mu\gamma_5\tau^3\psi)_R &= Z_A \bar{\psi}\gamma_\mu\gamma_5\tau^3\psi, \\ (\bar{\psi}\gamma_\mu\tau^3\psi)_R &= Z_V \bar{\psi}\gamma_\mu\tau^3\psi. \end{aligned} \tag{3.3}$$

[7]To be consistent with the H(4) invariance of the meson correlators, the matrix elements involving charged ($b = \pm$) or neutral ($b = 3$) mesons are normalized in Eqs. (3.4) and (3.5) with the corresponding charged or neutral meson mass.

occurs in the case of m_V. Here, the quantity that plays the role of ζ_π in the case of the pion mass is about 4 times smaller than the latter (as can be deduced e.g. from the data published in Refs. [29,36]). This correction leads to just a few percent effect in $R[m_V]$ owing to the comparatively larger value of m_V with respect to m_{π^3} (or $m_{\pi^\pm}$).

IV. CONCLUDING REMARKS

In this paper, we have proposed a theoretical explanation for the size of the O(a^2) flavor violating cutoff effects responsible for the large splitting between a neutral (m_{π^3}) and charged ($m_{\pi^\pm}$) pion mass seen in recent Mtm-LQCD dynamical simulations [2]. We have identified the origin of the additive O(a^2) cutoff effects appearing in $m^2_{\pi^3}$, which are absent in $m^2_{\pi^\pm}$ as the latter has discretization errors only of order $a^2\mu_q$, a^4 and higher. The magnitude of the O(a^2) lattice artifacts in the neutral pion mass is controlled, in the language of the Symanzik expansion, by the continuum matrix element $\langle\pi^3(\vec{0})|[\mathcal{L}_6^{\rm Mtm}(0) - (1/2)\times \int d^4x \mathcal{L}_5^{\rm Mtm}(x)\mathcal{L}_5^{\rm Mtm}(0)]|\pi^3(\vec{0})\rangle|_{\rm cont}$, which, if Mtm-LQCD is defined via the optimal critical mass estimate, is numerically dominated by $\zeta_\pi = \langle\pi^3(\vec{0})|\mathcal{L}_6^{\rm Mtm}|\pi^3(\vec{0})\rangle|_{\rm cont}$. In the vacuum saturation approximation, one gets the theoretical estimate $|\zeta_\pi| \sim 2\hat{G}^2_\pi \sim (560 \div 580\ {\rm MeV})^4$, up to an unknown multiplicative factor depending on the details of the lattice action and the number of dynamical quark flavors (actually one can argue that this coefficient grows linearly with N_f).

We have shown that numerical simulations of Mtm-LQCD with $N_f = 2$ light dynamical quarks yield values of $(r_0/a)^2 r_0^2 \Delta m^2_\pi|_L$ with negative sign and a magnitude that is in line with the above theoretical estimate. We have also provided evidence that among the many physical quantities recently measured in numerical simulations, only the neutral pion mass appears to be affected by large flavor-breaking discretization errors. Were it ever needed to reduce the relative lattice artifact on this particular quantity to, say, a ~5% level, while working, for instance, with a pion mass of about 250 MeV, simulations at lattice resolutions of about 0.03–0.04 fm would be required, based on the data and the a^2-scaling behavior discussed in this work.

Finally, we observe that, given the independence from the twist angle of the structure of the Symanzik effective action in the limit of vanishing quark mass, the analysis presented in this paper may have a bearing also on LQCD simulations employing standard (i.e. untwisted) Wilson fermions. Indeed, even in this formulation, O(a^2) cutoff effects of the same nature as those observed in Mtm-LQCD are expected to be present. In particular, a formula completely analogous to Eq. (2.1) holds true for the squared pion mass. Typically, these O(a^2) cutoff effects are reabsorbed in the definition of the current quark mass (which by construction vanishes simultaneously with the pion mass) and thus in the corresponding definition of critical mass. The consequences of this way of proceeding are in principle detectable in the form of O(a^2) cutoff effects in the masses of all the other hadrons and, more generally, in all the quantities that have a non-negligibly small dependence on the quark mass. Actually, in what observables exactly they will appear depends on the precise way the critical mass happens to have been determined (see the analysis in Appendix A).

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APPENDIX A: SYMANZIK EXPANSION AND CRITICAL MASS IN LQCD WITH WILSON FERMIONS

We consider $N_f = 2$ LQCD with quarks regularized as Wilson fermions. For generic values of the bare (twisted, μ_q, and untwisted, m_0) mass parameters the lattice action reads[8]

$$S_L = S_L^{\rm YM} + \bar{\chi}\Big[\gamma\cdot\tilde{\nabla} - \frac{a}{2}\nabla^*\nabla + c_{\rm SW}\frac{ia}{4}\sigma\cdot F + m_0 + i\mu_q\gamma_5\tau^3\Big]\chi, \tag{A1}$$

where $\tilde{\nabla}_\mu = \frac{1}{2}[\nabla_\mu + \nabla^*_\mu]$, with ∇_μ (∇^*_μ) the forward (backward) gauge covariant lattice derivative. For the sake of generality, we have also allowed for the presence of the clover term. We are especially interested in two specific regularizations of the Dirac-Wilson action comprised in (A1).

The first is the Mtm-LQCD regularization which is obtained from (A1) by setting $\mu_q = {\rm O}(a^0)$ and $m_0 = M^e_{\rm cr}$, where $M^e_{\rm cr}$ is some estimate of the critical mass. The physical interpretation of this scheme is most transparent

[8]We adopt the conventions and notations of Refs. [11,37,38]. In particular, the quark fields in the "physical" and "twisted" basis will be denoted by ψ, $\bar{\psi}$ and χ, $\bar{\chi}$, respectively.

in the quark basis resulting from the field transformation

$$\psi = \exp(i\pi\gamma_5\tau^3/4)\chi, \qquad \bar{\psi} = \bar{\chi}\exp(i\pi\gamma_5\tau^3/4), \tag{A2}$$

where the lattice action takes the form

$$S_L^{\mathrm{Mtm}} = S_L^{\mathrm{YM}} + \bar{\psi}\Big[\gamma\cdot\tilde{\nabla} - i\gamma_5\tau^3\Big(-\frac{a}{2}\nabla^*\nabla + c_{\mathrm{SW}}\frac{ia}{4}\sigma\cdot F + M_{\mathrm{cr}}^e\Big) + \mu_q\Big]\psi. \tag{A3}$$

This quark basis is referred to as the physical basis, because the quark mass term takes the form $\mu_q\bar{\psi}\psi$ with μ_q real [11].

The second is the (clover) standard Wilson fermion action, S_L^{cl}, which is obtained by setting $\mu_q = 0$ and $m_0 = m + M_{\mathrm{cr}}^e$ with m an $\mathrm{O}(a^0)$ quantity. With this choice, the most appropriate basis for discussing physics is the χ basis itself in which Eq. (A1) was written in the first place.

1. Symanzik expansion of Wilson fermion LQCD

The Symanzik effective Lagrangian associated to the Wilson action (A1) reads

$$\mathcal{L}_{\mathrm{Sym}} = \mathcal{L}_4 + \delta\mathcal{L}_{\mathrm{Sym}}, \tag{A4}$$

$$\mathcal{L}_4 = \mathcal{L}^{\mathrm{YM}} + \bar{\chi}[\not{D} + m + i\gamma_5\tau^3\mu_q]\chi, \tag{A5}$$

$$\delta\mathcal{L}_{\mathrm{Sym}} = a\mathcal{L}_5 + a^2\mathcal{L}_6 + \mathrm{O}(a^3), \tag{A6}$$

where the four-dimensional operator, $\mathcal{L}_4$, specifies the formal target theory in which continuum correlators are evaluated. The very definition of effective action (all the necessary logarithmic factors are understood) as a tool to describe the a dependence of lattice correlators implies that the mass parameters in $\mathcal{L}_4$, if not exactly vanishing, must be $\mathrm{O}(a^0)$ quantities. Thus all the lattice artifacts affecting M_{cr}^e will be described by higher dimensional operators in $\delta\mathcal{L}_{\mathrm{Sym}}$ of the form $a^k\delta_k\Lambda_{\mathrm{QCD}}^{k+1}\bar{\chi}\chi$, $k \geq 1$, with δ_k dimensionless coefficients, which are functions of the gauge coupling.

After using the equations of motion entailed by $\mathcal{L}_4$, the $\mathrm{O}(a)$ piece of $\delta\mathcal{L}_{\mathrm{Sym}}$ reads [4,20]

$$\mathcal{L}_5 = b_{5;\mathrm{SW}}\bar{\chi}i\sigma\cdot F\chi + \delta_1\Lambda_{\mathrm{QCD}}^2\bar{\chi}\chi + \mathrm{O}(m,\mu_q). \tag{A7}$$

The terms multiplied by powers of m and/or μ_q are not specified in Eq. (A7) as they are not of relevance for the topic discussed in this paper. We recall that the coefficients $b_{5;\mathrm{SW}}$ and δ_1 vanish if c_{SW} in Eq. (A1) is set to the value appropriate for Symanzik $\mathrm{O}(a)$ improvement.

The $\mathrm{O}(a^2)$ part of $\delta\mathcal{L}_{\mathrm{Sym}}$ has a more complicated expression, of the type

$$\mathcal{L}_6 = \sum_{i=1}^{3} b_{6;i}\Phi_{6;i}^{\mathrm{glue}} + b_{6;4}\bar{\chi}\gamma_\mu(D_\mu)^3\chi + \sum_{i=5}^{14} b_{6;i}\Phi_{6;i} + \delta_2\Lambda_{\mathrm{QCD}}^3\bar{\chi}\chi + \mathrm{O}(m,\mu_q), \tag{A8}$$

where the first three operators are purely gluonic, the fourth is a non-Lorentz invariant fermionic bilinear, and the remaining ones are four-fermion operators, which we choose to write in the form (equivalence with the list in [35] can be proved by using Fierz rearrangement)

$$\begin{aligned}
\Phi_{6;5} &= \frac{1}{4}(\bar{\chi}\chi)(\bar{\chi}\chi),\\
\Phi_{6;6} &= \frac{1}{4}\sum_b(\bar{\chi}\tau^b\chi)(\bar{\chi}\tau^b\chi),\\
\Phi_{6;7} &= \frac{1}{4}(\bar{\chi}i\gamma_5\chi)(\bar{\chi}\gamma_5\chi),\\
\Phi_{6;8} &= \frac{1}{4}\sum_b(\bar{\chi}i\gamma_5\tau^b\chi)(\bar{\chi}\gamma_5\tau^b\chi),\\
\Phi_{6;9} &= \frac{1}{4}(\bar{\chi}\gamma_\lambda\chi)(\bar{\chi}\gamma_\lambda\chi),\\
\Phi_{6;10} &= \frac{1}{4}\sum_b(\bar{\chi}\gamma_\lambda\tau^b\chi)(\bar{\chi}\gamma_\lambda\tau^b\chi),\\
\Phi_{6;11} &= \frac{1}{4}(\bar{\chi}\gamma_\lambda\gamma_5\chi)(\bar{\chi}\gamma_\lambda\gamma_5\chi),\\
\Phi_{6;12} &= \frac{1}{4}\sum_b(\bar{\chi}\gamma_\lambda\gamma_5\tau^b\chi)(\bar{\chi}\gamma_\lambda\gamma_5\tau^b\chi),\\
\Phi_{6;13} &= \frac{1}{4}(\bar{\chi}\sigma_{\lambda\nu}\chi)(\bar{\chi}\sigma_{\lambda\nu}\chi),\\
\Phi_{6;14} &= \frac{1}{4}\sum_b(\bar{\chi}\sigma_{\lambda\nu}\tau^b\chi)(\bar{\chi}\sigma_{\lambda\nu}\tau^b\chi).
\end{aligned} \tag{A9}$$

In closing this section, it is important to note that the form of the Symanzik effective Lagrangian enjoys some interesting degree of universality in the sense that formally, its zero mass limit ($m_0 - M_{\mathrm{cr}}^e = \mu_q = 0$) only depends on discretization details, like the form of the gauge action, the specific expression of the lattice derivatives, or the value of c_{SW}, but not on whether one shall be eventually dealing with standard or twisted Wilson fermions.

When quark mass terms are switched on, the QCD vacuum gets polarized driving spontaneous chiral symmetry breaking. The information about spontaneous chiral symmetry breaking effects is embodied in the Symanzik analysis by assigning to the continuum correlators in the expansion appropriate values consistent with the residual exact symmetries of the target QCD theory. In this way the relative "orientation" of the quark mass term with respect to the explicitly chirally breaking terms of the Symanzik low energy Lagrangian (describing the effects of the Wilson term present in the lattice action) becomes crucial for determining the size and the order in a of cutoff artifacts in correlation functions [4,11].

2. Critical mass in Wilson fermion LQCD

Both in the case of standard ($\mu_q = 0$) and twisted-mass [$\mu_q = \mathrm{O}(a^0)$] Wilson fermions, the critical mass is taken as the value of m_0 at which the partially conserved axial vector current (PCAC) mass vanishes. It is, however, useful to examine separately the two cases, since the resulting structure of lattice artifacts affecting these two determinations of the critical mass will be significantly different, as alluded to at the end of the previous section.

a. Critical mass in twisted-mass LQCD

In twisted-mass LQCD, the condition [which we write in the physical ψ basis (A2)]

$$a^3 \sum_{\vec{x}} \langle (\bar{\psi}\gamma_0 \tau^2 \psi)(\vec{x}, t)(\bar{\psi}\gamma_5 \tau^1 \psi)(0)\rangle|_L = 0 \qquad \text{(A10)}$$

leads to a determination of the critical mass, which is "optimal" ($M_{\mathrm{cr}}^{\mathrm{opt}}$) in the sense that with this choice, all the leading chirally enhanced cutoff effects [i.e. those of relative order $(a/\mu_q)^{2k}$, $k = 1, 2, \ldots$ with respect to the dominant term in the $a \to 0$ limit] are eliminated from lattice correlators [4].

In the spirit of the Symanzik expansion, the condition (A10) must be viewed as a relation holding true parametrically for generic values of a (and μ_q). As a consequence, it is equivalent to an infinite set of equations, where each equation results from the vanishing of the coefficient of the term proportional to a^k, $k = 0, 1, 2, \ldots$, in the expansion of the left-hand side of (A10).[9]

That the condition (A10) yields an acceptable estimate of the critical mass can be inferred from the observation that the first of these equations (the one which corresponds to the vanishing of the a^0 term) is nothing but the continuum relation

$$\int d^3x \langle (\bar{\psi}\gamma_0 \tau^2 \psi)(\vec{x}, t)(\bar{\psi}\gamma_5 \tau^1 \psi)(0)\rangle|_{\mathrm{cont}} = 0, \qquad \text{(A11)}$$

by which restoration of parity and isospin is enforced in the lattice theory. This means that, if [the O(a^0) term in] m_0 is chosen so as to fulfill Eq. (A10), then we will simultaneously have $m = 0$ in Eq. (A5) and the identification on the lattice of the operator $\bar{\psi}\gamma_0\tau^2\psi$ with the time component of the vector current, V_0^2. At this point to more clearly understand the further implications of Eq. (A10), it is convenient to explicitly write down the first few terms of its Symanzik expansion for which one gets

$$\begin{aligned} 0 = &-a \int d^3x \int d^4y \langle \mathcal{L}_5^{\mathrm{Mtm}}(y) V_0^2(x) P^1(0)\rangle|_{\mathrm{cont}} \\ &+ a \int d^3x \langle [\Delta_1 V_0^2(x) P^1(0) + V_0^2(x)\Delta_1 P^1(0)]\rangle|_{\mathrm{cont}} \\ &- a^2 \int d^3x \int d^4y \langle \mathcal{L}_6^{\mathrm{Mtm}}(y) V_0^2(x) P^1(0)\rangle|_{\mathrm{cont}} \\ &+ a^2 \int d^3x \langle [\Delta_2 V_0^2(x) P^1(0) + V_0^2(x)\Delta_2 P^1(0)]\rangle|_{\mathrm{cont}} \\ &+ \mathrm{O}(a^3). \end{aligned} \qquad \text{(A12)}$$

Equation (A12) has been written under the assumption that the O(a^0) piece of m_0 has been chosen so that condition (A11) is fulfilled. As a consequence [see Eq. (A7)] $\mathcal{L}_5^{\mathrm{Mtm}}$ is a parity-odd and flavor-breaking operator of the form

$$\begin{aligned} \mathcal{L}_5^{\mathrm{Mtm}} = &\, b_{5;\mathrm{SW}} \bar{\psi}\gamma_5\tau^3 \sigma \cdot F\psi - \delta_1 \Lambda_{\mathrm{QCD}}^2 \bar{\psi} i\gamma_5\tau^3\psi \\ &+ \mathrm{O}(\mu_q), \end{aligned} \qquad \text{(A13)}$$

while $\mathcal{L}_6^{\mathrm{Mtm}}$ [see Eq. (A8)] can be split into the sum of two contributions

$$\mathcal{L}_6^{\mathrm{Mtm}} = \mathcal{L}_6^{\mathrm{P\text{-}even}} - \delta_2 \Lambda_{\mathrm{QCD}}^3 \bar{\psi} i\gamma_5\tau^3\psi + \mathrm{O}(\mu_q), \qquad \text{(A14)}$$

with $\mathcal{L}_6^{\mathrm{P\text{-}even}}$ a parity-even operator. With the notation $\Delta_j O$ in Eq. (A12), we indicate the operators of dimension $d_O + j$ that correct to O(a^j) the (local) operator O. Their parity is equal to $(-1)^j$ times the parity of O (see the Appendix in [4]). We explicitly remark that in Eq. (A12), we have omitted the O(a^2) terms with two integrated insertions of $\mathcal{L}_5^{\mathrm{Mtm}}$ and the associated contact terms, because they all vanish by continuum parity. Finally, for the purpose of the present argument, we have ignored operators having coefficients proportional to μ_q.

At O(a), the condition implied by Eq. (A12) reduces to [4]

$$\begin{aligned} 0 = \int d^3x \int d^4y \langle [&b_{5;\mathrm{SW}} \bar{\psi}\gamma_5\tau^3\sigma \cdot F\psi \\ &- \delta_1 \Lambda_{\mathrm{QCD}}^2 \bar{\psi} i\gamma_5\tau^3\psi](y) V_0^2(x) P^1(0)\rangle|_{\mathrm{cont}} + \mathrm{O}(\mu_q), \end{aligned} \qquad \text{(A15)}$$

since the first term in the second line of Eq. (A12) gives a vanishing contribution to Eq. (A15) in the chiral limit, and there are no O(a) operator corrections to P^1 (i.e. $\Delta_1 P^1 = 0$).

In the chiral regime, where intermediate pion states dominate, one recognizes that Eq. (A15) leads to the condition which determines the O(a) piece of the optimal critical mass. We recall that with the definition

$$\xi_\pi = \xi_\pi(\mu_q) = \langle \Omega | \sum_{\ell=0}^{\infty} a^{2\ell} \mathcal{L}_{2\ell+5}^{\mathrm{Mtm}} | \pi^3(\vec{0})\rangle|_{\mathrm{cont}}, \qquad \text{(A16)}$$

[9] The practical problems in determining m_0 from (A10), which are related to subtleties associated to the exchange of continuum ($a \to 0$) and chiral ($\mu_q \to 0$) limit and to the possible limitations of the validity of the Symanzik expansion of the correlator (A10), have been discussed at length in Refs. [4,39] and will not be repeated here.

which to leading order in a reads $\xi_\pi \simeq \langle\Omega|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\rangle|_{\rm cont}$, Eq. (A15) becomes, in the chiral regime $\mu_q \ll \Lambda_{\rm QCD}$, the constraint [4]

$$\xi_\pi = \langle\Omega|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\rangle|_{\rm cont} + {\rm O}(a^2) = {\rm O}(\mu_q) + {\rm O}(a^2), \tag{A17}$$

which again should be looked at as an infinite set of equations, one for each power of a, with the leading one fixing δ_1 in terms of $b_{5;\rm SW}$.

At $\mathrm{O}(a^2)$, since by continuum parity invariance one can derive the equations

$$\int d^3x \int d^4y \langle \mathcal{L}_6^{\text{P-even}}(y) V_0^2(x) P^1(0)\rangle|_{\rm cont} = 0, \tag{A18}$$

$$\int d^3x \langle [\Delta_2 V_0^2(x) P^1(0) + V_0^2(x)\Delta_2 P^1(0)]\rangle|_{\rm cont} = 0, \tag{A19}$$

while the terms with the insertion of $\bar\psi i\gamma_5\tau^3\psi$ do not vanish

$$\int d^3x \int d^4y \langle \bar\psi i\gamma_5\tau^3\psi(y) V_0^2(x) P^1(0)\rangle|_{\rm cont} \neq 0, \tag{A20}$$

the condition implied by Eq. (A10) [or Eq. (A12)] yields $\delta_2 = 0$ in (A14). The important consequence of this argument is that the estimate of the critical mass provided by (A10) is not affected by $\mathrm{O}(a^2)$ corrections.

The above line of reasoning can be generalized to all orders in a leading to the conclusion that, if the critical mass is determined in twisted-mass LQCD by means of the condition (A10) [whose Symanzik expansion takes the form (A12)], the expansion of the critical mass will only display $\mathrm{O}(a^{2p+1})$, $p = 0, 1, \ldots,$ lattice corrections, with coefficients δ_{2p+1} determined by constraints analogous to (A15).

b. Critical mass in standard Wilson fermion LQCD

In the case of standard (clover) Wilson fermions, the condition for the vanishing of the PCAC mass is ($b = 1, 2, 3$, no sum over b)

$$\left.\frac{\tilde\partial_0 \sum_{\vec{x}} \langle i A_0^b(\vec{x}, t) P^b(0)\rangle}{2\sum_{\vec{x}}\langle P^b(\vec{x}, t)P^b(0)\rangle}\right|_L \equiv m_{\rm PCAC}|_L = 0 \quad \text{for } \mu_q = 0, \tag{A21}$$

which is analogous to Eq. (A10) with the crucial difference that now $\mu_q = 0$. The condition (A21) is in practice implemented by looking for the limiting value of m_0 at which $m_{\rm PCAC} \to 0^+$. We will call $M_{\rm cr}^{ew}$ the estimate of the critical mass obtained in this way.[10]

Setting $m_0 = M_{\rm cr}^{ew}$ in the standard Wilson action corresponds to have the continuum mass in $\mathcal{L}_4$ equal to zero. At the same time, lattice artifacts of order a^k, $k = 2, 3, \ldots$ in $M_{\rm cr}^{ew}$ will be correspondingly described by terms of the kind $a^k \delta_k^{ew} \Lambda_{\rm QCD}^{k+1} \bar\chi\chi$ in $\mathcal{L}_k$. The $\mathrm{O}(a)$ term is absent, if the lattice theory is clover improved. For the rest, unlike what we have shown to happen in twisted-mass LQCD (see Appendix A 2 a), discretization errors of any order in a will affect the critical mass determination provided by Eq. (A21).

As in the case of twisted-mass LQCD, here one must also look at the conditions coming from the vanishing of the PCAC mass as equations that fix the values of the coefficients δ_k^{ew} in terms of the matrix elements of $\mathcal{L}_k$ between one-pion states. For instance, at $\mathrm{O}(a^2)$ from the symmetries of the standard Wilson action (and the form of the associated Symanzik expansion) one cannot conclude anymore that δ_2^{ew} vanishes. Rather, the value of this parameter is fixed through Eq. (A21) by the condition

$$\langle\pi(\vec{0})|\mathcal{L}_6|\pi(\vec{0})\rangle|_{\rm cont} = 0, \tag{A22}$$

where $\mathcal{L}_6$ is the full six-dimensional operator of the Symanzik effective Lagrangian [given in Eq. (A8)] which, we recall, also includes the $\delta_2^{ew}\Lambda_{\rm QCD}^3\bar\chi\chi$ term. Equation (A22) follows from the fact that the lattice pion squared mass and $m_{\rm PCAC}|_L$ by construction vanish at the same value of m_0. Furthermore, these two quantities are found to be linearly proportional to a very good approximation in the region where they are both small, implying that possible additive cutoff artifacts affecting $m_{\rm PCAC}|_L$ and the squared pion mass are also proportional to each other.

APPENDIX B: $\mathrm{O}(a^2)$ CORRECTIONS TO THE SQUARED PION MASS

The correlator of interest for extracting the squared pion mass is the four-dimensional Fourier transform of the two-point subtracted[11] pseudoscalar correlator (no sum over $b = \pm, 3$), which reads

$$\Gamma_L^b(p) = a^4 \sum_x e^{ipx}\langle P^b(x)P^b(0)\rangle|_L. \tag{B1}$$

$\Gamma_L^b(p)$ has a pole at $p^2 = -m_{\pi^b}^2|_L$ with a residue given by $|G_{\pi^b}|_L^2$, where [see Eq. (2.11)]

[10] This nonperturbative estimate of the critical mass is the one that is implicitly adopted in the studies of standard (clover) Wilson LQCD where the renormalized quark mass is defined as $\hat m = Z_A Z_P^{-1} m_{\rm PCAC}$.

[11] Since we are interested in determining the structure of the cutoff corrections affecting the lattice pion mass, we can always imagine that contact terms, which do not display the pion pole, have been subtracted out. In the formulas that follow, the superscript "*subtracted*" is thus always understood.

$$G_{\pi^b}|_L = \langle\Omega|P^b|\pi^b(\vec{0})\rangle|_L. \tag{B2}$$

To proceed further, we need to write down the Symanzik expansion of $\Gamma_L(p)$ up to order a^2 included. This gives

$$\begin{aligned} a^4\sum_x e^{ipx}\langle P^b(x)P^b(0)\rangle|_L &= \int d^4x e^{ipx}\langle P^b(x)P^b(0)\rangle|_{\rm cont} + a^2\int d^4x e^{ipx}\langle\Delta_1 P^b(x)\Delta_1 P^b(0)\rangle|_{\rm cont} \\ &+ a^2\int d^4x e^{ipx}\langle\Delta_1 P^b(x)P^b(0)\int d^4y\mathcal{L}_5^{\rm Mtm}(y)\rangle|_{\rm cont} + a^2\int d^4x e^{ipx}\langle P^b(x)\Delta_1 P^b(0) \\ &\times\int d^4y\mathcal{L}_5^{\rm Mtm}(y)\rangle|_{\rm cont} + \frac{a^2}{2}\int d^4x e^{ipx}\langle P^b(x)P^b(0)\int d^4y\mathcal{L}_5^{\rm Mtm}(y)\int d^4y'\mathcal{L}_5^{\rm Mtm}(y')\rangle|_{\rm cont} \\ &- a^2\int d^4x e^{ipx}\langle\Delta_2 P^b(x)P^b(0)\rangle|_{\rm cont} - a^2\int d^4x e^{ipx}\langle P^b(x)\Delta_2 P^b(0)\rangle|_{\rm cont} \\ &- a^2\int d^4x e^{ipx}\langle P^b(x)P^b(0)\int d^4y\mathcal{L}_6^{\rm Mtm}(y)\rangle|_{\rm cont} + {\rm O}(a^4). \end{aligned} \tag{B3}$$

The absence of odd powers of the lattice spacing in this formula is guaranteed by the results of Ref. [11], as we are working at maximal twist. We will also assume that the critical mass has been determined in the optimal way described in Appendix A 2 a, so that by setting $m_0 = M_{\rm cr}^{\rm opt}$ the condition (A17) holds true. We also recall that the operators $\Delta_1 P^b$ and $\Delta_2 P^b$ are the dimension four and five terms that are needed to compensate for the O(a) and O(a^2) operator corrections arising from the contact of $\mathcal{L}_5^{\rm Mtm}(y)$ and $\mathcal{L}_6^{\rm Mtm}(y)$, respectively, with the operators localized at the points x and 0.

Since we are interested in the lattice corrections to the pion mass, we must look in the right-hand side (r.h.s.) of Eq. (B3) for the terms which may display the double pion pole factor[12] $(p^2 + m_\pi^2)^{-2}$.

Among the many terms in the r.h.s. of Eq. (B3), only the fifth and the last display the double pole we are after. Putting together Eqs. (2.11), (B2), and (B3) and taking the limit $p \to 0$ at small m_π^2 (but always parametrically larger than a^2 [4]), from the ensuing pion pole dominance we arrive at the formula

$$\begin{aligned} \frac{|G_{\pi^3}|^2}{m_{\pi^3}^2}\bigg|_L &= \frac{|G_\pi|^2}{m_\pi^2}\bigg|_{\rm cont} \\ &\times\left[1 - a^2\frac{\langle\pi^3(\vec{0})|\mathcal{L}_{6\&55}^{\rm Mtm}(0)|\pi^3(\vec{0})\rangle}{m_\pi^2}\bigg|_{\rm cont}\right] \\ &+ {\rm O}\left(\frac{a^2}{m_\pi^2}\right), \end{aligned} \tag{B4}$$

with

$$\mathcal{L}_{6\&55}^{\rm Mtm}(0) = \mathcal{L}_6^{\rm Mtm}(0) - \frac{1}{2}\int d^4x\mathcal{L}_5^{\rm Mtm}(x)\mathcal{L}_5^{\rm Mtm}(0). \tag{B5}$$

A simple Taylor series resummation leads precisely to Eq. (2.1) of the text, which we stress also agrees with the results derived in χPT [12,13,22,39].

We close the Appendix by noting that the absence of a contribution from $\langle\pi^\pm(\vec{0})|\mathcal{L}_6^{\rm Mtm}(0)|\pi^\pm(\vec{0})\rangle|_{\rm cont}$ in Eq. (2.6) is a consequence of the commutation relation[13]

$$[Q_A^\pm, \mathcal{L}_{\rm Sym}^{\rm Mtm}] = {\rm O}(\mu_q) = {\rm O}(m_\pi^2), \tag{B6}$$

from which one gets the SPT

$$\begin{aligned} &\langle\pi^\pm(\vec{0})|\mathcal{L}_6^{\rm Mtm}(0)|\pi^\pm(\vec{0})\rangle|_{\rm cont} \\ &= \frac{-i}{f_\pi}\langle\Omega|[Q_A^\pm, \mathcal{L}_6^{\rm Mtm}(0)]|\pi^\pm(\vec{0})\rangle|_{\rm cont} + {\rm O}(m_\pi^2) \\ &= {\rm O}(m_\pi^2). \end{aligned} \tag{B7}$$

APPENDIX C: EXPRESSION AND ESTIMATES OF $\Delta_{55}^{\pm,3}$

In this (long) Appendix, we present arguments showing that Δ_{55}^b, $b = 3, \pm$ [Eq. (2.5)] yield contributions to $m_{\pi^b}^2|_L$ [Eqs. (2.6) and (2.7)], which are parametrically (in the limit $m_\pi^2 \to 0$) and/or numerically negligible, provided Mtm-LQCD is defined by setting m_0 [see Eq. (A1)] at its optimal critical value determined by the condition (A10).

In Appendix C 1, we provide the expression of Δ_{55}^3 and $\Delta_{55}^\pm$ [Eq. (2.5)] based on standard field theoretical manipulations, i.e. insertion of intermediate states, or alternatively Lehmann-Symanzik-Zimmerman representation and reduction formulas, and, wherever applicable, SPT's [24,25]. In Appendix C 2, we give a numerical estimate of the magnitude of Δ_{55}^3 and $\Delta_{55}^\pm$ for the typical lattice volume and pion mass values relevant for the recent ETMC simulations. The details of our estimate of the key matrix

[12]For short from now, on we will simply write m_π^2 (with no isospin index as in the continuum target theory all three pions are mass-degenerate) for $m_\pi^2|_{\rm cont}$.

[13]In Mtm-LQCD, the flavor symmetry group is the "oblique" SU(2)$_{\rm ob}$ group generated by the charges Q_A^+, Q_A^-, and Q_V^3. These conserved charges are associated with the (one-point split) currents reported in Sec. 4.1 of Ref. [11]. In the notation of that paper we are dealing here with the case $r = 1$, $\omega_r = \pi/2$.

element ξ_π [Eqs. (A16) and (A17)], which controls the numerically dominant (in the small m_π^2 region) contributions to $\Delta_{55}^{3,\pm}$, are deferred to Appendix C 3.

1. The theoretical analysis of Δ_{55}^3 and $\Delta_{55}^\pm$

For the purposes of our study, we restrict attention to $N_f = 2$ QCD with light u and d quarks yielding light, weakly interacting pions. In this regime, on general grounds, one can write in the infinite volume limit the spectral decomposition of the continuum quantity Δ_{55}^3 [Eq. (2.5)] in the convenient form[14]

$$\Delta_{55}^3 = -\frac{\xi_\pi}{m_\pi^2}\langle\pi^3(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^3(\vec{0})\rangle - \frac{4\pi}{16\pi^3}\int_{2m_\pi}^{4m_\pi} dE\frac{k(E)}{E^2 - m_\pi^2}|\langle\pi^3(\vec{0})| \times \mathcal{L}_5^{\rm Mtm}|\mathcal{P}_{\pi\pi}^{(I_3=0)}\pi\pi, E\rangle|^2 + R_{55}^3, \tag{C1}$$

$$R_{55}^3 = -\sum_n \frac{|\langle\pi^3(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\sigma_n^0(\vec{0})\rangle|^2}{m_{\sigma_n^0}^2 - m_\pi^2} + \cdots, \tag{C2}$$

where we have explicitly separated out from the remainder, R_{55}^3, the contribution of the semidisconnected one-pion pole (sometimes referred to as "tadpole" in the following) and the contribution of the cut over two-pion states below the inelastic threshold. In order to have more manageable formulas, we have decided to reduce the initial integrations over the momenta of the two pions to the integration on the single center-of-mass energy variable, and we have set

$$k(E) = \sqrt{(E/2)^2 - m_\pi^2}. \tag{C3}$$

The remainder in Eq. (C2) comprises a sum over one-particle scalar states with zero isospin,[15] as well as contributions from heavier and/or more complicated multiparticle states which we have simply indicated by "$\cdots$." Our conventions are such that in Eq. (C1) the single-particle meson states α ($\alpha = \pi, \sigma_n^0, \ldots$) are introduced with the Lorentz covariant normalization ($b, b' = 1, 2, 3$ are SU(2) isospin labels)

$$\langle\alpha^b(\vec{p})|\alpha^{b'}(\vec{p}')\rangle = 2E_\alpha(\vec{p})(2\pi)^3\delta_{b,b'}\delta(\vec{p} - \vec{p}'), \quad E_\alpha(\vec{p}) = \sqrt{\vec{p}^2 + m_\alpha^2}. \tag{C4}$$

The states $|\mathcal{P}_{\pi\pi}^{(I_3=0)}\pi\pi, E\rangle$ are two-pion states with total energy E, zero total three-momentum, and a zero total isospin third component. In particular, the symbol $\mathcal{P}_{\pi\pi}^{(I_3=0)}$ denotes the isospin projector onto the two-pion states with a vanishing total third component ($I_3 = 0$). Here, we recall that two possible states contribute which one has to sum over, namely, the state with two neutral pions and that with one negatively and one positively charged pion.

Similarly, the expression of the (infinite volume limit) spectral decomposition of $\Delta_{55}^\pm$ [Eq. (2.5)] will read

$$\Delta_{55}^\pm = -\frac{\xi_\pi}{m_\pi^2}\langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^\pm(\vec{0})\rangle - \frac{4\pi}{16\pi^3}\int_{2m_\pi}^{4m_\pi} dE\frac{k(E)}{E^2 - m_\pi^2}|\langle\pi^\pm(\vec{0})| \times \mathcal{L}_5^{\rm Mtm}|\mathcal{P}_{\pi\pi}^{(\pm,3)}\pi\pi, E\rangle|^2 + R_{55}^\pm, \tag{C5}$$

$$R_{55}^\pm = -\sum_n \frac{|\langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\sigma_n^\pm(\vec{0})\rangle|^2}{m_{\sigma_n^\pm}^2 - m_\pi^2} + \cdots, \tag{C6}$$

with $\mathcal{P}_{\pi\pi}^{(\pm,3)}$ as the isospin projector onto the state of two pions having third component $\pm$ and 3.

On general grounds one expects the numerically dominating contributions to $\Delta_{55}^{3,\pm}$ to come from the interaction of the propagating pion [the initial and final particle in Eq. (2.5)] with a neutral pion created from the vacuum, i.e. from first term in the r.h.s. of Eqs. (C1) and (C5). In the next sections, we will show that this is indeed the case. The important observation is that in Mtm-LQCD with optimal critical mass, these dominant tadpole contributions are $\mathrm{O}(m_\pi^2)$ and moreover equal for Δ_{55}^3 and $\Delta_{55}^\pm$ up to (very small) $\mathrm{O}(m_\pi^4)$ terms; hence, they get canceled in the pion squared mass difference. The estimated leftover correction coming from the elastic two-pion cut as well as the remainders [Eqs. (C2) and (C6)] will be shown to be tiny.

We now examine in turn the various terms contributing to Δ_{55}^3 and $\Delta_{55}^\pm$ and discuss their parametric behavior in the small-m_π^2 regime. We shall see, in particular, that for symmetry reasons the contributions from the various intermediate states to $\Delta_{55}^\pm$ tend to be negligible compared to those contributing to Δ_{55}^3, with the exception of the tadpole term and the one coming from the lowest-lying two-pion intermediate state.

a. Tadpole

The first terms in Eqs. (C1) and (C5) are equal to leading order in the chiral expansion, as one can show e.g. by reducing the neutral pion in the ket state, yielding[16]

[14]For short in this Appendix, we will drop the subscript $|_{\rm cont}$ from continuum QCD quantities. Lattice quantities will still be labeled by the subscript $|_L$.

[15]Phenomenologically, the lightest of these states should be identified with the $a_0(980)$ meson. It should be kept in mind that, since in the actual simulation data we will be considering the lightest "pion" mass is about 300 MeV, the lattice state corresponding to the "$a_0(980)$" particle is expected to have a mass somewhat above 1 GeV.

[16]In this Appendix with the symbol $\sim$, we denote equality up to $\mathrm{O}(a^2)$ corrections, with the $\stackrel{\rm SPT}{=}$ equality up to $\mathrm{O}(m_\pi^2)$ terms and with the $\stackrel{\rm SPT}{\sim}$ equality up to $\mathrm{O}(a^2)$ and $\mathrm{O}(m_\pi^2)$ corrections.

$$\langle\pi^3(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^3(\vec{0})\rangle \overset{\rm SPT}{=} \langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^\pm(\vec{0})\rangle. \tag{C7}$$

An explicit estimate of the tadpole terms can be given on the basis of the SPT relations

$$\langle\pi^3(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^3(\vec{0})\rangle \overset{\rm SPT}{=} -\frac{1}{f_\pi^2}\langle\Omega|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\rangle = -\frac{\xi_\pi}{f_\pi^2}, \tag{C8}$$

from which one gets

$$\Delta_{55}^3|_{\rm tad} = -\frac{\xi_\pi}{m_\pi^2}\langle\pi^3(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^3(\vec{0})\rangle \overset{\rm SPT}{=} \frac{\xi_\pi^2}{f_\pi^2 m_\pi^2},$$
$$\Delta_{55}^\pm|_{\rm tad} = -\frac{\xi_\pi}{m_\pi^2}\langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\pi^3(\vec{0})\pi^\pm(\vec{0})\rangle \overset{\rm SPT}{=} \frac{\xi_\pi^2}{f_\pi^2 m_\pi^2}. \tag{C9}$$

We remark that when the untwisted mass, m_0, is fixed at its optimal value, Eq. (A17) holds [4], implying

$$\frac{\xi_\pi^2}{f_\pi^2 m_\pi^2} = {\rm O}(m_\pi^2), \tag{C10}$$

while in the opposite case one finds that this quantity tends to increase as we go towards the chiral limit, leaving large O(a^2/m_π^2) cutoff effects in the neutral as well as in the charged lattice pion mass.[17]

b. Two-pion cut below the inelastic threshold

In a finite three-dimensional volume, $V = L^3$, the integral over the two-pion cut can be rewritten as a sum over discrete states through the formal replacement

$$\int_{2m_\pi}^{4m_\pi} dE\frac{k(E)}{E^2 - m_\pi^2}\cdots \to \sum_{\ell=0}^{\ell_{\rm max}}\frac{1}{\rho_V(E_\ell)}\frac{k(E_\ell)}{E_\ell^2 - m_\pi^2}\cdots, \tag{C11}$$

where $\ell_{\rm max}$ is the number of allowed two-pion levels that can be hosted in the volume V below the inelastic threshold ($4m_\pi$). The relation between the allowed values of ℓ and the level energies is established combining Eq. (C3) with the formulas [43,44]

$$\ell\pi - \delta(k) = \phi(q), \qquad q = \frac{kL}{2\pi}, \qquad \ell \geq 0, \tag{C12}$$

where $\delta(k)$ denotes the s-wave $\pi\pi$ phase shift in the appropriate isospin channel and $\phi(q)$ is a known [44] kinematical function. Finally (see e.g. Ref. [45]),

$$\rho_V(E) = \frac{q\phi'(q) + k\delta'(k)}{4\pi k^2}E \tag{C13}$$

is the two-particle state density with $\delta'(k) = d\delta(k)/dk$ and $\phi'(q) = d\phi/dq$. At the volumes ($L = 2.1$ and $L = 2.8$ fm) that will be considered in Appendix C 2 and for the lightest pion mass ($m_{\pi^\pm} \sim 300$ MeV), one has $l_{\rm max} = 2$.

(i) $\ell = 0$—The contribution of the $\ell = 0$ term in the sum (C11) can be computed in an almost model-independent way observing that the lowest energy level corresponds to have the two pions at rest with $E_0 = 2m_\pi$.[18] Making use of the SPT's (C7) and (C8) and taking into account the presence of the isospin projectors $\mathcal{P}_{\pi\pi}^{(I_3=0)}$ and $\mathcal{P}_{\pi\pi}^{(\pm,3)}$ in Eqs. (C1) and (C5), respectively, one finds

$$\Delta_{55}^3|_{\ell=0} = -\frac{3h_0^2\xi_\pi^2}{(E_0^2 - m_\pi^2)f_\pi^4}\Bigg|_{E_0=2m_\pi}, \tag{C14}$$

$$\Delta_{55}^\pm|_{\ell=0} = -\frac{2h_0^2\xi_\pi^2}{(E_0^2 - m_\pi^2)f_\pi^4}\Bigg|_{E_0=2m_\pi}, \tag{C15}$$

where

$$h_0^2 = \frac{k(E_0)}{8\pi^2\rho_V(E_0)}\Bigg|_{E_0=2m_\pi} = \frac{1}{2m_\pi V}(1 + {\rm O}(1/L)) \tag{C16}$$

will be in the following approximated by its infinite volume limiting value, $(2m_\pi V)^{-1}$, which we remark is independent of the expression of the phase shift $\delta(k)$ appearing in $\rho_V(E)$.
Two observations are in order here. The first is that the quantities (C14) and (C15) only differ because different isospin combinations of two-pion intermediate states contribute. The second is that, as in the tadpole case discussed above, both contributions are of O(m_π^2), if Eq. (C10) holds, i.e. if the critical mass has been set to its optimal value. If this is not so, large and unequal, O(a^2/m_π^2) cutoff effects will be left out in the neutral, as well as in the charged, lattice pion mass.

(ii) $\ell \geq 1$—As we said, given the magnitude of L we consider, in the energy interval $2m_\pi < E < 4m_\pi$ two-pion states with $\ell = 1$ and $\ell = 2$ will contribute with terms of the form

$$\Delta_{55}^b|_\ell = -\frac{2h_\ell^2}{E_\ell^2 - m_\pi^2}\Big|\langle\pi^b(\vec{0})|\mathcal{L}_5^{\rm Mtm}|\mathcal{P}_{\pi\pi}^{(\ldots)}\pi\pi, E_\ell\rangle\Big|^2,$$
$$h_\ell^2 = \frac{k(E_\ell)}{8\pi^2\rho_V(E_\ell)} \tag{C17}$$

[17] This result is in agreement with the finding of theoretical studies [4,13,40] and indirectly confirmed by the observation of large, positive O(a^2) lattice artifacts in the quenched Mtm-LQCD computations [41,42] of the charged pion mass and the corresponding decay constant (computed from the WTI relation $f_{\pi^\pm} = 2\mu_q G_\pi/m_{\pi^\pm}^2$).

[18] Actually, there is a finite size correction proportional to the ($J = 0, I = 0$) $\pi\pi$ scattering length [43]. To be precise, one gets $E_0 = 2m_\pi - 4\pi a_0^0(m_\pi V)^{-1}(1 + {\rm O}(1/L))$.

with b equal to 3 or $\pm$ and $\mathcal{P}_{\pi\pi}^{(\dots)}$ standing for $\mathcal{P}_{\pi\pi}^{(I_3=0)}$ or $\mathcal{P}_{\pi\pi}^{(\pm,3)}$, respectively. Evaluation of $\Delta_{55}^{3}|_{\ell=1,2}$ is possible only at the price of making some reasonable assumption about the energy behavior of the pion matrix elements in Eq. (C17). The simplest thing is to assume that these matrix elements are constant in energy in the range $2m_\pi < E < 4m_\pi$. The quantities h_ℓ^2 in Eq. (C17) can be straightforwardly evaluated in terms of $k(E_\ell)$ and $\rho_V(E_\ell)$ for the ℓ values of interest, once a reasonable parametrization of the phase shift $\delta(k)$ (see Appendix C 2) is inserted in Eq. (C13).

Concerning $\Delta_{55}^{\pm}|_{\ell=1,2}$, the important remark is that these quantities in the chiral regime are suppressed by a factor of m_π^4 with respect to their neutral counterparts $\Delta_{55}^{3}|_{\ell=1,2}$. The result follows from Eq. (C17) by noting the SPT relation (actually valid for all $\ell > 0$)

$$if_\pi\langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\mathrm{Mtm}}|\mathcal{P}_{\pi\pi}^{(\pm,3)}\pi\pi, E_\ell\rangle = \langle\Omega|[Q_A^\pm, \mathcal{L}_5^{\mathrm{Mtm}}]|\mathcal{P}_{\pi\pi}^{(\pm,3)}\pi\pi, E_\ell\rangle = \mathrm{O}(m_\pi^2). \quad \text{(C18)}$$

As a consequence, assuming the validity of this SPT for $m_\pi \simeq 300 \div 400$ MeV, we shall neglect $\Delta_{55}^{\pm}|_{\ell=1,2}$ with respect to $\Delta_{55}^{3}|_{\ell=1,2}$ in our subsequent numerical estimates.

We also observe that, if $\mathcal{L}_5^{\mathrm{Mtm}}$ itself is an operator of $\mathrm{O}(\mu_q) = \mathrm{O}(m_\pi^2)$, as it happens in the LO-χPT description of Mtm-LQCD with optimal critical mass,[19] the r.h.s. of Eq. (C18) is actually an $\mathrm{O}(m_\pi^4)$ quantity for states with $E_\ell = \mathrm{O}(m_\pi)$, while $\langle\pi^3(\vec{0})|\mathcal{L}_5^{\mathrm{Mtm}}|\mathcal{P}_{\pi\pi}^{(I_3=0)}\pi\pi, E_\ell\rangle$ is $\mathrm{O}(m_\pi^2)$. In this situation one thus finds $\Delta_{55}^{\pm}|_{\ell=1,2} = \mathrm{O}(m_\pi^6)$ and $\Delta_{55}^{3}|_{\ell=1,2} = \mathrm{O}(m_\pi^2)$. The resulting m_π^4 suppression factor is in agreement with the general m_π^2 behavior [implied by the SPT (C18)] of the charged pion contribution with respect to the neutral one.

c. The remainder

The remainder comprises the two-pion cut integral from $4m_\pi$ to ∞ and the contribution from all other possible single and multiparticle intermediate states.

The first important observation is that all the contributions to $R_{55}^{\pm}$ are of $\mathrm{O}(m_\pi^4)$. This result can be derived in close analogy to Eq. (C18) above, namely, by reducing the charged pion in the matrix elements [see Eq. (C6)] $\langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\mathrm{Mtm}}|\alpha^\pm\rangle$, where $|\alpha^\pm\rangle$ is a state with a nonzero energy in the chiral limit [e.g. the one-particle scalar state $\sigma_n^\pm$ appearing in Eq. (C6)]. One gets, in fact

$$if_\pi\langle\pi^\pm(\vec{0})|\mathcal{L}_5^{\mathrm{Mtm}}|\alpha^\pm\rangle = \langle\Omega|[Q_A^\pm, \mathcal{L}_5^{\mathrm{Mtm}}]|\alpha^\pm\rangle = \mathrm{O}(m_\pi^2). \quad \text{(C19)}$$

A similar result does not hold for R_{55}^{3}, because the commutator $[Q_A^3, \mathcal{L}_5^{\mathrm{Mtm}}]$ does not vanish in the chiral limit. Based on Eq. (C19), we shall neglect the term $R_{55}^{\pm}$ with respect to R_{55}^{3} in the numerical estimates below.

In this context it should also be noted that the sum $\Delta_{55}^{\pm}|_{\ell=1} + \Delta_{55}^{\pm}|_{\ell=2} + R_{55}^{\pm}$, being a negative quantity, yields a (tiny) positive contribution to the phenomenologically negative [2,3] squared pion mass splitting. This term [see Eqs. (2.6) and (2.7)], if included in $\Delta_{55}^{\pm}$, would go in the direction of increasing the negative contribution of ζ_π that is necessary in order to reproduce the observed value of $m_{\pi^3}^2|_L - m_{\pi^\pm}^2|_L$.

Coming back to the evaluation of the remainder terms, we shall hence limit below our discussion to R_{55}^{3}. The latter, we recall, includes, besides terms from one-particle scalar intermediate states explicitly shown in Eq. (C2), also a cut contribution of the form

$$-\frac{4\pi}{16\pi^3}\int_{4m_\pi}^{\infty} dE\,\frac{k(E)}{E^2 - m_\pi^2}|\langle\pi^3(\vec{0})|\mathcal{L}_5^{\mathrm{Mtm}}|\mathcal{P}_{\pi\pi}^{(I_3=0)}\pi\pi, E\rangle|^2,$$

as well as negligible contributions from more complicated (and heavier) multiparticle intermediate states. The cut contribution above can be estimated by assuming the standard Källen-Lehmann (large energy) $1/E^2$ behavior for the modulus square of the $\mathcal{L}_5^{\mathrm{Mtm}}$ matrix elements and by setting the coefficient factor in front to a value that matches the contribution from the $\ell = 2$ two-pion intermediate state. As for the one-particle scalar state contribution, we make the plausible assumption that it is of the same (very small, see Appendix C 2) size as the cut contribution, and simply double the latter in order to get our numerical estimate of R_{55}^{3}.

Terms from multiparticle intermediate states of increasing mass are expected to give tiny and progressively smaller and smaller contributions, owing to explicit energy denominators and the asymptotic high-energy behavior of the matrix elements.

2. Numerical considerations

In this subsection, we want to provide a numerical estimate of the order of the magnitude of the difference $\Delta_{55}^{3} - \Delta_{55}^{\pm}$ relying on the results of the previous subsection and the numerical evaluation of ξ_π given in Appendix C 3.

We shall see that $\Delta_{55}^{\pm}$, which according to the considerations of Appendix C 1 is an $\mathrm{O}(m_\pi^2)$ quantity, takes a value much smaller than $a^{-2}\Delta m_\pi^2|_L^{\mathrm{Mtm}}$. Numerically, Δ_{55}^{3} is of similar size as $\Delta_{55}^{\pm}$, as the parametrically $\mathrm{O}(m_\pi^0)$ contributions from R_{55}^{3} are tiny and actually smaller than the $\mathrm{O}(m_\pi^2)$ terms.

These facts imply [see Eqs. (2.6) and (2.7)] that lattice corrections to the squared charged pion mass are also small

[19] In LO-χPT, there is only one operator (see e.g. Ref. [13]) with the same quantum numbers as $\mathcal{L}_5^{\mathrm{Mtm}}$ [Eq. (A13)]. Hence the condition $\xi_\pi = \langle\Omega|\mathcal{L}_5^{\mathrm{Mtm}}|\pi^3(\vec{0})\rangle = \mathrm{O}(\mu_q)$ implies that the unique effective operator representing $\mathcal{L}_5^{\mathrm{Mtm}}$ at LO of χPT must itself be proportional to the quark mass. Obviously for matrix elements involving states with increasing rest-frame energy E the LO-χPT description progressively looses its validity.

and of order $a^2m_\pi^2$ (or a^4), while the main contribution to the lattice artifacts of the squared neutral pion mass comes from ζ_π, as announced in the text (Sec. II). As we already said, in the difference $\Delta_{55}^3 - \Delta_{55}^\pm$ the contribution coming from the tadpole terms exactly cancels.

Using the value (C54) of ξ_π and the estimate $h_0^2 = (2m_\pi V)^{-1}$, we can provide an explicit numerical evaluation of the three contributions to Δ_{55}^3 and $\Delta_{55}^\pm$ described in Appendices C 1 a, C 1 b, and C 1 c. To arrive at this result, we also need to know the energies of the few lowest $\pi\pi$ levels living in our finite simulation box at the actual value of the simulated pion masses. In the situation corresponding to the lattice data used for our best estimate of ξ_π, we have $m_\pi \simeq 300$ MeV and $L \sim 2.1$ fm. We checked that results do not change significantly with the volume by repeating the same analysis for $L \sim 2.8$ fm. In order to compute k_ℓ and hence $E_\ell = 2\sqrt{k_\ell^2 + m_\pi^2}$ from Eq. (C12), as well as $\rho_V(E_\ell)$ from Eq. (C13), we parametrize the s-wave $\pi\pi$ phase shift in the form (suggested by LO-χPT [46])

$$\delta(k) = \frac{2k}{E}\cdot\frac{2E^2 - m_\pi^2}{32\pi f_0^2}, \qquad \frac{E^2}{4} = k^2 + m_\pi^2, \qquad \text{(C20)}$$

with $f_0 = 86$ MeV being the chiral limit value of the pion decay constant (as obtained from recent ETMC studies [2,3]). The formula (C20) (with m_π at its physical value 140 MeV) describes rather well the experimental $\pi\pi$-scattering data for center-of-mass energy E in the range $2m_\pi$ to $4m_\pi$ (see e.g. the phase-shift data compilation in Ref. [46]).

Following the discussion in Appendices C 1 a, C 1 b, and C 1 c, in terms of the reference scale $a_{\beta=3.9}^{-1}$, whose value is currently estimated [3] to be about 2.3 GeV, we obtain the following numerical results:

(i) *Tadpole*

$$\Delta_{55}^3|_{\rm tad} = \Delta_{55}^\pm|_{\rm tad} \stackrel{\rm SPT}{=} \frac{\xi_\pi^2}{f_\pi^2 m_\pi^2} \sim 0.00050^{+0.00032}_{-0.00024} a_{\beta=3.9}^{-4}, \qquad \text{(C21)}$$

where the quoted error reflects the uncertainty on ξ_π from Eq. (C54).

(ii) *Two-pion cut below the inelastic threshold*. For the $\ell = 0$ term, one obtains

$$\Delta_{55}^3|_{\ell=0} = -\frac{3h_0^2\xi_\pi^2}{3m_\pi^2 f_\pi^4} \sim -(0.000063^{+0.000040}_{-0.000030}) a_{\beta=3.9}^{-4}, \qquad \text{(C22)}$$

$$\Delta_{55}^\pm|_{\ell=0} = -\frac{2h_0^2\xi_\pi^2}{3m_\pi^2 f_\pi^4} \sim -(0.000042^{+0.000027}_{-0.000020}) a_{\beta=3.9}^{-4}. \qquad \text{(C23)}$$

For the $\ell > 0$ levels, one gets smaller and smaller contributions. A reasonable estimate of their order of magnitude is $-0.000020 a_{\beta=3.9}^{-4}$ and $-0.000015 a_{\beta=3.9}^{-4}$ for $\Delta_{55}^3|_\ell$ at $\ell = 1$ and $\ell = 2$, respectively, to which we attach a generous 50%–60% relative uncertainty. We neglect here $\Delta_{55}^\pm|_{\ell=1,2}$, which according to SPT arguments, are significantly smaller (m_π^4 suppressed) than their neutral counterparts.

(iii) *Remainder*. According to the results of Appendix C 1 c, we can limit consideration to R_{55}^3. Despite the difficulty of evaluating all the terms contributing to R_{55}^3, following the procedure discussed in Appendix C 1 c, we can reasonably estimate it to be about $-0.000080 a_{\beta=3.9}^{-4}$, with, as before, a 50%–60% relative statistical uncertainty. We thus find that R_{55}^3 is of the same order of magnitude as $\Delta_{55}^3|_{\ell=0}$ or $\sum_{\ell=1}^2 \Delta_{55}^3|_\ell$.

(iv) *Total*. Putting everything together, we finally get

$$\Delta_{55}^3 \simeq +(0.00032 \pm 0.00019 \pm 0.00008) a_{\beta=3.9}^{-4}, \qquad \text{(C24)}$$

$$\Delta_{55}^\pm \simeq +(0.00046 \pm 0.00027 \pm 0.00005) a_{\beta=3.9}^{-4}, \qquad \text{(C25)}$$

and

$$\Delta_{55}^3 - \Delta_{55}^\pm \simeq -(0.00014 \pm 0.00008 \pm 0.00004) a_{\beta=3.9}^{-4}. \qquad \text{(C26)}$$

The two "errors" quoted in the equations above reflect the uncertainty (dominantly of statistical nature) on the value of ξ_π from Appendix C 3 and the systematic indetermination inherent to the assumptions we made above about the energy behavior of the matrix elements of $\mathcal{L}_5^{\rm Mtm}$, respectively.

For the sake of comparison, here we only recall that (as one can infer from Fig. 1 and the value $r_0/a|_{\beta=3.9} \simeq 5.2$) at $m_\pi \simeq 300$ MeV direct lattice measurements yield $a_{\beta=3.9}^2 \Delta m_\pi^2|_{L;\beta=3.9}^{\rm Mtm} \simeq -0.0067(20)$, i.e. a number much bigger than $a_{\beta=3.9}^4\Delta_{55}^3$, or $a_{\beta=3.9}^4\Delta_{55}^\pm$. Comparisons of this kind are performed and discussed more thoroughly in Sec. II C.

3. Estimating ξ_π from lattice two-point correlators

We describe in this section the analysis, based on the Symanzik expansion, by which we arrive at a numerical estimate of the crucial continuum quantity ξ_π [Eqs. (A16) and (A17)] that has been employed in Appendix C 1 to parametrize the various terms contributing to $\Delta_{55}^\pm$ and Δ_{55}^3. Since in this numerical analysis we will be exploiting $N_f = 2$ Mtm-LQCD data at sufficiently small $m_\pi \simeq m_{\pi^\pm}|_L$ around 300 MeV, we feel safe to use SPT's to relate among themselves some of the (continuum QCD) matrix elements that appear in the Symanzik description of lattice quantities. The SPT approximation is correct up to $O(m_\pi^2)$ relative corrections, whose relevance is checked by going to heavier quark masses up to $m_{\pi^\pm}|_L \leq 450$ MeV. By extending the analysis from data at lattice resolution $a^{-1} = 2.3$ GeV ($\beta = 3.90$) to those at $a^{-1} = 2.9$ GeV ($\beta = 4.05$) and comparing (at the lowest-lying pion mass) results at box linear size $L \sim 2.1$ fm with those at $L \sim 2.8$ fm, we have checked that within our (large) statistical errors, the numerical estimates relevant for this paper display no significant discretization and/or finite size effects.

The key correlator we consider is[20]

$$C_{PS}^L(t) = \sum_{\vec{x}} \frac{1}{2}\langle P^3(\vec{x}, t) S^0(0)\rangle|_L - L^3 \frac{1}{2}\langle P^3(0)\rangle\langle S^0(0)\rangle|_L, \quad t > 0, \tag{C27}$$

which in the continuum limit is an $O(a)$ quantity because it violates parity (and isospin) invariance. The Symanzik expansion of its renormalized counterpart reads

$$\begin{aligned} -Z_{S^0} Z_P C_{PS}^L(t) &= a\left\langle \int d\vec{x} \hat{P}^3(\vec{x}, t) \int d^4 y \mathcal{L}_5^{\mathrm{Mtm}}(y) \frac{1}{2} \hat{S}^0(0) \right\rangle + O(a^3) \\ &= a\hat{G}_\pi \frac{\xi_\pi}{m_\pi^2} \langle \pi^3 | \frac{1}{2} \hat{S}^0 | \pi^3 \rangle \frac{e^{-m_\pi t}}{2m_\pi} + a\hat{G}_\pi \langle \pi^3 | \mathcal{L}_5^{\mathrm{Mtm}} | \sigma_{\mathrm{eff}}\rangle\langle \sigma_{\mathrm{eff}} | \frac{1}{2}\hat{S}^0 | \Omega\rangle \frac{1}{m_{\sigma_{\mathrm{eff}}}^2 - m_\pi^2}\left[\frac{e^{-m_\pi t}}{2m_\pi} - \frac{e^{-m_{\sigma_{\mathrm{eff}}} t}}{2m_{\sigma_{\mathrm{eff}}}}\right] \\ &\quad + a\frac{\xi_\pi}{m_\pi^2} \langle \pi^3 | \hat{P}^3 | \sigma_{\mathrm{eff}}\rangle\langle \sigma_{\mathrm{eff}} | \frac{1}{2}\hat{S}^0 | \Omega\rangle \frac{e^{-m_{\sigma_{\mathrm{eff}}} t}}{2m_{\sigma_{\mathrm{eff}}}} + O(a^3), \end{aligned} \tag{C28}$$

where $\hat{P}^3$ and $\hat{S}^0$ denote the renormalized operators P^3 and S^0, respectively, and G_π was defined in Eq. (2.11). The symbol $|\sigma_{\mathrm{eff}}\rangle$ represents the lightest (isosinglet) scalar state that can be created from the vacuum by the operator S^0. For the quark mass values and in the t range of interest for the present analysis of $C_{PS}^L(t)$ (because of the unfavourable signal-to-noise ratio inherent in the evaluation of the quark-disconnected piece of the correlator), we are in fact sensitive within errors only to the neutral pion and $|\sigma_{\mathrm{eff}}\rangle$ intermediate states. In a finite box and for sufficiently small quark masses, the symbol $|\sigma_{\mathrm{eff}}\rangle\langle\sigma_{\mathrm{eff}}|$ in the r.h.s. of Eq. (C28) is to be interpreted as

$$|\sigma_{\mathrm{eff}}\rangle\langle\sigma_{\mathrm{eff}}| = h_0^2 \sum_{b=1}^{3} |\pi^b\pi^b, m_{\sigma_{\mathrm{eff}}}\rangle\langle\pi^b\pi^b, m_{\sigma_{\mathrm{eff}}}|, \quad m_{\sigma_{\mathrm{eff}}} \simeq 2m_\pi. \tag{C29}$$

In the following, we shall write simply $|\sigma\rangle$ for $|\sigma_{\mathrm{eff}}\rangle$.

The three terms in the r.h.s. of Eq. (C28) come from the three different possible time orderings of the inserted operators. We have only retained the pole contributions from the two lightest states and the associated partially disconnected terms that must go along with them in order to comply with Lorentz invariance. Since in Mtm-LQCD with optimal critical mass all the leading terms (linear in a) in Eq. (C28) are of the same order in m_π, we have ignored here the $O(a)$ lattice corrections to the operators S^0 and P^3, because they would give contributions to the Symanzik expansion suppressed by an extra (relative) factor m_π^2[21] and are numerically small for the considered range of quark mass and t values.

With the help of Eqs. (C8) and (C29) as well as the SPT relations

$$\langle \pi^3 | \frac{1}{2}\hat{S}^0 | \pi^3\rangle \overset{\mathrm{SPT}}{=} \frac{1}{f_\pi}\hat{G}_\pi, \tag{C30}$$

$$\langle \pi^3 | \hat{P}^3 | \sigma\rangle \overset{\mathrm{SPT}}{=} -\frac{1}{f_\pi}\langle\Omega| \frac{1}{2}\hat{S}^0 |\sigma\rangle, \tag{C31}$$

the Symanzik expansion (C28) can be rewritten in the simpler form

$$\begin{aligned} Z_P Z_{S^0} C_{PS}^L(t) \overset{\mathrm{SPT}}{=} &-a\frac{e^{-m_\pi t}}{2m_\pi}\frac{\hat{G}_\pi^2 \xi_\pi}{f_\pi m_\pi^2}\left[1 - \frac{3h_0^2}{f_\pi^2}\frac{m_\pi^2}{m_\sigma^2 - m_\pi^2}\right] \\ &+ a\frac{e^{-m_\sigma t}}{2m_\sigma}\frac{\hat{G}_\pi^2 \xi_\pi}{f_\pi m_\pi^2}\frac{3h_0^2}{f_\pi^2}\left[1 - \frac{m_\pi^2}{m_\sigma^2 - m_\pi^2}\right] \\ &+ O(a^3), \end{aligned} \tag{C32}$$

where, as we shall see below, all the quantities, but ξ_π and the negligible $O(a^3)$ terms, can be directly evaluated from lattice data. Solving, in fact, the resulting equations yields an estimate of for ξ_π for each given quark mass μ_q and lattice resolution a.

[20]We recall that all the correlators we shall be dealing with are ''connected'' in the strict sense of Quantum Field Theory, though some contribution only through gluon exchanges.

[21]This is seen by noting that $\Delta_1 S^0 \propto a\mu_q P^3$, while $\Delta_1 P^3$ comprises a term proportional to $a\mu_q S^0$ and another one proportional to $F_{\mu\nu}\tilde{F}_{\mu\nu}$. This last term has $O(\mu_q)$ matrix elements between states involving only the vacuum and one or two neutral pions, as one can check by means of SPT's.

a. Evaluating ξ_π

Several two-point Green functions in the neutral pseudoscalar channel (where also quark-disconnected diagrams contribute) have been evaluated, among which

$$C^L_{PP}(t) = a^3\sum_{\vec{x}}\langle P^3(x)P^3(0)\rangle|_L - L^3\langle P^3(0)\rangle|_L\langle P^3(0)\rangle|_L, \tag{C33}$$

$$C^L_{SS}(t) = a^3\sum_{\vec{x}}\frac{1}{4}\langle S^0(x)S^0(0)\rangle|_L - L^3\frac{1}{4}\langle S^0(0)\rangle|_L\langle S^0(0)\rangle|_L, \tag{C34}$$

and

$$C^L_{PS}(t) = a^3\sum_{\vec{x}}\frac{1}{2}\langle P^3(x)S^0(0)\rangle|_L - L^3\frac{1}{2}\langle P^3(0)\rangle|_L\langle S^0(0)\rangle|_L, \tag{C35}$$

$$C^L_{SP}(t) = a^3\sum_{\vec{x}}\frac{1}{2}\langle S^0(x)P^3(0)\rangle|_L - L^3\frac{1}{2}\langle S^0(0)\rangle|_L\langle P^3(0)\rangle|_L, \tag{C36}$$

It should be noted that in connected correlators, the mixing of the bare operators P^3 and S^0 with the identity does not contribute.

All lattice correlators are simultaneously fitted to simple two-state ansatz of the form

$$C^L_{PS}(t) = c_5c_1\frac{\exp(-m_{\pi^3}|_L t)}{2m_{\pi^3}|_L} + d_5d_1\frac{\exp(-m_\sigma|_L t)}{2m_\sigma|_L}, \tag{C37}$$

$$C^L_{PP}(t) = c_5c_5\frac{\exp(-m_{\pi^3}|_L t)}{2m_{\pi^3}|_L} + d_5d_5\frac{\exp(-m_\sigma|_L t)}{2m_\sigma|_L}, \tag{C38}$$

$$C^L_{SS}(t) = c_1c_1\frac{\exp(-m_{\pi^3}|_L t)}{2m_{\pi^3}|_L} + d_1d_1\frac{\exp(-m_\sigma|_L t)}{2m_\sigma|_L}. \tag{C39}$$

Comparing the fit ansatz for the correlators $C^L_{PS,SS,PP}$ with the corresponding Symanzik expansions written to the leading order in a and in the form where only the neutral pion and/or the lightest scalar state contributions are retained (consistently with the numerical fact that within statistical errors only the contribution of these two states is visible), one obtains the following identifications:

$$c_5 \sim \langle\Omega|P^3|\pi^3(\vec{0})\rangle, \qquad d_1 \sim \langle\Omega|\frac{1}{2}S^0|\sigma\rangle, \tag{C40}$$

as well as

$$Z_{S^0}Z_Pc_1c_5 \overset{\mathrm{SPT}}{\sim} -a\frac{\hat{G}^2_\pi\xi_\pi}{f_\pi m^2_\pi}\left[1 - \frac{3h_0^2}{f_\pi^2}\frac{m^2_\pi}{m^2_\sigma - m^2_\pi}\right]. \tag{C41}$$

A similar equation between $Z_{S^0}Z_Pd_1d_5$ and the coefficient of the $e^{-m_\sigma t}/(2m_\sigma)$ term in the r.h.s. of Eq. (C32) can be obtained. This relation is, however, of minor interest given the substantial statistical error we have on the fitted coefficient d_5. Finally, the relevant dimensionless ratios Z_P/Z_{S^0} and $3h_0^2/f_\pi^2$ entering Eq. (C41) can be estimated via the formulas

$$\frac{Z_P}{Z_{S^0}} \sim \left|\frac{c_5}{G_{\pi^\pm}|_L}\right|, \qquad \frac{h_0^2}{f_\pi^2}\overset{\mathrm{SPT}}{\sim}\frac{1}{3}\left(\frac{d_1}{G_{\pi^\pm}|_L}\right)^2, \tag{C42}$$

where

$$G_{\pi^\pm}|_L = \langle\Omega|P^\pm|\pi^\pm(\vec{0})\rangle|_L, \tag{C43}$$

$$P^\pm = (P^1 \pm iP^2)/\sqrt{2}. \tag{C44}$$

The second of the Eqs. in (C42) is a consequence of the SPT (C30) and the relation

$$Z_Pd_1 \overset{\mathrm{SPT}}{\sim} \sqrt{3}\,h_0\langle\pi^3(\vec{0})|\frac{1}{2}\hat{S}^0|\pi^3(\vec{0})\rangle, \tag{C45}$$

which in turn follows from the identification of σ as a two-pion state [see Eq. (C29)]. It should also be recalled that both the renormalized operators $\hat{S}_0$ and $\hat{P}^\pm$ are related to their bare (subtracted) counterparts through the renormalization constant Z_P, which would then cancel in the ratio $d_1/G_{\pi^\pm}|_L$ if we were to write it in terms of renormalized quantities.

Combining together the relations (C40)–(C42), one arrives at an explicit formula for ξ_π, namely

$$a\xi_\pi \overset{\mathrm{SPT}}{\sim} -c_1\frac{f_{\pi^\pm}m^2_{\pi^\pm}}{G_{\pi^\pm}}\left[1 - \frac{d_1^2}{3G^2_{\pi^\pm}}\frac{3m^2_{\pi^\pm}}{m^2_\sigma - m^2_{\pi^\pm}}\right]^{-1}\Bigg|_L, \tag{C46}$$

where the charged pion sector O(a^0) quantities $m_{\pi^\pm}|_L$, $G_{\pi^\pm}|_L$ and

$$f_{\pi^\pm}|_L \equiv 2\mu_q(G_{\pi^\pm}m^{-2}_{\pi^\pm})|_L \tag{C47}$$

can be evaluated much more accurately (at level of 1% or better) than the corresponding neutral sector quantities, $m_\sigma|_L$, d_1 and c_1 (we recall that c_1 vanishes linearly in a as $a \to 0$). From the analysis of the neutral pseudoscalar channel correlators specified in Eqs. (C33) to (C36), we can extract $m_\sigma|_L$ that, within statistical errors (ranging from 10% to 20% depending on statistics) turns out to be equal to $2m_{\pi^\pm}|_L$ at all the values of μ_q and at the two different lattice resolutions we consider (see Table II below). Using the relation (C47) and setting $m_\sigma|_L = 2m_{\pi^\pm}|_L$, Eq. (C46) takes the simple form

$$a\xi_\pi \overset{\mathrm{SPT}}{\sim} -c_12\mu_q\left[1 - \frac{d_1^2}{3G_{\pi^\pm}|_L^2}\right]^{-1}, \tag{C48}$$

or alternatively,

TABLE II. Quantities entering Eqs. (C46)–(C49). The labels for the parameter sets have self-explanatory names and the corresponding columns follow the same order as the list of parameter sets in Eqs. (C50)–(C52). The statistical errors come from a standard bootstrap analysis on blocked data, so as to properly take into account autocorrelation of consecutive measurements.

$(\beta, a\mu_q)\|_{L/a}$	$(3.9, .0040)\|_{24}$	$(3.9, .0064)\|_{24}$	$(3.9, .0085)\|_{24}$	$(3.9, .0040)\|_{32}$
# meas.	880	240	248	184
$am_{\pi^\pm}\|_L$	0.1359(7)	0.1694(4)	0.1940(5)	0.1338(3)
$a^2G_{\pi^\pm}\|_L\sqrt{2}$	0.1501(25)	0.1581(16)	0.1643(15)	0.1484(11)
$am_{\pi^3}\|_L$	0.103(4)	0.134(10)	0.163(8)	0.107(7)
$am_\sigma\|_L$	0.234(25)	0.391(46)	0.449(47)	0.284(47)
$a^2c_1\sqrt{2}$	−0.021(4)	−0.018(6)	−0.011(6)	−0.019(5)
$a^2d_1\sqrt{2}$	−0.12(2)	−0.22(5)	−0.25(6)	−0.15(3)
$c_1r_0^3a^{-1}\sqrt{2}$	−3.0(6)	−2.6(9)	−1.6(9)	−2.7(7)
$\xi_\pi r_0^4$	0.10(2)	0.14(5)	0.10(4)	0.08(2)
$(\beta, a\mu_q)\|_{L/a}$	$(4.05, .0030)\|_{32}$	$(4.05, .0060)\|_{32}$		
# meas.	192	188		
$am_{\pi^\pm}\|_L$	0.1038(6)	0.1432(6)		
$a^2G_{\pi^\pm}\|_L\sqrt{2}$	0.0898(18)	0.0972(12)		
$am_{\pi^3}\|_L$	0.090(6)	0.125(6)		
$am_\sigma\|_L$	0.231(37)	0.232(55)		
$a^2c_1\sqrt{2}$	−0.014(3)	−0.010(6)		
$a^2d_1\sqrt{2}$	−0.10(2)	−0.09(3)		
$c_1r_0^3a^{-1}\sqrt{2}$	−4.0(9)	−2.9(1.7)		
$\xi_\pi r_0^4$	0.13(2)	0.16(9)		

$$a\xi_\pi \overset{\text{SPT}}{\sim} - c_1 2\mu_q\left[1 - \frac{h_0^2}{f_{\pi^\pm}|_L^2}\right]^{-1}. \tag{C49}$$

The latter expression of ξ_π is exploited to obtain the numerical estimates presented below.

b. Numerical results

We report in Table II in lattice units the results for the quantities entering Eqs. (C46)–(C49). These numbers are obtained from the analysis of the correlators (C33)–(C36), as well as their charged pseudoscalar meson analogs, evaluated on the gauge configurations taken from the $N_f = 2$ ETMC ensembles with the following bare parameters:

$$\beta = 3.9 (a \simeq 0.09\ \text{fm}), \qquad L/a = 24: \quad a\mu_q = 0.0040, 0.0064, 0.0085, \tag{C50}$$

$$\beta = 3.9 (a \simeq 0.09\ \text{fm}), \qquad L/a = 32: \quad a\mu_q = 0.0040, \tag{C51}$$

$$\beta = 4.05 (a \simeq 0.07\ \text{fm}), \qquad L/a = 32: \quad a\mu_q = 0.0030, 0.0060. \tag{C52}$$

The values of $a\mu_q$ above are known [3,5] to correspond to quark mass values (in the $\overline{MS}$ scheme at a scale of 2 GeV) in the range from 20 to 40 MeV. At $\beta = 3.9$ and $a\mu_q = 0.0040$, data at two different volumes allow us to check that our estimates of ξ_π are not significantly affected by finite size effects. The results at the two β values can be compared by expressing quantities in units of r_0 (extrapolated to zero quark mass limit) with the help of the estimates [3,7])

$$r_0/a|_{\beta=3.9} = 5.22(2), \qquad r_0/a|_{\beta=4.05} = 6.61(3). \tag{C53}$$

In order to ease such a comparison, for the case of c_1, which is a dimension two and O(a) quantity, we also quote the value of $c_1r_0^3a^{-1}$, the latter being by construction a dimensionless and O(a^0) quantity.[22] For the key quantity ξ_π, we quote for the same reasons $r_0^4\xi_\pi$. In Table II, we also give for each ensemble the number of measurements (# meas.) of the neutral pseudoscalar meson channel correlators.

Inspection of Table II shows that the most accurate results are obtained for $\beta = 3.9$, $a\mu_q = 0.0040$, where the number of measurements of neutral pseudoscalar meson channel correlators is the largest, and we also have data

[22]The statistical error on $c_1r_0^3a^{-1}$ is completely dominated by that on a^2c_1.

on two different physical volumes. From the results at $\beta = 3.9$, $a\mu_q = 0.0040$ and using Eq. (C49), we obtain our best ξ_π estimate, namely

$$\xi_\pi \overset{\mathrm{SPT}}{\sim} 0.00014(4)a^{-4}_{\beta=3.9} \Leftrightarrow r_0^4\xi_\pi \overset{\mathrm{SPT}}{\sim} 0.10(3), \qquad \text{(C54)}$$

from which Eqs. (C21)–(C26) follow. One checks in Table II that this result remains stable within statistical errors at increasing values of the quark mass.

If we were to use for ξ_π the expression (C48), instead of Eq. (C49), results consistent with Eq. (C54) would be obtained, though with a larger statistical errors due to the fact that $d_1/(\sqrt{3}G_{\pi^\pm})|_L$ is a quantity of order one with a sizeable uncertainty from d_1, the effect of which is enhanced in the factor $(1 - \frac{d_1^2}{3G_{\pi^\pm}|_L^2})^{-1}$. For instance, at $\beta = 3.9$, $a\mu_q = 0.0040$ and $L/a = 24$ (the statistically most precise data set), we would get $\xi_\pi = 0.00015(5)a^{-4}_{\beta=3.9}$.

Results about the various quantities entering Eqs. (C46)–(C49) are also shown in Table II, as a check of their quark mass dependence and scaling with a. For instance, in the case of c_1, we find by inspection that the values of $c_1 r_0^3 a^{-1}$ display within errors good scaling and no visible quark mass dependence. This last property is consistent with the use of SPT's we made in order to arrive at Eq. (C48). The situation for d_1 is similar, but with somewhat increasing statistical uncertainties at higher quark masses. The statistically very precise matrix element $G_{\pi^\pm}|_L$, shows instead a mild quark mass dependence, as its value is seen to change by not more than 10% in the quark mass range we have considered.

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