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

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We show that the size of the O(a^2) flavour violating cutoff artifacts that have been found to affect the value of the neutral pion mass in simulations with maximally twisted Wilson fermions is controlled by a continuum QCD quantity that is fairly large and is determined by the dynamical mechanism of spontaneous chiral symmetry breaking. One can argue that the neutral pion mass is the only physical quantity blurred by such cutoff effects. O(a^2) corrections of this kind are also present in standard Wilson fermion simulations, but they can either affect the determination of the pion mass or be shifted from the latter to other observables, depending on the way the critical mass is evaluated.

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1. Introduction and main results

Numerical data for the mass of the neutral pion in maximally twisted Lattice QCD (Mtm-LQCD) [1] simulations show unnaturally large lattice artifacts [2] [1], despite the fact that on general grounds they are expected to be O(a^2) corrections [7, 8]. This is in striking contrast with the smallness of the cutoff effects observed not only in the mass of the charged pions, which are related through the Goldstone theorem to exactly conserved lattice currents [9], but also in all the other so far measured hadronic observables. Quite remarkably small lattice artifacts are found even in matrix elements where the neutral pion is involved [10, 11].

In this talk, relying on arguments based on the Symanzik analysis [12] of lattice cutoff effects, we give an explanation of the origin of such peculiar corrections, showing that they are a general feature of any Wilson-like fermion regularization, whether twisted or not, and their appearance in the pion mass or instead in other observables depends on the choice of the twisted angle (zero or $\pi/2$) and the way the critical mass is determined.

In sect. 2 we recall the properties of the Symanzik approach for the description of cutoff effects in LQCD with Wilson fermions and we discuss how the critical mass is determined. In sect. 3 we illustrate the nature of O(a^2) artifacts in Mtm-LQCD and in sect. 4 how they show up in the standard Wilson fermion regularization. We end with some concluding remarks in sect. 5.

2. Symanzik expansion and critical mass in Wilson fermion LQCD

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

$$S_L = S_L^{\rm YM} + \bar\chi \left[\gamma\cdot\widetilde\nabla - \frac{a}{2}\nabla^*\nabla + c_{\rm SW}\frac{ia}{4}\sigma\cdot F + m_0 + i\mu\gamma_5\tau^3\right]\chi\,, \tag{2.1}$$

where for the sake of generality we have also introduced the clover term. In this talk we are interested in two specific cases comprised in (2.1).

• Mtm-LQCD, which is obtained from (2.1), by setting $\mu = {\rm O}(a^0)$ and $m_0 = M_{\rm cr}^e$, where $M_{\rm cr}^e$ is some estimate of the critical mass. The physical interpretation of this regularization is most transparent in the so-called “physical basis”, resulting from the field transformation

$$\psi = \exp(i\pi\gamma_5\tau^3/4)\chi\,,\quad \bar\psi = \bar\chi\exp(i\pi\gamma_5\tau^3/4) \Longrightarrow \tag{2.2}$$

$$S_L^{\rm Mtm} = S_L^{\rm YM} + \bar\psi\left[\gamma\cdot\widetilde\nabla - i\gamma_5\tau^3\left(-\frac{a}{2}\nabla^*\nabla + c_{\rm SW}\frac{ia}{4}\sigma\cdot F + M_{\rm cr}^e\right) + \mu\right]\psi\,. \tag{2.3}$$

• The clover standard Wilson fermions action, $S_L^{\rm cl}$, which is obtained by setting $\mu = 0$ and $m_0 = m + M_{\rm cr}^e$ with m an O(a^0) quantity. With this choice the most appropriate basis for discussing physics is the χ-basis itself in which eq. (2.1) was written in the first place.

[1] The neutral to charged pion mass splitting measured in the unquenched Mtm-LQCD simulations carried out in ref. [2] with the tree-level improved Symanzik gauge action turns out to be smaller (and of opposite sign) than the quenched result [3] where the standard plaquette gauge action was used. This finding is interesting in view of the established relation [4, 5] between the magnitude of this splitting and the strength of metastabilities detected in the theory at much too coarse lattice spacings [6].

B) The Symanzik effective Lagrangian associated to the Wilson LQCD action (2.1) reads

$$\mathscr{L}_{\rm Sym} = \mathscr{L}_4 + \delta\mathscr{L}_{\rm Sym}\,, \tag{2.4}$$

$$\mathscr{L}_4 = \mathscr{L}^{\rm YM} + \bar\chi[\not{D} + m + i\gamma_5\tau^3\mu]\chi\,, \qquad \delta\mathscr{L}_{\rm Sym} = a\mathscr{L}_5 + a^2\mathscr{L}_6 + {\rm O}(a^3)\,, \tag{2.5}$$

where the four-dimensional operator (all the necessary logarithmic factors are understood) specifies the continuum theory in which correlators are evaluated. The very definition of effective action, as a tool to describe the a dependence of lattice correlators, implies that the mass parameters in $\mathscr{L}_4$, if not exactly vanishing, must be $\mathrm{O}(a^0)$ quantities. Thus all the lattice artifacts affecting $M^e_{\rm cr}$ will be described by operators of the form $a^k\Lambda^{k+1}_{\rm QCD}\bar\chi\chi$, $k=1,2,\ldots$ in $\delta\mathscr{L}_{\rm Sym}$.

After using the equations of motion of $\mathscr{L}_4$, the $\mathrm{O}(a)$ piece of $\delta\mathscr{L}_{\rm Sym}$ reads ($b_{5;\rm SW}$ and δ_1 are O(1) coefficients)

$$\mathscr{L}_5 = b_{5;\rm SW}\bar\chi i\sigma\cdot F\chi + \delta_1\Lambda^2_{\rm QCD}\bar\chi\chi + {\rm O}(m,\mu)\,. \tag{2.6}$$

The terms multiplied by powers of m and/or μ are not specified in eq. (2.6) because they are not of relevance for the topic discussed in this note. We recall that the coefficient $b_{5;\rm SW}$ vanishes, if $c_{\rm SW}$ in eq. (2.1) is set to the value appropriate for Symanzik $\mathrm{O}(a)$ improvement.

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

$$\mathscr{L}_6 = \sum_{i=1}^{3} b_{6;i}\Phi^{\rm glue}_{6;i} + b_{6;4}\bar\chi\gamma_\mu(D_\mu)^3\chi + \sum_{i=5}^{14} b_{6;i}\Phi_{6;i} + \delta_2\Lambda^3_{\rm QCD}\bar\chi\chi + {\rm O}(m,\mu)\,, \tag{2.7}$$

where the first three operators are purely gluonic, the fourth is a chiral (but not Lorentz) invariant fermionic bilinear and the remaining ones are four fermion operators, which we find useful to write in the form (equivalence with the list in [13] can be proved using Fierz rearrangement)

$$\begin{array}{ll}
\Phi_{6;5} = (\bar\chi\chi)(\bar\chi\chi)\,, & \Phi_{6;6} = \sum_b(\bar\chi\tau^b\chi)(\bar\chi\tau^b\chi)\,,\\
\Phi_{6;7} = (\bar\chi\gamma_5\chi)(\bar\chi\gamma_5\chi)\,, & \Phi_{6;8} = \sum_b(\bar\chi\gamma_5\tau^b\chi)(\bar\chi\gamma_5\tau^b\chi)\,,\\
\Phi_{6;9} = (\bar\chi\gamma_\lambda\chi)(\bar\chi\gamma_\lambda\chi)\,, & \Phi_{6;10} = \sum_b(\bar\chi\gamma_\lambda\tau^b\chi)(\bar\chi\gamma_\lambda\tau^b\chi)\,,\\
\Phi_{6;11} = (\bar\chi\gamma_\lambda\gamma_5\chi)(\bar\chi\gamma_\lambda\gamma_5\chi)\,, & \Phi_{6;12} = \sum_b(\bar\chi\gamma_\lambda\gamma_5\tau^b\chi)(\bar\chi\gamma_\lambda\gamma_5\tau^b\chi)\,,\\
\Phi_{6;13} = (\bar\chi\sigma_{\lambda\nu}\chi)(\bar\chi\sigma_{\lambda\nu}\chi)\,, & \Phi_{6;14} = \sum_b(\bar\chi\sigma_{\lambda\nu}\tau^b\chi)(\bar\chi\sigma_{\lambda\nu}\tau^b\chi)\,.
\end{array} \tag{2.8}$$

C) Both in the case of standard Wilson and twisted mass fermions the condition which determines the critical mass is the vanishing of the PCAC mass. Let us examine these two cases separately.

1) tm-LQCD – The condition (it is convenient to rotate the quark fields to the ψ-basis (2.2))

$$a^3\sum_{\vec x}\langle(\bar\psi\gamma_0\tau^2\psi)(\vec x,t)(\bar\psi\gamma_5\tau^1\psi)(0)\rangle\Big|_L = 0 \tag{2.9}$$

leads to a determination of the critical mass which is "optimal" ($M^{\rm opt}_{\rm cr}$) in the sense that with this choice all the leading chirally enhanced cutoff effects are eliminated from lattice correlators [9].

In the spirit of the Symanzik approach the condition (2.9) must be viewed as a relation holding true parametrically for generic values of a (and μ). As a result, it is equivalent to an infinite set of equations, each equation corresponding to the vanishing of the coefficient of the term a^k, $k=0,1,2,\ldots$. From the vanishing of the a^0 term one gets

$$\int d^3x\,\langle(\bar\psi\gamma_0\tau^2\psi)(\vec x,t)(\bar\psi\gamma_5\tau^1\psi)(0)\rangle\Big|_{\rm cont} = 0\,, \tag{2.10}$$

by which restoration of parity and isospin is enforced. This means that, if (the $\mathrm{O}(a^0)$ piece of) m_0 is chosen so as to verify eq. (2.9), then we will simultaneously have $m=0$ in (2.5) and the identification on the lattice of $\bar{\psi}\gamma_0\tau^2\psi$ with the (time component of the) vector current V_0^2 (the identification of $\bar{\psi}\gamma_5\tau^1\psi$ with the pseudoscalar density P^1 being trivial). The further implications of eq. (2.9) are conveniently exposed looking at its Symanzik expansion. In ref. [9] it was proved that at $\mathrm{O}(a)$ (2.9) implies the condition

$$\xi_\pi \equiv a\,\langle\Omega|\mathscr{L}_5^{\mathrm{Mtm}}|\pi^3(\vec{0})\rangle\Big|_{\mathrm{cont}} + \mathrm{O}(a^3) = \mathrm{O}(a\mu) + \mathrm{O}(a^3)\,, \tag{2.11}$$

$$\mathscr{L}_5^{\mathrm{Mtm}} = b_{5;SW}\,\bar{\psi}\gamma_5\tau^3\sigma\cdot F\psi - \delta_1\Lambda^2_{\mathrm{QCD}}\,\bar{\psi}i\gamma_5\tau^3\psi + \mathrm{O}(\mu)\,. \tag{2.12}$$

Eq. (2.11) should be read as a constraint fixing δ_1. At $\mathrm{O}(a^2)$ the only relevant term [11] is the one where $V_0^2P^1$ is inserted with (the integrated density) $\mathscr{L}_6^{\mathrm{Mtm}}$. The latter in the ψ-basis has the expression

$$\mathscr{L}_6^{\mathrm{Mtm}} = \mathscr{L}_6^{\mathrm{P-even}} - \delta_2\Lambda^3_{\mathrm{QCD}}\,\bar{\psi}i\gamma_5\tau^3\psi + \mathrm{O}(\mu^2)\,, \tag{2.13}$$

with $\mathscr{L}_6^{\mathrm{P-even}}$ parity-even. Since in the continuum limit (because of parity invariance) one gets $\int d^3x\int d^4y\langle\mathscr{L}_6^{\mathrm{P-even}}(y)V_0^2(x)P^1(0)\rangle|_{\mathrm{cont}}=0$, the condition implied by (2.9) yields $\delta_2=0$, owing to $\int d^3x\int d^4y\langle\bar{\psi}i\gamma_5\tau^3\psi(y)V_0^2(x)P^1(0)\rangle|_{\mathrm{cont}}\neq 0$. It follows from this analysis that the estimate of the critical mass provided by (2.9) is not affected by $\mathrm{O}(a^2)$ effects. These arguments can be generalized to all orders in a and show that $M_{\mathrm{cr}}^{\mathrm{opt}}$ can only display $\mathrm{O}(a^{2p+1})$, $p=0,1,\ldots$ corrections. The latter are determined by constraints, like (2.11), that fix the value of the coefficients δ_{2p+1} in front of $\bar{\psi}i\gamma_5\tau^3\psi$.

2) Standard clover Wilson fermions – The condition for the vanishing of the PCAC mass is

$$\frac{\tilde{\partial}_0\sum_{\vec{x}}\langle A_0^b(\vec{x},t)P^b(0)\rangle}{2\sum_{\vec{x}}\langle P^b(\vec{x},t)P^b(0)\rangle}\Big|_L \equiv m_{\mathrm{PCAC}}\Big|_L = 0 \quad @\mu=0\,, \tag{2.14}$$

which apart from the normalization and a trivial time derivative is exactly eq. (2.9) (though written in the χ-basis) with the only difference that now $\mu=0$. This condition is in practice implemented by looking for the limiting value of m_0 for which $m_{\mathrm{PCAC}}|_L\to 0^+$.

The vanishing of the twisted mass is at the origin of all the differences resulting from the two ways of subtracting the Wilson term. In fact, if μ is set to zero, from the symmetries of the Wilson theory and the associated Symanzik expansion one cannot conclude anymore that δ_2 vanishes. Rather at $\mathrm{O}(a^2)$ eq. (2.14) fixes the value of δ_2 through the condition

$$\langle\pi(\vec{0})|\mathscr{L}_6^{\mathrm{cl}}|\pi(\vec{0})\rangle|_{\mathrm{cont}} = 0\,, \tag{2.15}$$

where $\mathscr{L}_6^{\mathrm{cl}}$ is the full six-dimensional operator of the Symanzik Lagrangian associated to the clover improved Wilson fermion regularization (including the contribution of the two fermion operator $a^2\delta_2\Lambda^3_{\mathrm{QCD}}\bar{\chi}\chi$). In general discretization errors of any order in a will affect the critical mass determination (2.14) (except those linear in a owing to clover improvement).

3. Neutral and charged pion mass in Mtm-LQCD

• *Neutral pion mass* – The quantity of interest for the study of the neutral pion mass is the zero-momentum four-dimensional Fourier transform of the two-point (subtracted) correlator

$$\Gamma_L(p) = a^4\sum_x e^{ipx}\langle P^3(x)P^3(0)\rangle\Big|_L\,. \tag{3.1}$$

It is immediate to recognize that at $p=0$ and in the limit of very small lattice pion mass one gets

$$\Gamma_L(0) = \frac{|G_{\pi^3}|^2}{m^2_{\pi^3}}\Big|_L, \qquad G_{\pi^3}\Big|_L = \langle \Omega | P^3(0) | \pi^3(\vec{0})\rangle\Big|_L . \tag{3.2}$$

From the Symanzik expansion of $\Gamma_L(0)$ through orders a^2 included one can prove [11] that, even in the absence of the clover term, thanks to the optimal choice of the critical mass (see sect. 2), one arrives at the equation

$$\frac{|G_{\pi^3}|^2}{m^2_{\pi^3}}\Big|_L = \frac{|G_{\pi}|^2}{m^2_{\pi}}\Big|_{\rm cont}\Big(1 - a^2 \frac{\langle \pi^3(\vec{0})|\mathscr{L}_6^{\rm Mtm}|\pi^3(\vec{0})\rangle}{m^2_\pi}\Big|_{\rm cont}\Big) + \mathrm{O}(\frac{a^2}{m^2_\pi}), \tag{3.3}$$

where the continuum pion mass has been simply indicated by m_π. Consistently with the results of χPT [14, 15, 4, 16, 17], a simple Taylor resummation leads to the key formulae of this note

$$m^2_{\pi^3}|_L = m^2_\pi + a^2\zeta_\pi + \mathrm{O}(a^2 m^2_\pi, a^4), \qquad \zeta_\pi \equiv \langle \pi^3(\vec{0})|\mathscr{L}_6^{\rm Mtm}|\pi^3(\vec{0})\rangle|_{\rm cont}, \qquad \mathscr{L}_6^{\rm Mtm} = \mathscr{L}_6^{\rm P-even}. \tag{3.4}$$

• *Estimating O(a^2) lattice artifacts in* $m^2_{\pi^3}|_L$ – To estimate the size of the O(a^2) artifacts (3.4) we need to compute ζ_π in the chiral limit. This can be done under the assumption that a sufficiently accurate estimate of ζ_π can be obtained in the vacuum saturation approximation (VSA). Quenched studies show that VSA works quite well for matrix elements of four-fermion operators between pseudo-scalar states [18]. We must then identify the operators in (2.8) that have non-vanishing matrix elements between π^3 states as $m_\pi \to 0$ and give a non-zero contribution in the VSA. An example is $P^3P^3 = (\bar\psi\gamma_5\tau^3\psi)(\bar\psi\gamma_5\tau^3\psi)$ which corresponds in the list (2.8) to the operator $(\bar\chi\chi)(\bar\chi\chi)$. Noticeably one can prove that the matrix elements between π^3 states of the four-fermion operators in $\mathscr{L}_6^{\rm Mtm}$ of interest for our estimate of ζ_π are all proportional to $|\langle\pi^3(\vec{0})|P^3|\Omega\rangle|^2_{\rm cont}$ in the limit $m^2_\pi \to 0$. Thus up to a numerical factor in the VSA we can write $a^2\zeta_\pi \sim a^2|\hat G_\pi|^2$, with $\hat G_\pi$ the continuum (renormalized) analog of the quantity defined in (3.2).

An estimate of $\hat G_\pi$ can be obtained either by a direct lattice measurement of $a^2 G_\pi$ [2] or exploiting the WTI $2\hat m_q\langle\Omega|\hat P^3|\pi^3\rangle|_{\rm cont} = f_\pi m^2_\pi$. Using the results of [2, 11], the two evaluations turn out to be numerically well consistent yielding $|\hat G_\pi|^2 \sim (570\ \mathrm{MeV})^4$, a number $\sim 20-25$ times larger than the typical scale $\Lambda^4_{\rm QCD} \sim (250\ \mathrm{MeV})^4$.

• *Charged pion mass* – Replacing the isospin index 3 in eq. (3.1) with either 1 or 2, one finds

$$m^2_{\pi^\pm}|_L = m^2_\pi + a^2\langle\pi^\pm(\vec{0})|\mathscr{L}_6^{\rm Mtm}|\pi^\pm(\vec{0})\rangle|_{\rm cont} + \mathrm{O}(a^2m^2_\pi, a^4) = m^2_\pi + \mathrm{O}(a^2m^2_\pi, a^4). \tag{3.5}$$

The last equality follows from the invariance of $\mathscr{L}_{\rm Sym}^{\rm Mtm}$ under $\mathrm{SU}(2)_{\rm ob} \equiv (Q_A^1, Q_A^2, Q_V^3)$ and it is in perfect agreement with χPT [4, 16, 17] and the similar result derived in ref. [9]. The lattice square pion mass splitting in Mtm-LQCD can thus be estimated up to terms of O($a^2m^2_\pi, a^4$) with the result

$$\begin{aligned}\Delta m^2_\pi\Big|_L^{\rm Mtm} &= m^2_{\pi^3}\Big|_L - m^2_{\pi^\pm}\Big|_L \sim a^2\zeta_\pi \sim a^2(570\ \mathrm{MeV})^4 \\ &\sim (140\ \mathrm{MeV})^2\ @\ a^{-1} \sim 2.3\,\mathrm{GeV}.\end{aligned} \tag{3.6}$$

This number compares very nicely with the value of the splitting $(180(40)\ \mathrm{MeV})^2$ reported in [2].

• *Where else does ζ_π enter?* – Given the impact we have seen it has on the lattice expression of the neutral pion mass, an important question to ask is where else (besides $m^2_{\pi^3}|_L$ and all related energy factors) can the key parameter ζ_π appear in the Symanzik expansion of lattice quantities. The answer requires a detailed analysis which we have no space to report here [11]. The outcome of it is that to all practical purposes the only interesting place where ζ_π enters is just $m^2_{\pi^3}|_L$.

4. Pion mass and O(a^2) artifacts with standard Wilson fermions

Proceeding as before, one gets for the (clover improved) standard Wilson pions the formula

$$m_\pi^2|_L = m_\pi^2 + a^2\langle\pi(\vec{0})|\mathscr{L}_6^{\rm cl}|\pi(\vec{0})\rangle|_{\rm cont} + {\rm O}(a^2 m_\pi^2, a^3)\,, \tag{4.1}$$

where isospin indexes are understood owing to the SU(2)$_V$ flavour symmetry of the lattice Wilson theory. No O(a) terms are present ($b_{5;SW} = \delta_1 = 0$ in (2.6)) as we are assuming clover improvement.

The particular way in which the critical mass is fixed reflects itself into the form of the Symanzik effective Lagrangian of the lattice theory. Here we will examine two choices. The first corresponds to the standard procedure where the critical mass is determined from eq. (2.14). The second is somewhat more exotic and corresponds to fixing the critical mass by using the determination provided by Mtm-LQCD.

• *The standard way of fixing the critical mass* – At O(a^2) the condition for the vanishing of $m_{\rm PCAC}|_L$ implies the relation (2.15), which fixes δ_2 in terms of other parameters of the theory and in particular of the matrix elements of the four-fermion operators (2.8) between one-pion states.

Given the uniqueness of the Symanzik effective action (eqs. (2.4), (2.5)) for Wilson fermions (close to the chiral limit), a theoretical analysis similar to that we have sketched in sect. 3, together with the numerical estimate of $\hat{G}_\pi$, shows that there are sizable contributions in the r.h.s. of the eq. (2.15). As a result chances are that $\delta_2 \gg 1$ because this coefficient has to compensate for the large value of ζ_π. The consequences of this situation are twofold.

1) No O(a^2) artifacts will affect the value of the lattice pion mass because they are absent in $m_{\rm PCAC}|_L$ thanks to (2.15) and (as it follows by taking the limit $t \to \infty$ in eq. (2.14)) one has

$$m_\pi^2 \frac{f_\pi}{2|G_\pi|}\Big|_L = m_{\rm PCAC}\Big|_L\,. \tag{4.2}$$

2) On the contrary, in other observables, like for instance the mass (square mass) of the baryonic (mesonic) state h, there will appear O(a^2) terms proportional to $\Lambda^3_{\rm QCD}\langle h|\bar{\chi}\chi|h\rangle$ times the possibly large number δ_2.

• *Using the critical mass of Mtm-LQCD* – If the estimate of the critical mass as determined in tm-LQCD is instead employed, since, as recalled above, only odd powers of a come into play, the term $a^2\Lambda^3_{\rm QCD}\bar{\chi}\chi$ will not appear in the Symanzik Lagrangian. As a result one will have $\delta_2 = 0$ and the O(a^2) corrections to the square pion mass in eq. (4.1) will not be zero. But now, no O(a^2) corrections stemming from $a^2\Lambda^3_{\rm QCD}\bar{\chi}\chi$ will affect other observables.

5. Concluding remarks

In this talk we have argued that there are peculiar O(a^2) cutoff effects in LQCD with Wilson fermions which have a dynamical origin related to the mechanism of spontaneous chiral symmetry breaking. In Mtm-LQCD they only affect the neutral pion mass making it substantially different from that of the charged pion. If the standard Wilson fermion regularization is employed, where these discretization errors will show up will depend upon the way the critical mass is determined. With the usual determination, pion masses are free from these lattice artifacts, but the latter will appear in other physical quantities, such as hadronic masses. If, instead, the critical mass as determined in tm-LQCD is employed such O(a^2) terms will only affect the value of the pion mass.

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