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Cutoff effects in maximally twisted LQCD

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The Symanzik analysis of correlators in lattice QCD with maximally twisted Wilson fermions reveals that there exist cutoff artifacts which tend to become large as the quark mass gets small. We show that these effects can be reduced to a negligible level by either introducing the clover term in the action or, as already suggested in the literature, by a suitable choice of the critical mass. Recent simulation data support these conclusions.

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1. Introduction and main results

Although in lattice QCD at maximal twist (Mtm-LQCD) O(a) discretization effects (actually all O(a^{2k+1}), $k \geq 0$ effects) are absent or easily eliminated [1, 2, 3, 4], it turns out that correlators are affected by dangerous artifacts of relative order a^{2k}, $k \geq 1$, which are enhanced by inverse powers of the (squared) pion mass, as the latter becomes small. In fact, when analyzed in terms of the Symanzik expansion, lattice expectation values exhibit, as $m_\pi^2 \to 0$, what we will call "infrared (IR) divergent" cutoff effects with a behaviour of the form

$$\langle O \rangle\Big|_{m_q}^{L} = \langle O \rangle\Big|_{m_q}^{\mathrm{cont}} \Big[1 + \mathrm{O}\Big(\frac{a^{2k}}{(m_\pi^2)^h}\Big)\Big]\,, \quad 2k \geq h \geq 1 \; (k,h \text{ integers})\,, \tag{1.1}$$

where we have assumed that the lattice correlator admits a non-trivial continuum limit. Powers of Λ_{QCD} required to match physical dimensions are often understood in the following.

We shall see that artifacts of the type (1.1) are reduced to terms that are at worst of order $a^2(a^2/m_\pi^2)^{k-1}$, $k \geq 1$, if the action is O(a) improved *à la* Symanzik, or alternatively the critical mass is chosen in some "optimal" way.

The idea that a suitable definition of critical mass exists which can lead to a smoothing out of chirally enhanced lattice artifacts or perhaps be of help in getting improvement was already put forward in the context of chiral perturbation theory (χPT) in refs. [5] and [6], respectively.

An important consequence of our analysis is that the strong (order of magnitude) inequality $m_q > a\Lambda_{\mathrm{QCD}}^2$, invoked in ref. [2] can be relaxed to the weaker relation $m_q > a^2\Lambda_{\mathrm{QCD}}^3$, before large cutoff effects are possibly met while lowering the quark mass at fixed a. The works of refs. [5, 6], and most recently refs. [7, 8], which are based on lattice chiral perturbation theory, lead to essentially equivalent conclusions about cutoff effects in pion quantities in the parameter region $m_q > a^2\Lambda_{\mathrm{QCD}}^3$. They also yield interesting predictions on the possible Wilson fermions phase scenarios [9, 10] and results, when m_q is of order a^2 or smaller.

A thorough discussion on the effectiveness of Mtm-LQCD in killing O(a) discretization errors and the ability of the optimal choice of the critical mass in diminishing the magnitude of lattice artifacts at small quark mass can be found in [11, 12] and in the work of refs. [13, 14]. As for Mtm-LQCD with clover-improved quark action, the promising quenched tests presented some years ago in [15] have been recently extended in [16] down to pion masses of 300 MeV or lower, confirming the absence of large cutoff effects.

The outline of this presentation is as follows. In Section 2 we analyze the form of the Symanzik expansion of lattice correlators beyond O(a) and explain why and how 'IR divergent" cutoff effects arise in this context. In section 3 we discuss two ways of killing all the leading "IR divergent" cutoff effects and we describe the structure of the left-over "IR divergent" terms. Finally in Section 4 we collect some remarks on the peculiar structure of the lattice artifacts affecting lattice hadronic energies and in particular pion masses. Conclusions can be found in Section 5.

2. Symanzik analysis of "IR divergent" cutoff artifacts

The study of cutoff artifacts affecting lattice correlators in Mtm-LQCD can be elegantly made in the language of the Symanzik expansion. A full analysis of cutoff effects beyond O(a) is of course extremely complicated. Fortunately it is not necessary, if we limit the discussion to the terms that are enhanced as the quark mass m_q is decreased.

• *The Symanzik LEEA of Mtm-LQCD* - The expression of the fermionic action of Mtm-LQCD in the physical quark basis is given in [2, 3]. The low energy effective action (LEEA), $S_{\rm Sym}$, of the theory can be conveniently written in the form

$$S_{\rm Sym} = \int d^4y \Big[\mathscr{L}_4(y) + \sum_{k=0}^{\infty} a^{2k+1}\ell_{4+2k+1}(y) + \sum_{k=1}^{\infty} a^{2k}\ell_{4+2k}(y)\Big], \tag{2.1}$$

where $\mathscr{L}_4 = \frac{1}{2g_0^2}{\rm tr}(F\cdot F) + \bar\psi(\gamma\cdot D + m_q)\psi$ is the target continuum QCD Lagrangian. Based on the symmetries of Mtm-LQCD a number of interesting properties enjoyed by $S_{\rm Sym}$ can be proved which are summarized below.

1. Lagrangian densities of even dimension, ℓ_{2k}, in eq. (2.1) are parity-even, while terms of odd dimension, ℓ_{2k+1}, are parity-odd and twisted in iso-spin space. Thus the latter have the quantum numbers of the neutral pion.

2. The term of order a in eq. (2.6), ℓ_5, is given by the linear combination

$$\ell_5 = \delta_{5,SW}\,\ell_{5,SW} + \delta_{5,m^2}\,\ell_{5,m^2} + \delta_{5,e}\,\ell_{5,e}\,, \tag{2.2}$$

$$\ell_{5,SW} = \frac{i}{4}\bar\psi[\sigma\cdot F]i\gamma_5\tau_3\psi\,, \quad \ell_{5,m^2} = m_q^2\bar\psi i\gamma_5\tau_3\psi\,, \quad \ell_{5,e} = \Lambda^2_{\rm QCD}\bar\psi i\gamma_5\tau_3\psi\,, \tag{2.3}$$

where the coefficients $\delta_{5,SW}$, δ_{5,m^2} and $\delta_{5,e}$ are dimensionless quantities, odd in r. The operator $\ell_{5,e}$ arises from the need to describe order a uncertainties entering any non-perturbative determination of the critical mass and goes together with $\ell_{5,SW}$. Both $\ell_{5,SW}$ and $\ell_{5,e}$ could be made to disappear from (2.1) by introducing in the Mtm-LQCD action the SW (clover)-term [17] with the appropriate non-perturbatively determined c_{SW} coefficient [18] and at the same time setting the critical mass to its correspondingly O(a) improved value.

3. Higher order ambiguities ($k \geq 1$) in the critical mass, which will all contribute to $\mathscr{L}_{\rm odd}$, are described by terms proportional to odd powers of a of the kind

$$a^{2k+1}\,\delta_{4+2k+1,e}\,\ell_{4+2k+1,e} = a^{2k+1}\,\delta_{4+2k+1,e}\,(\Lambda_{\rm QCD})^{2k+2}\,\bar\psi i\gamma_5\tau_3\psi\,. \tag{2.4}$$

• *Describing Mtm-LQCD correlators beyond O(a)* - We are interested in the Symanzik description of the lattice artifacts affecting connected expectation values of n-point, multi-local, multiplicative renormalizable (m.r.) and gauge-invariant operators $O(x_1,x_2,\ldots,x_n) = \prod_{j=1}^n O_j(x_j) \equiv O(x)$, $x_1 \neq x_2 \neq \ldots \neq x_n$, which we take to have continuum vacuum quantum numbers, so as to yield a non trivially vanishing result as $a \to 0$. In order to ensure automatic O(a) improvement [2] we shall assume that O is parity invariant in which case its Symanzik expansion will contain only even powers of a. Schematically we write

$$\langle O(x)\rangle\Big|_{m_q}^{L} = \langle[O(x) + \Delta_{\rm odd}O(x) + \Delta_{\rm even}O(x)]e^{-\int d^4y[\mathscr{L}_{\rm odd}(y)+\mathscr{L}_{\rm even}(y)]}\rangle\Big|_{m_q}^{\rm cont}, \tag{2.5}$$

$$\mathscr{L}_{\rm odd} = \sum_{k=0}^{\infty} a^{2k+1}\ell_{4+2k+1}\,, \qquad \mathscr{L}_{\rm even} = \sum_{k=1}^{\infty} a^{2k}\ell_{4+2k}\,. \tag{2.6}$$

The operators $\Delta_{\rm odd}O$ ($\Delta_{\rm even}O$) have an expansion in odd (even) powers of a. They can be viewed as the n-point operators necessary for the on-shell improvement of O [19, 18].

• *Pion poles and "IR divergent" cutoff effects* - Although a complete analysis of all the "IR divergent" cutoff effects is very complicated, the structure of the leading ones ($h = 2k$ in eq. (1.1)) is rather simple, as they only come from continuum correlators where $2k$ factors $\int d^4y\,\mathscr{L}_{\rm odd}(y)$ are inserted. More precisely the leading "IR divergent" cutoff effects are identified on the basis of the following result [4].

In the Symanzik expansion of $\langle O(x)\rangle|^L_{m_q}$ at order a^{2k} ($k \geq 1$) there appear terms with a $2k$-fold pion pole and residues proportional to $|\langle\Omega|\mathscr{L}_{\rm odd}|\pi^0(\mathbf{0})\rangle|^{2k}$, where $\langle\Omega|$ and $|\pi^0(\mathbf{0})\rangle$ denote the vacuum and the one-π^0 state at zero three-momentum, respectively. Putting different factors together, each one of these terms can be seen to be schematically of the form (recall $\mathscr{L}_{\rm odd} = {\rm O}(a)$)

$$\Big[\Big(\frac{1}{m_\pi^2}\Big)^{2k}(\xi_\pi)^{2k}\mathscr{M}[O;\{\pi^0(\mathbf{0})\}_{2k}]\Big]^{\rm cont}_{m_q}, \qquad \xi_\pi = \Big|\langle\Omega|\mathscr{L}_{\rm odd}|\pi^0(\mathbf{0})\rangle\Big|^{\rm cont}_{m_q}, \tag{2.7}$$

where we have generically denoted by $\mathscr{M}[O;\{\pi^0(\mathbf{0})\}_{2k}]$ the $2k$-particle matrix elements of O, with each of the $2k$ particles being a zero three-momentum neutral pion.

Less "IR divergent" cutoff effects (those with h strictly smaller than $2k$ in eq. (1.1)) come either from terms with some extra $\int d^4y\mathscr{L}_{\rm even}(y)$ insertions or from contributions of more complicated intermediate states other than straight zero three-momentum pions or from both. In the first case one gets extra a powers (not all "compensated" by corresponding pion poles), while in the second one loses some $1/m_\pi^2$ factor.

It is important to remark that the appearance of pion poles like the ones in eq. (2.7) in no way means that the lattice correlators diverge as $m_q \to 0$, but only that the Symanzik expansion we have employed appears to have a finite radius of convergence (on this point see the remarks of ref. [8]).

3. Reducing "IR divergent" cutoff artifacts

Recalling that $\mathscr{L}_{\rm odd} = a\,\ell_5 + {\rm O}(a^3)$, the previous analysis shows that at leading order in a the residue of the most severe multiple pion poles is proportional to $|\langle\Omega|\ell_5|\pi^0(\mathbf{0})\rangle|^{2k}$. It is an immediate conclusion then that the leading "IR divergent" cutoff effects can all be eliminated from lattice data if we can either reduce ℓ_5 to only ℓ_{5,m^2} in (2.2) or set ξ_π to zero.

• *Improving the Mtm-LQCD action by the SW-term* - The obvious, field-theoretical way to eliminate ℓ_5 from the LEEA of Mtm-LQCD consists in making use of the O(a) improved action [17, 18, 19]. In this case lattice correlation functions will admit a Symanzik description in terms of a LEEA where the operators $\ell_{5,SW}$ and $\ell_{5,e}$ are absent, and ℓ_5 is simply given by ℓ_{5,m^2}. The left-over contributions arising from the insertions of ℓ_{5,m^2} in $\langle O\rangle|^{\rm cont}_{m_q}$ yield terms that are at most of order $(am_q^2/m_\pi^2)^{2k} \simeq (am_q)^{2k}$, hence negligible in the chiral limit. It is instead the next odd operator in the Symanzik expansion, $a^3\ell_7$, which comes into play.

A detailed combinatoric analysis based on the structure of the non-leading "IR divergent" cutoff effects [4] reveals that the worst lattice artifacts left behind in correlators after the "clover cure" are of the kind $a^2(a^2/m_\pi^2)^{k-1}$, $k \geq 1$.

• *Optimal choice of the critical mass* - The alternative strategy to kill the leading "IR divergent" cutoff effects consists in leaving the Mtm-LQCD action unimproved, but fixing the critical mass through the condition

$$\lim_{m_q\to 0^+}\xi_\pi(m_q) = \lim_{m_q\to 0^+}\Big|\langle\Omega|\mathscr{L}_{\rm odd}|\pi^0(\mathbf{0})\rangle\Big|^{\rm cont}_{m_q} \;=\; 0\,. \tag{3.1}$$

The meaning of (3.1) is simple. It amounts to fix, for $k \geq 0$, the order a^{2k+1} contribution in the counter-term, $M_{\rm cr}\bar\psi^L i\gamma_5\tau_3\psi^L$, so that its vacuum to one-$\pi^0(\mathbf{0})$ matrix element compensates, in the limit $m_q \to 0$, the similar matrix element of the sum of all the other operators making up ℓ_{4+2k+1}.

A concrete procedure designed to implement condition (3.1) in actual simulations was discussed in ref. [4]. It consists in determining the critical mass by requiring the lattice correlator $a^3\sum_{\mathbf{x}}\langle V_0^2(x)P^1(0)\rangle|^L_{m_q}$ $(x_0 \neq 0)$ to vanish in the chiral limit, where $V_0^2 = \bar\psi\gamma_0\frac{\tau_2}{2}\psi$ is the vector current with iso-spin index 2 and $P^1 = \bar\psi\gamma_5\frac{\tau_1}{2}\psi$ the pseudo-scalar density with iso-spin index 1. In the continuum this correlator is zero by parity for any value of m_q. On the lattice the breaking of parity (and iso-spin) due to the twisting of the Wilson term makes it non-vanishing by pure discretization artifacts, which have the form of a power series expansion in ξ_π/m_π^2.

The important conclusion of the analysis presented in [4] is that it is not necessary (nor possible) to really go to $m_q \to 0$. It is enough to have the critical mass determined by the vanishing of the above correlator at the current simulation quark mass, provided we stay in the region $m_q > a^2$. In these conditions we will have $\xi_\pi(m_q) = \mathrm{O}(am_\pi^2)$ with all the leading "IR divergent" cutoff effects reduced to finite O(a^{2k}) terms. As for the subleading ones, a non-trivial diagrammatic analysis shows that the worst of them, left behind after the "optimal critical mass cure", are reduced to only $a^2(a^2/m_\pi^2)^{k-1}$, $k \geq 1$, effects, just like in the case where the clover term is employed.

4. Artifacts on hadronic energies and pion masses

In the language of the Symanzik expansion discretization artifacts on hadronic energies are described by a set of diagrams where at least one among the inserted $\int\mathscr{L}_{\rm odd}$ factors gets necessarily absorbed in a multi-particle matrix element, with the consequence that it is not available for producing a pion pole. As a consequence, at fixed order in a, the most "IR divergent" lattice corrections to continuum hadronic energies contain one overall factor $1/m_\pi^2$ less than the leading "IR divergent" cutoff effects generically affecting correlators. For instance, to order a^2 the difference between lattice and continuum energy of the hadron α_n reads [4]

$$\Delta E_{\alpha_n}(\mathbf{q})\Big|_{a^2} \propto \left[\frac{a^2}{m_\pi^2}\mathrm{Re}\left(\frac{\langle\Omega|\ell_5|\pi^0(\mathbf{0})\rangle\langle\pi^0(\mathbf{0})\alpha_n(\mathbf{q})|\ell_5|\alpha_n(\mathbf{q})\rangle}{2E_{\alpha_n}(\mathbf{q})}\right)+\mathrm{O}(a^2)\right]^{\rm cont}_{m_q}, \tag{4.1}$$

where $\mathrm{O}(a^2)$ denotes "IR finite" corrections. It should be noted that this "IR divergent" lattice artifact is reduced to an "IR finite" correction after anyone of the two "cures" described in Sect. 3.

Specializing the formula (4.1) to the case of pions, one obtains the interesting result that the difference between charged and neutral pion (square) masses is a finite O(a^2) quantity even if the critical mass has not been set to its optimal value or the clover term has been introduced. The reason is that the leading "IR divergent" contributions shown in (4.1) are equal for all pions (as one can prove by standard soft pion theorems [20]), hence cancel in the (square) mass difference. This conclusion is in agreement with detailed results from chiral perturbation theory (see refs. [10] and [5]), as well as with the first numerical estimates of the pion mass splitting in Mtm-LQCD [21].

5. Conclusions

When analyzed in terms of the Symanzik expansion, lattice correlators in Mtm-LQCD show "IR divergent" cutoff effects which tend to become large as the quark mass gets small. Extending the works of refs. [6, 5], we have shown that, not only if the critical mass is chosen in some "optimal" way but also if the action is clover improved, such lattice artifacts are strongly reduced to terms that are at worst of the type $a^2(a^2/m_\pi^2)^{k-1}$, $k \geq 1$. The latter result implies that the continuum extrapolation of lattice data is smooth at least down to values of the quark mass satisfying the order of magnitude inequality $m_q > a^2\Lambda^3_{\rm QCD}$.

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