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Chirally improving Wilson fermions 1. $O(a)$ improvement

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Abstract: We show that it is possible to improve the chiral behaviour and the approach to the continuum limit of correlation functions in lattice QCD with Wilson fermions by taking arithmetic averages of correlators computed in theories regularized with Wilson terms of opposite sign. Improved hadronic masses and matrix elements can be obtained by similarly averaging the corresponding physical quantities separately computed within the two regularizations. To deal with the problems related to the spectrum of the Wilson-Dirac operator, which are particularly worrisome when Wilson and mass terms are such as to give contributions of opposite sign to the real part of the eigenvalues, we propose to use twisted-mass lattice QCD for the actual computation of the quantities taking part to the averages. The choice $\pm\pi/2$ for the twisting angle is particularly interesting, as $O(a)$ improved estimates of physical quantities can be obtained even without averaging data from lattice formulations with opposite Wilson terms. In all cases little or no extra computing power is necessary, compared to simulations with standard Wilson fermions or twisted-mass lattice QCD.

Keywords: Lattice Gauge Field Theories, Kaon Physics, Lattice QCD.

Contents

1. Introduction

The two major limitations of the standard Wilson formulation of lattice QCD (LQCD) [1] are related to the non-negligible magnitude of the systematic errors associated to discretization effects and the complicated pattern of operator mixing induced by the explicit breaking of chiral symmetry due to the presence of the Wilson term in the lattice action [2]–[4]. Consequently a lot of effort has gone in the direction of reducing errors related to the finiteness of the lattice spacing, a, with the full implementation of the Symanzik program [5] up to $O(a)$ corrections [6]–[10] and in developing formulations in which chiral symmetry is exact at the level of the regularized action [11]–[14].

Elimination of $O(a)$ effects can be in principle fully achieved. The standard approach developed in refs. [6]–[10] requires, besides a suitable improvement of operators, the introduction in the standard Wilson LQCD action of the so-called Sheikholeslami-Wohlert (SW) term,

$$S_{\rm SW}^{\rm L} = a^5 c_{\rm SW}(g_0^2) \sum_x \bar\psi(x) \frac{i}{4} \sigma_{\mu\nu} P_{\mu\nu}(x) \psi(x) \,, \tag{1.1}$$

with an appropriate value of the coefficient function $c_{\rm SW}(g_0^2)$ depending on the detailed form of the pure gauge action and Wilson term.[1] All the above modifications, particularly in the unquenched case, make $O(a)$ improved computations significantly more CPU-time demanding than standard Wilson simulations. This is even more so if the evaluation of off-shell or gauge non-invariant correlators is attempted [10].

[1] In eq. (1.1) $P_{\mu\nu}$ is any lattice discretization of the gauge field strength [15], g_0 is the bare gauge coupling and we define $\sigma_{\mu\nu} = i[\gamma_\mu, \gamma_\nu]/2$, with $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ and $\gamma_\mu^\dagger = \gamma_\mu$.

Fully chiral invariant lattice actions have been also constructed [12]–[14], where the Ginsparg-Wilson relation [11] is exactly implemented and a first exploration of their numerical potentiality has been carried out [16]–[18]. Overlap, domain-wall and fixed-point fermions have been put at work with rather encouraging results, though the extra computational effort required with respect to the standard Wilson case is in most cases very large. Of course this comparison is not totally fair because the quality of data produced with fermions obeying the Ginsparg-Wilson relation looks superior to that usually obtainable with standard Wilson fermions.

If one does not want to make use of chirally invariant fermions, because of their relatively heavy computational cost, a nice alternative is to use twisted-mass lattice QCD (tm-LQCD) [19, 20], which represents a cheap but effective solution to the problem of exceptional configurations occurring in quenched (or partially quenched) simulations. Recently it has been shown, in fact, that tm-LQCD can be judiciously used to alleviate both the numerical difficulties associated to $O(a)$ discretization errors [21, 22] and the mixing problem of Wilson fermions in the calculation of B_K and the CP-conserving $\Delta S = 1$ weak matrix elements [19, 23, 24].

The present one is the first of two companion papers in which we propose a simple strategy to get from simulations employing Wilson fermions (or rather, as we shall see, twisted Wilson fermions) lattice data that are free of $O(a)$ discretization effects and have a somewhat smoother and more chiral behaviour near the continuum limit than data obtained in unimproved standard Wilson or tm-LQCD simulations.

In this paper we show that, if quarks are arranged in $\mathrm{SU}(2)_\mathrm{f}$ flavour doublets, $O(a)$ discretization effects are absent from the average of correlators (Wilson average, WA) computed with lattice actions having Wilson terms of opposite sign and a common value of the subtracted (unrenormalized) lattice quark mass

$$m_q = M_0 - M_{\mathrm{cr}}\,, \tag{1.2}$$

where M_0 is the bare mass. For short in the following we will occasionally call m_q the "excess" quark mass.

Absence of $O(a)$ discretization errors in WA's is proved by referring to the Symanzik expansion of (connected, on-shell) lattice correlators in terms of continuum Green functions and exploiting the relations derived by matching the "$\mathcal{R}_5$-parity" of lattice correlators under the transformation

$$\mathcal{R}_5 : \begin{cases} \psi \to \psi' = \gamma_5 \psi \\ \bar\psi \to \bar\psi' = -\bar\psi\gamma_5 \end{cases} \tag{1.3}$$

to the $\mathcal{R}_5$-parities of the related continuum Green functions. $\mathcal{R}_5$ is an element of the chiral $\mathrm{SU}(2)_L \otimes \mathrm{SU}(2)_R$ group, for it can be expressed as the product of the following three transformations $u_V^{(1)}(\pi) = \exp(i\pi\tau_1/2)$, $u_V^{(2)}(\pi) = \exp(i\pi\tau_2/2)$, $u_A^{(3)}(\pi) = \exp(i\pi\gamma_5\tau_3/2)$, with τ_1, τ_2, τ_3 the Pauli matrices. Obviously $[\mathcal{R}_5]^2 = \mathbb{1}$.

The improvement of WA's is the result of the use of simple dimensional and symmetry considerations combined with certain algebraic identities holding between pairs of correlators computed with opposite signs of M_0 and r. These identities come from a generalized spurion analysis, which in turn follows from the fact that the lattice fermionic action is left invariant if the field transformation (1.3) is accompanied by a simultaneous change of sign of M_0 and the coefficient, r, sitting in front of the Wilson term. From these considerations one can prove that the Symanzik coefficients necessary to match lattice correlators to the continuum ones have such properties under $r \to -r$ that all $O(a)$ corrections to the continuum result cancel in WA's.

An important point to stress is that, in order for the formal counting of powers of a yielded by the relevant Symanzik expansion to be meaningful, it is necessary that one is dealing with expectation values of multiplicatively renormalizable (m.r.) lattice operators.

The obvious problem with the approach we have described is the existence of real eigenvalues of the massless Wilson-Dirac (WD) operator with magnitude much smaller than the inverse lattice cutoff. For realistic values of the lattice spacing, the existence of such spurious eigenvalues (in particular those that are negative at $m_q = 0$) has been shown to be at the origin of the occurrence of zero modes of the massive ($m_q > 0$) WD operator[2] on the so-called "exceptional" configurations [26, 27]. The problem becomes more severe when the relative sign of the coefficients of Wilson and quark mass terms is such that they give opposite contributions to the real part of the spectrum of the WD operator. The remedy to this situation, which we will for short refer to as the problem of "spurious fermionic modes", is to use tm-LQCD [19, 20]. Fully $O(a)$ improved lattice data for energy levels (hence hadronic masses), matrix elements and renormalization constants can be obtained, without the need of computing anyone of the usual lattice improvement coefficients, if one takes averages of correlators evaluated with tm-LQCD actions having twisted Wilson terms of opposite sign.

The procedure we propose is very flexible as it is based on the freedom of regularizing different flavours with Wilson terms of different chiral phases. Its extension to mass non-degenerate quarks is discussed in ref. [28]. In the second of this series of paper [29] we show that, without loosing $O(a)$ improvement, this freedom can be appropriately exploited to have a real and positive fermionic determinant, while at the same time canceling all finite and power divergent contributions due to mixing with operators of "wrong chirality" (i.e. those due to the breaking of chiral symmetry induced by the presence of the Wilson term in the lattice action) in the calculation of the CP-conserving matrix elements of the effective weak hamiltonian. These results confirm and largely extend arguments given in refs. [19, 24].

The present paper is logically divided in two parts. In the first part (sections 2 and 3) we derive our results momentarily ignoring problems with the spectrum of the WD operator. This key issue will be taken up in the second part (sections 4 to 6) where, after an introduction to tm-LQCD, we prove that with appropriate choices of twisting none of the nice results derived for Wilson fermions is lost. On the contrary, if the special choice $\pm\pi/2$ for the twisting angle is made, simple symmetry considerations imply that many interesting physical quantities can be extracted from lattice data that are automatically $O(a)$ improved with no need of taking any WA.[3]

[2] For a first hint to the existence of such a problem see ref. [25].

[3] We are indebted to M. Della Morte for his precious help in numerical tests concerning the problem with

The detailed plan of the paper is as follows. In section 2, after briefly reviewing the standard Wilson formulation of LQCD, we show that the critical mass, $M_{\rm cr}$, changes sign if the sign in front of the Wilson term is reversed. This is done by providing an argument both in perturbation theory (PT) and in the presence of spontaneous chiral symmetry breaking (SχSB). In section 3 we outline the basic ideas of the present approach by showing that averages of lattice correlators computed in theories with Wilson terms of opposite sign and a common value of m_q are $O(a)$ improved. We also prove that similar averages of hadronic masses, matrix elements and renormalization constants analogously lead to $O(a)$ improved quantities. We present in section 4 a general discussion of tm-LQCD with special attention to the non-singlet Ward-Takahashi identities (WTI's) of the theory. In section 5 the idea of improvement through WA's is extended to tm-LQCD and the partial breaking of parity invariance that occurs in this regularization is carefully analyzed. We show that it is possible to attribute to the eigenstates of the transfer matrix a parity label that in the continuum limit turns out to coincide with the standard parity quantum number. In section 6 we discuss the remarkable simplifications that occur if the choice $\pm\pi/2$ for the twisting angle is made and we prove that many interesting physical quantities are automatically $O(a)$ improved. Conclusions and an outlook of future lines of investigations can be found in section 7. We leave in a number of appendices certain more technical arguments and a detailed discussion of the improvement of the non-singlet axial WTI's for standard Wilson fermions.

2. Wilson fermions and γ_5-chirality

LQCD for one flavour doublet ($N_{\rm f} = 2$) of quarks, as formulated by Wilson [1], is expressed in terms of the (euclidean) partition function

$$Z_{\rm LQCD} = \int \mathcal{D}\mu(\psi,\bar\psi,U)\, e^{-[S^{\rm L}_{\rm YM}(U)+S^{\rm LW}_{\rm F}(\psi,\bar\psi,U)]}\,, \tag{2.1}$$

where $\mathcal{D}\mu(\psi,\bar\psi,U)$ is the functional integration measure, $S^{\rm L}_{\rm YM}(U)$ is any sensible lattice regularization of the Yang-Mills action and

$$\begin{aligned} S^{\rm LW}_{\rm F}(\psi,\bar\psi,U) &= a^4\sum_x\Big[-\frac{1}{2a}\sum_\mu[\bar\psi(x)U_\mu(x)(r-\gamma_\mu)\psi(x+\mu)+ \\ &\qquad + \bar\psi(x+\mu)U^\dagger_\mu(x)(r+\gamma_\mu)\psi(x)] + \bar\psi(x)\left(M_0+\frac{4r}{a}\right)\psi(x)\Big] \\ &\equiv a^4\sum_x \bar\psi(x)\left[\frac{1}{2}\sum_\mu\gamma_\mu(\nabla^\star_\mu+\nabla_\mu) - a\frac{r}{2}\sum_\mu\nabla^\star_\mu\nabla_\mu + M_0\right]\psi(x) \end{aligned} \tag{2.2}$$

is the standard Wilson fermion action. In the last line of eq. (2.2) we have introduced the usual definitions of forward and backward lattice covariant derivatives

$$\begin{aligned} \nabla_\mu\psi(x) &\equiv \frac{1}{a}\left[U_\mu(x)\psi(x+a\hat\mu)-\psi(x)\right] \\ \nabla^*_\mu\psi(x) &\equiv \frac{1}{a}\left[\psi(x)-U^\dagger_\mu(x-a\hat\mu)\psi(x-a\hat\mu)\right]. \end{aligned} \tag{2.3}$$

spurious fermionic modes of the WD operator and the question of $O(a)$ improvement of hadronic masses.

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In all our formulae the sum over flavour indices is understood. In this paper we restrict to the case in which M_0 is taken to be proportional to the unit matrix in flavour space. It is, however, possible to extend the following arguments to encompass the case of non-degenerate quark masses. This will be done in refs. [28, 29].

The piece of the action proportional to r is to the so-called Wilson term. It is an "irrelevant" operator of mass dimension 5, needed to solve the fermion doubling problem. Its presence explicitly breaks the $\mathrm{SU}(2)_L \otimes \mathrm{SU}(2)_R$ chiral symmetry of the (naive discretization of the) fermionic action. The symmetry is only recovered, at tree level, when M_0 and a go to 0. In higher orders of PT powers of the factor a in front of the Wilson term may be compensated by $1/a^p$ divergencies in loops, leading to finite or even divergent r-dependent contributions. This means that the formal chiral properties of continuum QCD are lost: the limit $M_0 \to 0$ does not correspond to the chiral limit and operators naively belonging to different chiral representations mix among themselves. A complicated renormalization procedure is needed in order to recover perturbatively (and non-perturbatively) chiral symmetry in the continuum limit [4].

These are intrinsic problems that do not depend on how fast the continuum is reached. The same kind of problems appears, in fact, in the improved version of LQCD [6, 7, 8, 9], even if, in the limit $a \to 0$, $O(a)$ corrections are absent from lattice estimates of physical quantities.

We are interested in computing expectation values of the type ($x_1 \neq x_2 \neq \ldots \neq x_n$)

$$\langle O(x_1, x_2, \ldots, x_n) \rangle\Big|_{(r,M_0)} = \frac{1}{Z_{\mathrm{LQCD}}} \int \mathcal{D}\mu(\psi, \bar{\psi}, U)\, e^{-[S^{\mathrm{L}}_{\mathrm{YM}} + S^{\mathrm{LW}}_{\mathrm{F}}]}\, O(x_1, x_2, \ldots, x_n)\,, \quad (2.4)$$

with $O(x_1, x_2, \ldots, x_n)$ a gauge invariant, multi-local and m.r. operator built in terms of the fundamental fields of the theory (quarks and gluons). We will also assume that O has in the continuum limit a Lorentz (rather, in euclidean metric, an SO(4)) covariant structure. The subscript (r, M_0) on the l.h.s. of eq. (2.4) means that the expectation value is taken with the specified values of the Wilson parameter, r, and bare quark mass, M_0.[4] Here and in the rest of the paper we will always restrict to connected correlation functions, though this will not be explicitly indicated in our subsequent equations.

The key observation of this work is that under the $\mathcal{R}_5$ transformation (1.3) the fermionic action (2.2) goes into itself, if at the same time we change sign to the Wilson term (i.e. to r) and M_0. In the spirit of the spurion analysis, a quick way of studying the situation is to consider r and M_0 momentarily as fictitious fields and consider the combined transformation

$$\mathcal{R}_5^{\mathrm{sp}} \equiv \mathcal{R}_5 \times [r \to -r] \times [M_0 \to -M_0] \quad (2.5)$$

as a symmetry of the lattice theory. In this situation it is easy to prove that any m.r. operator will be either even or odd under $\mathcal{R}_5^{\mathrm{sp}}$. The argument goes as follows. Given the

[4] Throughout the paper to lighten the notation we will drop, unless necessary for clarity, the dependence upon the bare coupling constant, g_0. Also with a little abuse of notation we will use the same symbol O for the operator on the Hilbert space and the function of the elementary fields that appear under the functional integral.

bare operator, O_B, one can always assume that the latter is either even or odd under $\mathcal{R}_5$, because $[\mathcal{R}_5]^2 = \mathbb{1}$. Since $\mathcal{R}_5^{\rm sp}$ is a spurionic symmetry of the action, the renormalization procedure will necessarily give rise to a m.r. operator, O, which under $\mathcal{R}_5^{\rm sp}$ has exactly the same parity O_B has under $\mathcal{R}_5$. This parity will be denoted in the following as $(-1)^{P_{\mathcal{R}_5}[O]}$ and called the $\mathcal{R}_5$-parity of O, while $P_{\mathcal{R}_5}[O]$ will be referred to as the γ_5-chirality of O.

In general O will be given by a linear combination of bare operators with finite or power divergent coefficients having a parametric dependence on r and M_0. In this linear combination operators that under $\mathcal{R}_5$ have a parity opposite to that of O_B (if any) will necessarily appear multiplied by mixing coefficients odd under $[r \to -r] \times [M_0 \to -M_0]$.

This argument implies that the expectation value of a m.r. operator must satisfy the relation

$$\langle O(x_1, x_2, \ldots, x_n)\rangle\Big|_{(r,M_0)} = (-1)^{P_{\mathcal{R}_5}[O]}\langle O(x_1, x_2, \ldots, x_n)\rangle\Big|_{(-r,-M_0)}, \tag{2.6}$$

where, we recall, the sign inversion of r and M_0 has to be performed both in the action and in the mixing coefficients. This result can be proved by performing the change of fermionic integration variables induced by (1.3) in the functional integral defining the l.h.s. of eq. (2.6).

From this discussion one also concludes that the renormalization constant of O, Z_O, must be even under $r \to -r$ in order for the renormalized operator, $\hat{O} = Z_O O$, to have the same γ_5-chirality as O (and O_B). We will see in section 3.3 how it is possible to extract from lattice data non-perturbative estimates of renormalization constants that are even in r and $O(a)$ improved.

The interest of eq. (2.6) lies in the fact that from it one can prove that discretization effects associated to the presence of the Wilson term in the action, induce in correlators $O(a)$ corrections having well defined properties under $r \to -r$ (r-parity for short). The latter are such that averages of Green functions computed in lattice theories with opposite values of r have a faster approach to the continuum limit and a better chiral behaviour than the two correlators separately.

Ideas in this direction were already put forward in the literature long time ago in the papers of ref. [30, 31, 32].[5]

To give a precise basis to the line of arguments sketched above, it is necessary to start by establishing the r-parity property of $M_{\rm cr}(r)$. Since Wilson's lattice theory (2.1) is invariant under the spurionic transformation $\mathcal{R}_5^{\rm sp}$ (see eq. (2.5)), the mass action counterterm $a^4 \sum_x \bar{\psi}(x) M_{\rm cr}(r)\psi(x)$ must be naturally chosen so as to maintain this spurionic invariance. From this simple but crucial remark, given the definition of $\mathcal{R}_5$, it is immediately concluded that the critical mass must be an odd function of r

$$M_{\rm cr}(-r) = -M_{\rm cr}(r)\,. \tag{2.7}$$

For the reader's convenience, we illustrate how this this key property is born out by the definitions of $M_{\rm cr}$ that are commonly employed either in PT or at the non-perturbative level, where SχSB is expected to take place in the large volume regime.

[5]We thank S. Aoki and S. Sint for having brought these papers to our attention.

To avoid mixing up different issues we will present the whole discussion in this and next section by temporarily ignoring the problems with the spectrum of the WD operator. We will take up this crucial question in the second part of this paper beginning from section 4.

2.1 Critical mass in PT

We start from the formal definition of the lattice quark propagator, Σ^{-1}, in momentum space

$$[\Sigma(p;r,M_0)]^{-1} \equiv a^4 \sum_x e^{ip\cdot x} \langle \psi(0)\bar{\psi}(x)\rangle\Big|_{(r,M_0)} . \tag{2.8}$$

Performing the change of fermionic functional integration variables induced by the transformation (1.3), one gets the lattice identity

$$\Sigma(p;r,M_0) = -\gamma_5 \Sigma(p;-r,-M_0)\gamma_5 . \tag{2.9}$$

In the continuum inspired decomposition (where we ignore obvious logarithmic factors irrelevant for this argument)

$$\Sigma(p;r,M_0) = i\Sigma_1(p^2;r,M_0)\,\not{p} + \Sigma_2(p^2;r,M_0) + \mathrm{O}(a) , \tag{2.10}$$

the critical mass is defined as the value of M_0 which solves the equation

$$\Sigma_2(0;r,M_0) = 0 . \tag{2.11}$$

Introducing the decomposition (2.10) in (2.9), we derive the simple relations

$$\Sigma_1(p^2;r,M_0) = \Sigma_1(p^2;-r,-M_0) \tag{2.12}$$

$$\Sigma_2(p^2;r,M_0) = -\Sigma_2(p^2;-r,-M_0) . \tag{2.13}$$

To any order in perturbation theory Σ_1 and Σ_2 are smooth functions of M_0 and $r \neq 0$, which are defined for arbitrary values of M_0 and $|r| \leq 1$. It follows that, if a certain value of M_0 is a solution of (2.11) for a given r, then $-M_0$ solves the same equation with r replaced by $-r$. In other words, barring unexpected patterns of multiple solutions to eq. (2.11), we recover eq. (2.7), in agreement with the argument given in ref. [31].

2.2 Critical mass beyond PT

In the presence of SχSB $M_{\rm cr}$ can be defined as the value of M_0 at which the pion mass vanishes. This definition is implemented numerically by studying the large $t > 0$ behaviour of the two-point correlator

$$G_\pi(t;r,M_0) = a^3 \sum_{\mathbf{x}} \langle P^b(\mathbf{x},t)P^b(0)\rangle\Big|_{(r,M_0)} , \tag{2.14}$$

where

$$P^b = \bar{\psi}\gamma_5 \frac{\tau_b}{2}\psi \tag{2.15}$$

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is the pseudo-scalar quark density with flavour index b ($b = 1, 2, 3$). Performing in the expectation value (2.14) the change of functional integration variables (1.3), one finds

$$G_\pi(t; r, M_0) = G_\pi(t; -r, -M_0)\,. \tag{2.16}$$

As implied by reflection positivity (see section 2.3 below and appendix B), we assume that the mass, m_π, of the lightest state contributing to (2.16) can be non-perturbatively, equally well defined for positive and negative values of M_0 and for $|r| \leq 1$. Then to comply with the behaviour implied by eq. (2.16) in the $t \to \infty$ limit, we must have

$$m_\pi(-r, -M_0) = m_\pi(r, M_0)\,. \tag{2.17}$$

From the definition of $M_{\rm cr}$ the relation (2.7) again follows.

In deriving this non-perturbative result we have implicitly assumed that, once g_0^2 and r are given, there always exists a *unique* value of M_0 where the pion mass vanishes. Careful analyses of cutoff effects in lattice QCD with Wilson fermions [31, 33] actually suggest that, depending on details of the lattice theory and the value of g_0^2, the mass of the neutral pion can either vanish at two "critical" values of M_0 (with the charged pions being massless for M_0 in the interval between them)[6] or never vanish and just have a minimum at some value of M_0 (in this situation charged pions remain degenerate with the neutral state). In the latter case, the value of M_0 at which m_π is minimal can be defined as $M_{\rm cr}(r)$. This definition satisfies eq. (2.7). In the former case, instead, the two "critical values" of M_0 turn out to differ by an amount that is $O(a^2)$ in the scaling limit.[7] In this case any of the two "critical" values can be chosen as $M_{\rm cr}(r)$: e.g. the larger for $r > 0$ and the smaller for $r < 0$. This choice is consistent with eq. (2.17) and thus with eq. (2.7).

As expected, we find that for the purpose of making the subtracted Wilson term in the action, $\bar\psi[-a(r/2)\sum_\mu \nabla^*_\mu\nabla_\mu + M_{\rm cr}(r)]\psi$, a truly dimension five operator the quantity $M_{\rm cr}(r)$ can always be taken odd in r.

It goes without saying that, if PCAC is used to define $M_{\rm cr}$, an equally good and r-odd determination is obtained (see Appendix A), only differing by $O(a)$ terms from that based on the behaviour of the pion mass, described before.

2.3 A comment on reflection positivity

An important question in the framework of the computational strategy we are proposing is whether reflection positivity [34, 35] remains valid for the Wilson lattice theory in which the sign of r is reversed. Reflection positivity is a crucial property for being able to extract energies and matrix elements from lattice correlators, because it ensures that a consistent hamiltonian formalism can be set up at finite lattice spacing (even though the explicit construction of a transfer matrix may be technically difficult or not available).

It has been shown in refs. [35, 36] that the "link" reflection positivity of the lattice action is a sufficient condition to define a Hilbert space of states with positive metric and

[6] We restrict attention to the branch of the Aoki phase closest to $M_0 = 0$ (see ref. [31, figure 9]).

[7] Such an $O(a^2)$ quantity is in general not odd in r. We thank the referee for drawing our attention to this point.

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prove the existence of a positive, self-adjoint operator that can be viewed as the square of the transfer matrix. We recall that link reflection, as opposed to "site" reflection [37, 38], refers to reflection of lattice points across a time-hyperplane not containing lattice sites.

The standard fermionic Wilson action (2.2) is known to be link reflection positive for all (real) values of g_0^2, M_0 and $|r| \leq 1$ [36]. Actually in refs. [35, 36] a stronger result was proved which implies that even the general tm-LQCD action of eq. (4.1) is link reflection positive for $|r| \leq 1$. This fact is of special relevance for our work, where the problems with the spectrum of the standard WD operator are avoided by making recourse to tm-LQCD (see section 4).

In appendix B for completeness we give some useful definitions and summarize a few results about reflection positivity and lattice transfer matrix.

3. Removing $O(a)$ cutoff effects

In this section we propose a way of extracting $O(a)$ improved estimates of physical quantities from lattice correlation functions, which does not require the knowledge of anyone of the usual improvement coefficients.

Let us consider the expectation value of a gauge invariant, multi-local, m.r. operator which, as we discussed in section 2, without loss of generality can be taken to have a definite γ_5-chirality. In fact, while multi-local operators made out only of bosonic local factors are necessarily eigenstates of $\mathcal{R}_5^{\rm sp}$, the general case of multi-local operators containing also baryonic local factors can be treated by splitting the operator into a $\mathcal{R}_5$-even and a $\mathcal{R}_5$-odd part and applying separately to each of them the arguments we present in the following.

We start by noting that, since $M_{\rm cr}(r)$ is odd in r, the excess quark mass m_q, eq. (1.2), changes sign under $M_0 \to -M_0$ and $r \to -r$. The transformation $\mathcal{R}_5^{\rm sp}$ under which the Wilson action is invariant can then be also written as

$$\mathcal{R}_5^{\rm sp} = \mathcal{R}_5 \times [r \to -r] \times [m_q \to -m_q] \,. \tag{3.1}$$

Correspondingly, the relation (2.6), which expresses the implications of the spurionic symmetry $\mathcal{R}_5^{\rm sp}$ on lattice correlators, takes the form

$$\langle O \rangle \Big|_{(r,m_q)} = (-1)^{P_{\mathcal{R}_5}[O]} \langle O \rangle \Big|_{(-r,-m_q)} \,, \tag{3.2}$$

where, by slightly changing the notation employed in the previous section, we have indicated the parameters that specify the fermionic action by using, besides r, the excess quark mass, $m_q = M_0 - M_{\rm cr}$, instead of the bare mass M_0.

In order to discuss the issue of $O(a)$ improvement we need to make reference to the notion of effective theory introduced by Symanzik and use the related Symanzik expansion of lattice correlators in terms of correlators of the continuum theory [5]. Schematically up to $O(a)$ terms, one can write for the lattice expectation value of a m.r. operator the expansion

$$\langle O \rangle \Big|_{(r,m_q)} = [\zeta_O^O(r) + a m_q \xi_O^O(r)] \langle O \rangle \Big|_{(m_q)}^{\rm cont} + a \sum_\ell (m_q)^{n_\ell} \eta_{O_\ell}^O(r) \langle O_\ell \rangle \Big|_{(m_q)}^{\rm cont} + \mathrm{O}(a^2) \,. \tag{3.3}$$

The label $|^{\rm cont}_{(m_q)}$ in the correlators appearing on the r.h.s. of eq. (3.3) is meant to recall that they are continuum Green functions renormalized at the scale a^{-1}. They are computed employing the continuum QCD action, regularized by using, e.g., a second lattice regularization with lattice spacing much smaller than a. Consistently, the parameter m_q on the r.h.s. is to be interpreted as the continuum value of the quark mass at the subtraction point a^{-1}. Even in the limit of vanishing lattice spacing, the previous equation has a logarithmically divergent a-dependence. This divergency can be disposed of by multiplying both sides of eq. (3.3) by the renormalization constant of the operator O. The coefficients ζ, ξ and η are finite functions of r and g_0^2. All these coefficients are necessary to match the lattice correlator on the l.h.s. to the continuum Green functions on the r.h.s. of (3.3).

The sum over ℓ is extended over all operators, $O_\ell \neq O$, with (mass) dimension ($d[O]$ is the dimension of O)

$$d[O_\ell] = d[O] - n_\ell + 1\,, \tag{3.4}$$

having the same unbroken quantum numbers of O. The obvious positivity of $d[O]$ and $d[O_\ell]$ puts an upper bound, $n_{\rm max}$, to the possible values of $n_\ell \geq 0$. Two types of correlators will contribute to the sum over ℓ: correlators in which products of local operators are inserted and correlators where O is inserted with space-time integrated local densities. The former are related to the improvement of the single local factors making up O, while the latter owe their origin from the need of improving the action [8].

A careful discussion of the structure of the Symanzik expansion will be given in appendix A, where we present a detailed analysis of the improvement of flavour non-singlet axial WTI's.

In the light of eq. (3.2) we want to compare the expansion (3.3) with the similar one obtained after changing sign to r and m_q. To this end we observe that

1. in the r.h.s. of eq. (3.3) m_q appears not only explicitly in some of the factors that multiply the continuum correlators, but, as we have explicitly indicated in the formulae, also through the dependence of the continuum action on m_q;

2. the transformation (1.3) is part of the chiral group and, acting on the continuum action, is equivalent to changing the sign of m_q; since $[\mathcal{R}_5]^2 = \mathbb{1}$, the operators O_ℓ can always be taken to have well defined γ_5-chiralities, $P_{\mathcal{R}_5}[O_\ell]$; consequently their continuum expectation values will have a definite parity under $m_q \to -m_q$, namely

$$\langle O_\ell \rangle\Big|^{\rm cont}_{(m_q)} = (-1)^{P_{\mathcal{R}_5}[O_\ell]} \langle O_\ell \rangle\Big|^{\rm cont}_{(-m_q)}\,. \tag{3.5}$$

Using (3.5), one gets from (3.3)

$$\begin{aligned}\langle O\rangle\Big|_{(-r,-m_q)} &= (-1)^{P_{\mathcal{R}_5}[O]}[\zeta_O^O(-r) - am_q\xi_O^O(-r)]\langle O\rangle\Big|^{\rm cont}_{(m_q)} + \\ &+ a\sum_\ell (-1)^{P_{\mathcal{R}_5}[O_\ell]+n_\ell}(m_q)^{n_\ell}\eta^O_{O_\ell}(-r)\langle O_\ell\rangle\Big|^{\rm cont}_{(m_q)} + \mathrm{O}(a^2)\,. \end{aligned} \tag{3.6}$$

Inserting the expansions (3.3) and (3.6) in eq. (3.2) and equating $O(a^0)$ and $O(a)$ terms, one obtains the relations

$$\zeta_O^O(r) - \zeta_O^O(-r) = 0\,, \tag{3.7}$$

$$\begin{aligned} am_q[\xi_O^O(r) + \xi_O^O(-r)]\langle O\rangle\Big|_{(m_q)}^{\rm cont} + \\ +a\sum_\ell (m_q)^{n_\ell}\Big[\eta_{O_\ell}^O(r) - (-1)^{P_{\mathcal{R}_5}[O]+P_{\mathcal{R}_5}[O_\ell]+n_\ell}\eta_{O_\ell}^O(-r)\Big]\langle O_\ell\rangle\Big|_{(m_q)}^{\rm cont} = 0\,. \end{aligned} \tag{3.8}$$

We now want to show that eqs. (3.7) and (3.8) imply the formula (Wilson average - WA)

$$\langle O\rangle\Big|_{(m_q)}^{WA} \equiv \frac{1}{2}\Big[\langle O\rangle\Big|_{(r,m_q)} + \langle O\rangle\Big|_{(-r,m_q)}\Big] = \zeta_O^O(r)\langle O\rangle\Big|_{(m_q)}^{\rm cont} + \mathrm{O}(a^2)\,. \tag{3.9}$$

We recall again than in the above equation the prescription of changing the sign of r must be extended to the whole r-dependence present in the expectation value, i.e. to the r-dependence of the action and of the mixing coefficients making up O in terms of bare operators.

To prove eq. (3.9) we first observe that from eq. (3.3), by changing only sign to r, one gets

$$\begin{aligned} \langle O\rangle\Big|_{(r,m_q)} + \langle O\rangle\Big|_{(-r,m_q)} &= \Big[\zeta_O^O(r) + \zeta_O^O(-r)\Big]\langle O\rangle\Big|_{(m_q)}^{\rm cont} + \\ &+ a\,m_q\Big[\xi_O^O(r) + \xi_O^O(-r)\Big]\langle O\rangle\Big|_{(m_q)}^{\rm cont} + \\ &+ a\sum_\ell (m_q)^{n_\ell}\Big[\eta_{O_\ell}^O(r) + \eta_{O_\ell}^O(-r)\Big]\langle O_\ell\rangle\Big|_{(m_q)}^{\rm cont} + \mathrm{O}(a^2)\,. \end{aligned} \tag{3.10}$$

In appendix C we prove that simple symmetry considerations imply the validity of the relation

$$P_{\mathcal{R}_5}[O] + P_{\mathcal{R}_5}[O_\ell] + n_\ell = 1 \bmod(2)\,. \tag{3.11}$$

Consequently all $O(a)$ terms on the r.h.s. of eq. (3.10) vanish owing to the relation (3.8), while the $O(a^0)$ terms add up to the desired continuum result thanks to eq. (3.7), thus proving our statement.

It is worth noting that a compact way of summarizing the results obtained above is to say that the Symanzik coefficients ζ are even functions of r, while all the others (ξ and η) are odd. These properties immediately follow from the vanishing of the sum of terms in the last two lines of eq. (3.10) (owing to eqs. (3.8) and (3.11)), thanks to the fact that in each term r and space-time dependences are completely factorized.

Making use of eq. (3.2) in the second term of the formula (3.9), we can rewrite the latter in the equivalent form (mass average — MA)[8]

$$\begin{aligned} \langle O\rangle\Big|_{(m_q)}^{MA} &\equiv \frac{1}{2}\Big[\langle O\rangle\Big|_{(r,m_q)} + (-1)^{P_{\mathcal{R}_5}[O]}\langle O\rangle\Big|_{(r,-m_q)}\Big] \\ &= \zeta_O^O(r)\langle O\rangle\Big|_{(m_q)}^{\rm cont} + \mathrm{O}(a^2)\,, \end{aligned} \tag{3.12}$$

[8]We thank M. Testa for a very useful discussion on this point.

which says that an $O(a)$ improved lattice correlator can be obtained by taking the sum with an appropriate relative sign of the two correlators computed within the same lattice regularization (same value of r) but with opposite sign of the excess quark mass, m_q.

Since, as we have seen, eqs. (3.9) and (3.12) are identical, in the following we will often refer to either one of them as Wilson average.

3.1 Comments

A few observations on the general strategy we have outlined above are in order here. A first remark concerns the key property characterizing the operators to which our method is applicable. Two others have to do with the question of whether $O(a)$ discretization effects in $M_{\rm cr}$ may jeopardize the results we have obtained and the delicate problem of taking the $m_q \to 0$ limit in eqs. (3.9) and (3.12).

3.1.1 Multiplicative renormalizability and improvement

At the beginning of section 3 we restricted our consideration to m.r. (gauge invariant) operators, O. Indeed the Symanzik expansion (3.3), in the way we have written and exploited it, is only valid if O is (apart from a possible logarithmically divergent renormalization factor) a finite operator. If this is not the case, negative powers of the lattice spacing would appear in the r.h.s. of the expansion, together with dreadful terms arising from the interference of $O(a)$ (and higher) discretization effects with power divergencies. In this situation the naive counting of powers of a is not anymore valid and the Symanzik expansion is not immediately useful for our purposes.[9]

3.1.2 $O(a)$ discretization effects in $M_{\rm cr}$

While in PT, to any order in g_0^2, $M_{\rm cr}$ can be defined to an arbitrary accuracy in the lattice spacing, this is not so non-perturbatively. Beyond PT, $M_{\rm cr}$ can be determined, in the presence of SχSB, by looking at the behaviour of the pion masses (as discussed in section 2.2) or, more in general, as the value where the axial currents are conserved (PCAC). In any case the critical mass can only be known up to discretization errors whose magnitude depends on the condition chosen to determine it and the details of its computational implementation. Then an obvious question to ask is whether these ambiguities may invalidate the argument about improvement presented above.

We show in appendix D that, although $M_{\rm cr}$ can only be known with $O(a)$ discretization errors (unless the theory is fully improved à la Symanzik, something which obviously we do not imagine to be doing in the present context), the formulae for Wilson (eq. (3.9)) — or mass (eq. (3.12)) — averages lead to $O(a)$ improvement as claimed above.

3.1.3 The limit $m_q \to 0$

In the presence of SχSB the chiral symmetry is not realized *à la* Wigner and, as the mass goes to zero, the chiral phase of the vacuum is driven by the phase of the quark mass term.

[9] We will take back this question in [29], when dealing with power divergent operators, like the effective weak hamiltonian, and show how one can go around this problem.

The same must be true on the lattice, thus ideally the continuum limit should be taken before letting $m_q \to 0$. As a result, taking the chiral limit is a numerically delicate matter (see also section 5.4.1).[10]

In practice in order to ensure that on the lattice the chiral phase of the vacuum is determined by the quark mass term proportional to m_q, and not by the Wilson term, it is necessary to work with lattice parameters satisfying

$$m_q \Lambda_{\rm QCD}^{-1} \gg a\Lambda_{\rm QCD}\,, \tag{3.13}$$

in the unimproved case, or possibly under the weaker condition

$$m_q \Lambda_{\rm QCD}^{-1} \gg a^2\Lambda_{\rm QCD}^2\,, \tag{3.14}$$

if one is dealing with $O(a)$ improved correlators. When conditions like (3.13) or (3.14) are not fulfilled, renormalized lattice quantities may strongly differ from their continuum limit counterpart, thus resulting of little use in extracting information about the underlying theory.

To analyze the subtleties of taking the limit $m_q \to 0$ in our approach it is convenient to first discuss the non-physical case in which there is no SχSB.

- In the absence of SχSB there would be no problem in setting $m_q = 0$ and from (3.2) one would get
$$\langle O\rangle\Big|_{(r,m_q=0)} = (-1)^{P_{\mathcal{R}_5}[O]}\langle O\rangle\Big|_{(-r,m_q=0)}\,. \tag{3.15}$$
This relation is telling us that expectation values of operators with $P_{\mathcal{R}_5}[O] = 0$ (mod 2) are automatically $O(a)$ improved. Indeed all the operators O_ℓ that are left over after taking the limit $m_q \to 0$ (i.e. those with $n_\ell = 0$) in the Symanzik expansion of O are necessarily $\mathcal{R}_5$-odd (see eq. (C.2) with $d[O_\ell] = d[O] + 1$), hence have a vanishing continuum expectation value. So there are actually no non-zero $O(a)$ contributions in the Symanzik expansion of the lattice expectation value of O if $P_{\mathcal{R}_5}[O] = 0 \pmod 2$. On the other hand for operators having $P_{\mathcal{R}_5}[O] = 1 \pmod 2$ the WA yields a quantity which is identically zero, in agreement with the expected continuum result.

- In the presence of SχSB the chiral phase of the vacuum matters and, since the theory is non-analytic at $m_q = 0$, eq. (3.15) does not make sense anymore, rather the limit $m_q \to 0$ should be approached under the condition (3.13), or (3.14) if correlators are $O(a)$ improved. In this situation a direct analysis of the m_q-dependence of $\langle O\rangle|_{(r,m_q)}$, based on the parities of the continuum expectation values under $m_q \to -m_q$ (see eq. (3.5)), confirms the validity of eq. (3.12).

The remarks of this section suggest that in practice, for each value of g_0^2, the cutoff effects on quantities sensitive to SχSB may become quite large when m_q goes below some threshold value. This threshold value should be determined by numerical experiments and will depend

[10]We wish to thank R. Sommer for drawing our attention to this important point.

in general on the observable under consideration. As a consequence, performing a chiral fit of lattice data obtained at fixed g_0^2 becomes difficult and possibly inappropriate, if data at too small values of m_q are included. The safe region is determined by the order of magnitude inequality (3.13) or rather, for improved quantities, (3.14). It is reassuring to note that for realistic lattice spacings, say $a \leq 0.1\,\mathrm{fm}$, the bound (3.14) is satisfied down to pretty low values of m_q, of the order of 10 Mev.

3.2 Matrix elements and hadronic masses

An immediate consequence of the absence of $O(a)$ discretization effects in Wilson averaged correlators is the observation that improved hadronic masses and matrix elements can be similarly obtained by taking averages of the corresponding quantities, extracted from the individual terms in the l.h.s. of equations like (3.9) (or equivalently (3.12)), i.e. by averaging the values of the masses and matrix elements computed in separate simulations performed with standard Wilson actions having opposite values of r and fixed m_q (or fixed r and opposite values of m_q).

This remark is very important as it yields a simple and practical prescription to extract improved physical quantities from Monte Carlo simulations. It also solves an apparent paradox of the approach we propose.[11] The problem has to do with the observation that different regularizations, as the ones provided by Wilson lattice actions with opposite Wilson terms, will lead at finite a to slightly different values for the masses of intermediate states. Now suppose that we consider the spatially integrated two-point Green function of some local, m.r. (bosonic) operator, Φ_h, with definite γ_5-chirality and the quantum numbers appropriate to create the state h ($|h\rangle$) from the vacuum ($|\Omega\rangle$). We have proved that to get $O(a)$ improved quantities, one has to average correlators computed with opposite values of r. In particular we expect to be able to extract improved masses from the average

$$G_{hh}(t)\Big|_{(m_q)}^{WA} = \frac{1}{2}\Big[G_{hh}(t; r, m_q) + G_{hh}(t; -r, m_q)\Big]\,, \tag{3.16}$$

with

$$G_{hh}(t; r, m_q) = a^3 \sum_{\mathbf{x}} \langle \Phi_h(\mathbf{x}, t)\Phi_h^\dagger(0)\rangle\Big|_{(r,m_q)}\,. \tag{3.17}$$

Here the operator $\Phi_h^\dagger$ is defined in terms of the lattice reflection operator, Θ, appropriate to euclidean metric (see appendix B for details), so as to guarantee the validity of the relation $\langle\alpha|\Phi_h^\dagger|\beta\rangle = \langle\beta|\Phi_h|\alpha\rangle^\star$ for generic states $|\alpha\rangle$ and $|\beta\rangle$.

If we take at finite a the limit $t \to \infty$ of $G_{hh}(t)|_{(m_q)}^{WA}$, we seem to run into a paradox. On the one hand, in fact, as $t \to \infty$ one of the two correlators, namely that in which the lowest lying state has the lighter mass, will dominate over the second. On the other hand, one single correlator is not in general $O(a)$ improved by itself. Moreover at finite lattice spacing it is not obvious that one can extract hadronic masses from the large time behaviour of the Wilson averaged correlator, $G_{hh}(t)|_{(m_q)}^{WA}$, as the latter does not admit a spectral decomposition in the usual sense.

[11] We would like to thank R. Sommer for a useful discussion on this question.

The solution of this problem lies in the remark that for the purpose of getting $O(a)$ improvement of physical quantities via WA's the limits $t \to \infty$ and $a \to 0$ do not really commute. In fact, if we let $|t| \to \infty$ at fixed a, the corrections of order $a|t|$ are no longer small. As a result the expansion in a breaks down and the continuum limit cannot be taken. This simply means that the continuum limit $a \to 0$ must be taken first. This observation, however, is not immediately useful for the purpose of actually extracting improved masses and matrix elements from lattice data.

To see how one should proceed in practice let us fix the attention on the spatial Fourier Transform (FT)

$$G_{hh}(\mathbf{k}, t; \pm r, m_q) = a^3 \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle \Phi_h(\mathbf{x}, t)\Phi_h^\dagger(0)\rangle\Big|_{(\pm r, m_q)} . \tag{3.18}$$

From the general principles of quantum mechanics and the existence of a lattice hamiltonian for any $|r| \leq 1$ (see section 2.3), it follows [34, 35] that the following spectral representation ($t > 0$) must hold

$$G_{hh}(\mathbf{k}, t; \pm r, m_q) = \sum_n \frac{e^{-E_{h,n}(\mathbf{k};\pm r, m_q)t}}{2E_{h,n}(\mathbf{k}; \pm r, m_q)} |R_{h,n}(\mathbf{k}; \pm r, m_q)|^2 , \tag{3.19}$$

where the $E_{h,n}(\mathbf{k}; \pm r, m_q)$'s denote the energies of the (covariantly normalized) states $|h, n, \mathbf{k}\rangle|_{(\pm r, m_q)}$ in the two regularizations we are comparing and

$$R_{h,n}(\mathbf{k}; \pm r, m_q) = \langle \Omega | \Phi_h | h, n, \mathbf{k}\rangle|_{(\pm r, m_q)} . \tag{3.20}$$

For combinations of operators and states such that $R_{h,n}(\mathbf{k}; \pm r, m_q)$ is non-vanishing in the continuum limit, we expect for sufficiently small a

$$E_{h,n}(\mathbf{k}; \pm r, m_q) = E^{\rm cont}_{h,n}(\mathbf{k}, m_q) + \delta^{\pm}_{h,n} , \quad \delta^{\pm}_{h,n} = \mathrm{O}(a) , \tag{3.21}$$

$$|R_{h,n}(\mathbf{k}; \pm r, m_q)|^2 = |\zeta^{\Phi_h}_{\Phi_h}(r)|^2 |R^{\rm cont}_{h,n}(\mathbf{k}, m_q)|^2 (1 + \epsilon^{\pm}_{h,n}) , \quad \epsilon^{\pm}_{h,n} = \mathrm{O}(a) . \tag{3.22}$$

From the absence of $O(a)$ terms in the average

$$G_{hh}(\mathbf{k}, t)\Big|^{WA}_{(m_q)} = \frac{1}{2}\Big[G_{hh}(\mathbf{k}, t; r, m_q) + G_{hh}(\mathbf{k}, t; -r, m_q)\Big] \tag{3.23}$$

and the arbitrariness of t, one gets

$$\delta^{+}_{h,n} + \delta^{-}_{h,n} = \mathrm{O}(a^2) \tag{3.24}$$

$$\epsilon^{+}_{h,n} + \epsilon^{-}_{h,n} = \mathrm{O}(a^2) \tag{3.25}$$

and consequently

$$\frac{1}{2}\Big[E_{h,n}(\mathbf{k}; r, m_q) + [r \to -r]\Big] = E^{\rm cont}_{h,n}(\mathbf{k}, m_q) + \mathrm{O}(a^2) , \tag{3.26}$$

$$\frac{1}{2}\Big[|R_{h,n}(\mathbf{k}; r, m_q)|^2 + [r \to -r]\Big] = |\zeta^{\Phi_h}_{\Phi_h}(r)|^2 |R^{\rm cont}_{h,n}(\mathbf{k}, m_q)|^2 + \mathrm{O}(a^2) . \tag{3.27}$$

The practical recipe suggested by these equations is to first extract energies (hence masses, $E_{h,n}(\mathbf{0};r,m_q) = M_{h,n}(r,m_q)$) and matrix elements separately from the two terms in the r.h.s. of eq. (3.23) and then take the WA of the corresponding quantities to get rid of $O(a)$ cutoff effects.

We show in appendix E that the argument leading to eq. (3.26) directly applies to the energy of baryonic states, with no need of splitting the interpolating operators into $\mathcal{R}_5$-even and -odd parts.

A somewhat more elaborate argument can be made to show that it is possible to take the "square root" of eq. (3.22) before computing the average, thus getting the simpler relations

$$\frac{1}{2}\Big[R_{h,n}(\mathbf{k};r,m_q) + [r\to -r]\Big] = \zeta_{\Phi_h}^{\Phi_h}(r) R_{h,n}^{\rm cont}(\mathbf{k},m_q) + \mathrm{O}(a^2)\,, \tag{3.28}$$

which say that $R_{h,n}(\mathbf{k};r,m_q)$ and $R_{h,n}(\mathbf{k};-r,m_q)$ only differ by $O(a)$ terms that are odd in r.[12]

3.2.1 Generalization to three-point correlators

The above line of arguments can be generalized to encompass the case of three-point correlators. Let us consider the double FT

$$G_{hBh'}(\mathbf{k},t,\mathbf{k}',t';\pm r,m_q) = a^6 \sum_{\mathbf{x},\mathbf{x}'} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{x}'} \langle \Phi_h(\mathbf{x},t) B(0) \Phi_{h'}^\dagger(\mathbf{x}',t')\rangle\Big|_{(\pm r,m_q)}\,, \tag{3.29}$$

where, like Φ_h, also B is a local, m.r. operator. With an obvious extension of the previous notations we can write for the spectral decomposition of $G_{hBh'}$ ($t>0$, $t'<0$)

$$\begin{aligned} G_{hBh'}(\mathbf{k},t,\mathbf{k}',t';\pm r,m_q) &= \sum_{n,n'} \frac{e^{-E_{h,n}(\mathbf{k};\pm r,m_q)t}}{2E_{h,n}(\mathbf{k};\pm r,m_q)} \frac{e^{E_{h',n'}(\mathbf{k}';\pm r,m_q)t'}}{2E_{h',n'}(\mathbf{k}';\pm r,m_q)}\,\cdot \\ &\cdot R_{h,n}(\mathbf{k};\pm r,m_q)\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|_{(\pm r,m_q)} R^\star_{h',n'}(\mathbf{k}';\pm r,m_q)\,. \end{aligned} \tag{3.30}$$

$O(a)$ improvement of the correlator (3.29) via WA, together with eqs. (3.26) and (3.27) (or rather (3.28)), imply the set of relations

$$\frac{1}{2}\Big[\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|_{(r,m_q)} + [r\to -r]\Big] = \zeta_B^B(r)\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|_{(m_q)}^{\rm cont} + \mathrm{O}(a^2)\,. \tag{3.31}$$

Eqs. (3.31) prove that WA's of matrix elements of local operators with definite γ_5-chirality between pairs of states having arbitrary three-momenta are $O(a)$ improved.

3.3 Renormalization constants

In agreement with the general argument about the r-dependence of renormalization constants given in section 2 (below eq. (3.2)), we explicitly show that, in a mass independent renormalization scheme, the lattice renormalization constant, Z_B, of a m.r. local operator, B, can (and should) be defined as an even function of r. Furthermore we prove that Z_B can be determined non-perturbatively with only $O(a^2)$ discretization errors.

[12] If there is only one operator that can create from the vacuum the state $|h,n,\mathbf{k}\rangle|_{(r,m_q)}$, a suitable choice for its phase is sufficient to obtain eq. (3.28). When there are several such operators, consideration of all the related two-point correlators is necessary.

To define the renormalization constant of the m.r. operator, B, let us fix our attention on the correlator

$$G_B(x;r,m_q) = \langle \Phi_B(x) B(0) \rangle\Big|_{(r,m_q)}\,, \tag{3.32}$$

with Φ_B a m.r. operator located at $x \neq 0$, with the same unbroken quantum numbers and $\mathcal{R}_5$-parity as B. Schematically, mimicking the standard continuum construction, one can get a non-perturbative estimate of the lattice renormalization constant of B using the formula

$$Z_B(a\mu,r) \frac{\langle \Phi_B(x) B(0) \rangle\Big|_{(r,0)}}{[\langle \Phi_B(x) \Phi_B(0) \rangle\Big|_{(r,0)}]^{1/2}}\Bigg|_{|x|=\mu^{-1}} = \frac{\langle \Phi_B(x) B(0) \rangle\Big|_{(r,0)}}{[\langle \Phi_B(x) \Phi_B(0) \rangle\Big|_{(r,0)}]^{1/2}}\Bigg|^{\rm tree}_{|x|=\mu^{-1}}\,, \tag{3.33}$$

where μ plays the role of subtraction point. At the cost of introducing some infrared regulator, all correlators in (3.33) are evaluated at $m_q = 0$. This is not in conflict with what we said in section (3.1.3), because the phenomenon of SχSB is not expected to affect in any way the value of renormalization constants.

Eq. (3.33) automatically implies that $Z_B(a\mu, r)$ is even in r, because each correlator in (3.33) is $\mathcal{R}_5$-even. Any other definition of renormalization constant will have to be even in r, otherwise the renormalized lattice operator, $\hat{B} = Z_B B$, could not have the same $\mathcal{R}_5$ (hence chiral) transformation properties as the corresponding continuum operator.

In actual simulations one has to relax the condition $m_q = 0$, unless the Schrödinger functional setup is employed. But one may define at non-vanishing mass a renormalization constant, $Z_B(a\mu, am_q, r)$, still employing a formula like (3.33). To avoid introducing a new symbol, we gave to this determination of the renormalization constant the same name we used before, in view of the fact that $Z_B(a\mu, 0, r) = Z_B(a\mu, r)$. The important point is that $Z_B(a\mu, am_q, r)$ is no longer even in r and near to the continuum limit differs from $Z_B(a\mu, r)$ by $O(am_q)$ terms.

An $O(a)$ improved r-even estimate, $Z_B^{\rm I}$, can be however obtained either from the equation

$$Z_B^{\rm I}(a\mu, am_q, r) \frac{\langle \Phi_B(x) B(0) \rangle\Big|^{WA}_{(m_q)}}{[\langle \Phi_B(x) \Phi_B(0) \rangle\Big|^{WA}_{(m_q)}]^{1/2}}\Bigg|_{|x|=\mu^{-1}} = \frac{\langle \Phi_B(x) B(0) \rangle\Big|^{WA}_{(m_q)}}{[\langle \Phi_B(x) \Phi_B(0) \rangle\Big|^{WA}_{(m_q)}]^{1/2}}\Bigg|^{\rm tree}_{|x|=\mu^{-1}}\,, \tag{3.34}$$

or, as we did in the case of masses and matrix elements, by taking the WA of the unimproved estimates computed with fermionic actions having Wilson terms of opposite signs. In formulae

$$Z_B^{\rm I}(a\mu, am_q, r) = \frac{1}{2}\Big[Z_B(a\mu, am_q, r) + Z_B(a\mu, am_q, -r)\Big] + {\rm O}(a^2)\,. \tag{3.35}$$

The arguments developed in this section apply, in particular, to the renormalization constants of the pseudo-scalar and scalar quark densities, Z_P and Z_{S^0} (we recall that $z_m Z_P^{-1} = Z_{S^0}^{-1}$ [39, 8] is the quark mass renormalization constant, see eq. (A.8) of appendix A), as well as the renormalization constants of the vector and axial vector currents, Z_V and Z_A.

Also the renormalization constant of the gauge coupling, Z_g, is even in r. A simple way of seeing it is to observe that the whole r-dependence of Z_g is through the fermionic determinant, which at $m_q = 0$ is even in r.

Concretely Z_g could be computed by making reference to the quark-antiquark potential, $V_{q\bar{q}}$, using the equations

$$Z_g\left(\frac{a}{d}, r\right) g_0^2 = g_{q\bar{q}}^2\left(\frac{a}{d}, r\right), \tag{3.36}$$

$$\frac{C_F}{4\pi} g_{q\bar{q}}^2\left(\frac{a}{d}, r\right) = \frac{\partial V_{q\bar{q}}(d/a, r)}{\partial d}, \tag{3.37}$$

where $C_F = 4/3$ for the gauge group $\mathrm{SU}(3)_\mathrm{c}$ and $V_{q\bar{q}}$ can be extracted from the expectation value of two Polyakov loops located at spatial distance d (d^{-1} plays the rôle of subtraction point, μ). In a mass independent renormalization scheme, we can go in the chiral limit and observe that the Polyakov loop correlation function is even in r. The same holds for $\partial V_{q\bar{q}}(d/a, r)/\partial d$ and consequently for $Z_g(a/d, r)$. At $m_q \neq 0$ an $O(a)$ improved r-even determination of Z_g can be obtained through an average of the type (3.35).

We close this section by remarking that, in the context of the standard $O(a)$ improvement à la Symanzik, the improvement coefficients c_{SW} [6], b_m and b_g [8, 9] are necessarily odd under $r \to -r$. Similarly odd must be the improvement coefficients of quark bilinears [9, 10, 40]. These results follow from the observation that the structure of $O(a)$ terms in the unimproved Wilson theory is dictated by the spurionic invariance of the lattice Wilson action under $\mathcal{R}_5^{\mathrm{sp}}$. In particular, since these terms must be invariant under $\mathcal{R}_5^{\mathrm{sp}}$, they can only be canceled by similarly $\mathcal{R}_5^{\mathrm{sp}}$ invariant improvement counterterms added to either the action or the operators. To conclude that c_{SW}, b_m, b_g are r-odd, it is thus sufficient to observe that they multiply $O(a)$ improvement terms in the action which are odd under $\mathcal{R}_5 \times (m_q \to -m_q)$. Similarly quark bilinear improvement coefficients are all r-odd, because the $O(a)$ terms they go along with have transformation properties under $\mathcal{R}_5 \times (m_q \to -m_q)$ opposite to that of the quark bilinear in which they appear. This argument can be extended to a generic operator with the result that all improvement coefficients are r-odd.

Actually one can go one step further and make use of this kind of spurion analysis to deduce the r-parity properties of the coefficients of "wrong chirality" mixings. This topic will be central in the discussion of ref. [29].

4. Twisted mass LQCD

In this and the following sections we want to extend the idea of Wilson averaging to tm-LQCD. For completeness and to set our notations, we start by giving a short introduction to tm-LQCD which extends the presentation of ref. [20].

4.1 The action

For the purpose of this paper it is convenient to begin with a slightly more general expression of the lattice regularized action than the ones discussed in refs. [19, 20]. We consider a fermionic action of the form

$$S_{\rm F}^{\rm L-tm}[\psi,\bar\psi,U] = a^4\sum_x \bar\psi(x)\Big[\frac{1}{2}\sum_\mu \gamma_\mu(\nabla^\star_\mu+\nabla_\mu) - a\frac{r}{2}\sum_\mu \nabla^\star_\mu\nabla_\mu \exp(-i\omega_r\gamma_5\tau_3) + \\ + M_0' + M_0''(-i\gamma_5\tau_3)\Big]\psi(x)\,, \tag{4.1}$$

describing an $\mathrm{SU}(2)_{\rm f}$ flavour doublet of mass degenerate quarks.[13] Besides r, three more real parameters, M_0', M_0'' and ω_r, appear in eq. (4.1), though, as we shall see, only two are actually relevant.

As for the question of reflection positivity of tm-LQCD, it was shown in ref. [36] that the most general form of a (link) reflection positive (bilinear) fermionic action is such as to include the expression (4.1) for all values of g_0^2, M_0', M_0'' and $|r|\le 1$ (see appendix B for more details).

The standard Wilson action (in the notations of eq. (2.2)) is recovered setting $\omega_r = 0, M_0''=0$, while tm-LQCD as formulated in [19] is obtained for $\omega_r=0, M_0'=m_0$ and $M_0''=-\mu_q$. The spurionic symmetry of $S_{\rm F}^{\rm L-tm}$ analog of (2.5) takes the form

$$\mathcal{R}_5^{\rm sp} \equiv \mathcal{R}_5\times[r\to -r]\times[M_0'\to -M_0']\times[M_0''\to -M_0'']\,. \tag{4.2}$$

It is immediately seen that under the (non-anomalous) chiral change of variables

$$\begin{cases}\psi(x)\to\psi'(x)=T(\theta)^{-1}\psi(x)\\ \bar\psi(x)\to\bar\psi'(x)=\bar\psi(x)T(\theta)^{-1}\end{cases} \tag{4.3}$$

with

$$T(\theta)=\exp(i\theta\gamma_5\tau_3/2)\,, \tag{4.4}$$

the fermionic action (4.1) transforms as follows

$$S_{\rm F}^{\rm L-tm}[\psi,\bar\psi,U] \longrightarrow a^4\sum_x \bar\psi(x)\Big[\frac{1}{2}\sum_\mu\gamma_\mu(\nabla^\star_\mu+\nabla_\mu) - a\frac{r}{2}\times \\ \times\sum_\mu \nabla^\star_\mu\nabla_\mu\exp[-i(\omega_r+\theta)\gamma_5\tau_3] + M_0'\cos\theta - M_0''\sin\theta + \\ + (M_0''\cos\theta + M_0'\sin\theta)(-i\gamma_5\tau_3)\Big]\psi(x)\,. \tag{4.5}$$

With an eye to the standard expression of the formal continuum Dirac action, one can without loss of generality use this freedom to somewhat simplify the form of the regularized lattice action (4.1). It goes without saying that in computing expectation values of the kind (2.4), the fields in the action as well as those in O must be simultaneously rotated, should one be willing to make use of (4.3).

[13] The case of non-degenerate masses requires some special considerations and will be discussed in refs. [28, 29].

At $M_0' = M_0'' = 0$ the action (4.1) is invariant under the discrete transformation ($x_P = (-\mathbf{x}, t)$)

$$\mathcal{P}_{\omega_r} : \begin{cases} U_0(x) \to U_0(x_P) \qquad U_k(x) \to U_k^\dagger(x_P - a\hat{k}) \quad k = 1,2,3 \\ \psi(x) \to T(\omega_r)\gamma_0 T(\omega_r)^{-1}\psi(x_P) \\ \bar{\psi}(x) \to \bar{\psi}(x_P)T(\omega_r)^{-1}\gamma_0 T(\omega_r) \end{cases} \tag{4.6}$$

and the continuous ones ($b = 1,2,3$, no sum over b)

$$\mathcal{I}^b_{\omega_r}(\theta) : \begin{cases} \psi(x) \to T(\omega_r)\exp(i\theta_b\tau_b/2)T(\omega_r)^{-1}\psi(x) \\ \bar{\psi}(x) \to \bar{\psi}(x)T(\omega_r)^{-1}\exp(-i\theta_b\tau_b/2)T(\omega_r) \end{cases} \tag{4.7}$$

In connection with these formulae we note that $\mathcal{P}_{\omega_r}$ is the "rotated" version of the standard parity operation ($\mathcal{P}_{\omega_r=0} = \mathcal{P}$, see eq. (5.4) below) and that the factors T and T^{-1} in (4.7) cancel if $b = 3$.

The (1-point split) currents associated with the flavour transformations (4.7) are

$$\begin{aligned} J^b_\mu(x) &= \frac{1}{2}\Big[\bar{\psi}(x)\frac{\tau_b}{2}[\gamma_\mu T(\omega_r)^{-2} - r]U_\mu(x)\psi(x+a\hat{\mu}) + \\ &\qquad + \bar{\psi}(x+a\hat{\mu})\frac{\tau_b}{2}[\gamma_\mu T(\omega_r)^{-2} + r]U_\mu^\dagger(x)\psi(x)\Big], \qquad b = 1,2 \end{aligned} \tag{4.8}$$

$$\begin{aligned} J^3_\mu(x) &= \frac{1}{2}\Big[\bar{\psi}(x)\frac{\tau_3}{2}[\gamma_\mu - rT(\omega_r)^{-2}]U_\mu(x)\psi(x+a\hat{\mu}) + \\ &\qquad + \bar{\psi}(x+a\hat{\mu})\frac{\tau_3}{2}[\gamma_\mu + rT(\omega_r)^{-2}]U_\mu^\dagger(x)\psi(x)\Big]. \end{aligned} \tag{4.9}$$

Of course J^3_μ is a vector current, which is conserved even when the condition $M_0' = M_0'' = 0$ is not fulfilled. The other two currents are mixtures of vector and axial currents with flavour indices 1 and/or 2, whose relative magnitude depends on the value of the angle ω_r. We will discuss in section 4.2 the structure of the non-singlet WTI's of tm-LQCD.

The action (4.1) is also invariant under charge conjugation

$$\mathcal{C} : \begin{cases} U_\mu(x) \to U_\mu^*(x) \\ \psi(x) \to i\gamma_0\gamma_2\bar{\psi}^T(x) \\ \bar{\psi}(x) \to -\psi^T(x)i\gamma_0\gamma_2 \end{cases} \tag{4.10}$$

and the two discrete transformations

$$\mathcal{P}_F^{1,2} : \begin{cases} U_0(x) \to U_0(x_P) \qquad U_k(x) \to U_k^\dagger(x_P - a\hat{k}) \quad k = 1,2,3 \\ \psi(x) \to i\gamma_0\tau_{1,2}\psi(x_P) \\ \bar{\psi}(x) \to -i\bar{\psi}(x_P)\tau_{1,2}\gamma_0 \end{cases} \tag{4.11}$$

Charge conjugation and $\mathcal{P}_F^2$ invariances rule out action counterterms of the form $a^4 \times \sum_x \bar{\psi}(x)\sum_\mu \gamma_\mu(\nabla^*_\mu + \nabla_\mu)\gamma_5\,\tau\,\psi(x)$ with τ any matrix in flavour space. In analogy with the definitions (4.11), we could also introduce the transformation $\mathcal{P}_F^3$. The latter, however, as soon as $\omega_r \neq 0$ or $M_0'' \neq 0$, is not a symmetry of the action (4.1).

The existence, at vanishing M_0' and M_0'', of the symmetries (4.6) and (4.7) implies in particular that radiative corrections can only generate (possibly divergent) mass terms invariant under $\mathcal{P}_{\omega_r}$ and $\mathcal{I}^{1,2}_{\omega_r}$. Consequently the critical mass will contribute the lattice action a single term having the form $\bar{\psi} M_{\rm cr} \exp(-i\omega_r\gamma_5\tau_3)\psi$ with $M_{\rm cr}$ the critical mass of the standard Wilson theory. To prove this statement it is convenient to first rewrite the action (4.1) in the form

$$S_{\rm F}^{\rm L-tm}[\psi,\bar{\psi},U] = a^4 \sum_x \bar{\psi}(x)\Big[\frac{1}{2}\sum_\mu \gamma_\mu(\nabla^\star_\mu + \nabla_\mu) + \Big(-a\frac{r}{2}\sum_\mu \nabla^\star_\mu\nabla_\mu + M_{\rm cr}(r)\Big) \times \\ \times \exp(-i\omega_r\gamma_5\tau_3) + m_q \exp(i\omega_m\gamma_5\tau_3)\Big]\psi(x)\,, \tag{4.12}$$

where both Wilson and mass term are twisted. To get eq. (4.12) from (4.1) we have introduced besides the excess quark mass

$$M_0' - M_{\rm cr}\cos\omega_r = m_q\cos\omega_m\,, \tag{4.13}$$

also the excess twisted quark mass

$$M_0'' - M_{\rm cr}\sin\omega_r = -m_q\sin\omega_m \tag{4.14}$$

with $m_q \geq 0$. Physics is unaffected if we subject (4.12) to the transformation (4.3) with $\theta = -\omega_r$ (change of variables in the functional integral). In the new variables the fermionic action reads

$$S_{\rm F}^{\rm tm-LQCD}[\chi,\bar{\chi},U] = a^4 \sum_x \bar{\chi}(x)\Big[\frac{1}{2}\sum_\mu \gamma_\mu(\nabla^\star_\mu + \nabla_\mu) + \Big(-a\frac{r}{2}\sum_\mu \nabla^\star_\mu\nabla_\mu + M_{\rm cr}(r)\Big) + \\ + m_q \exp[i(\omega_m+\omega_r)\gamma_5\tau_3]\Big]\chi(x)\,. \tag{4.15}$$

We gave it the name $S_{\rm F}^{\rm tm-LQCD}$ because with the identifications

$$m_q\cos(\omega_m+\omega_r) \to m_q \tag{4.16}$$

$$m_q\sin(\omega_m+\omega_r) \to \mu_q \tag{4.17}$$

eq. (4.15) is precisely the tm-LQCD action of ref. [19]. In the form (4.15) it is clear that $M_{\rm cr}$ cannot depend on ω_r (nor on ω_m), because the whole ω_r (and ω_m) dependence is brought by the excess quark mass term. The argument also shows that the value of the critical mass is the same as for the standard Wilson theory.

Going back for a while to the form (4.12) of the tm-LQCD action, it is worth noting that 1) the transformations $\mathcal{P}_{\omega_r}$ and $\mathcal{I}^b_{\omega_r}$, $b=1,2$, are exact symmetries if $m_q = 0$ for any ω_r and, if $\omega_r = -\omega_m$, even when $m_q \neq 0$, provided m_q is a multiple of the identity in flavour space; 2) since the currents given by the eqs. (4.8) and (4.9) are conserved in the massless limit, they do not suffer of any renormalization. We will make use of this observation in section 6.2.

Starting from the action (4.12), we might equally well set the phase of $m_q\bar{\psi}\psi$ to zero by bringing it fully to the Wilson term with a rotation (4.3) of an angle ω_m. Precisely because in this basis the quark mass term has the canonical form, we will call it the "physical" basis. In this basis the action takes the form

$$S_{\rm F}^{\rm L,ph}[\psi_{\rm ph},\bar{\psi}_{\rm ph},U] = a^4\sum_x \bar{\psi}_{\rm ph}(x)\Big[\frac{1}{2}\sum_\mu \gamma_\mu(\nabla^\star_\mu+\nabla_\mu)+\Big(-a\frac{r}{2}\sum_\mu \nabla^\star_\mu\nabla_\mu + M_{\rm cr}(r)\Big)\times$$
$$\times\exp(-i\omega\gamma_5\tau_3)+m_q\Big]\psi_{\rm ph}(x) \qquad (4.18)$$

and, to avoid any possible confusion, the quark fields have been denoted by $\psi_{\rm ph},\bar{\psi}_{\rm ph}$. Eq. (4.18) shows that physics can all be extracted from lattice quantities that only depend on three real parameters, m_q, r and the combination

$$\omega = \omega_m + \omega_r \bmod (2\pi)\,. \qquad (4.19)$$

In particular the fermion determinant, $\mathcal{D}_F$, has the expression

$$\mathcal{D}_F = \det\Big[(D_{\rm W}^{\rm cr}+m_q\cos\omega)^\dagger(D_{\rm W}^{\rm cr}+m_q\cos\omega)+m_q^2\sin^2\omega\Big]\,, \qquad (4.20)$$

$$D_{\rm W}^{\rm cr} = \sum_\mu\Big[\frac{1}{2}\gamma_\mu(\nabla^\star_\mu+\nabla_\mu)-a\frac{r}{2}\nabla^\star_\mu\nabla_\mu\Big]+M_{\rm cr}(r)\,. \qquad (4.21)$$

Eq. (4.20) shows that the fermion determinant is real and positive [41] and no zero modes can occur if $m_q,\omega\neq 0$.

Ending this section, we wish to remark that the tm-LQCD action (4.18) with $|\omega|=\pi/2$ is closely related to the action first proposed by Osterwalder and Seiler (OS) [35].[14] There is, however, a key difference between the OS proposal and tm-LQCD. While in the action of ref. [35] quarks of different flavours are all twisted with the same angle, in tm-LQCD quarks of different flavours appear combined in pairs and the twisting involves a traceless flavour matrix, which for degenerate quarks is conveniently chosen to be τ_3 (besides, tm-LQCD is defined for any twisting angle in the 0-2π range). This specific pairing of quarks is crucial to guarantee the validity of two related properties, which are not satisfied by the OS action [42, 43]: positivity of the fermionic determinant (see eq. (4.20)) and independence from the twisting angle of all the continuum renormalized correlation functions.

The second property can be proved in different ways. One way is to rely on universality arguments [19] and notice that for GW fermions a twist in the mass term of the non-singlet type, like the one we are considering here, can always be let to disappear from the lattice action by a non-anomalous chiral transformation. This is the same as saying that in the continuum limit physics will not be dependent on the value of the twisting angle. An equivalent, perhaps more direct, way is to notice that in tm-LQCD, through a chiral change of fermionic variables in the path integral, one can always bring the whole twist on the "subtracted" Wilson term (see eq. (4.18)). The latter on the basis of symmetry

[14] The use of the OS formulation to solve the problem of exceptional configurations was first suggested in ref. [27].

and power counting arguments can only mix with dimension 5 operators (in particular it cannot mix with $i\mathrm{Tr}[F_{\mu\nu}\tilde{F}_{\mu\nu}]$, because of the different transformation properties under $\mathcal{P}_F^{1,2}$ (eq. (4.11)), thus it appears as a truly irrelevant operator. On the contrary, if one considers a fermion regularization with a flavour singlet twisted Wilson term, like the one proposed in [35], a term proportional to $i\int d^4x\,\mathrm{Tr}[F_{\mu\nu}\tilde{F}_{\mu\nu}](x)$ multiplied by the twisting angle will occur in the effective gauge action. In this situation the corresponding continuum theory will explicitely depend on the twisting angle, with the latter playing the role of the θ-angle of the vacuum [43].

4.2 Non-singlet Ward-Takahashi identities

In this section we want to write down explicitly the expression of the renormalized operators (currents and quark densities) entering the flavour non-singlet WTI's of the theory described by the general fermionic action (4.12), where both the Wilson and the mass term are twisted. The results that we present below can be derived in various equivalent ways. One possibility is to follow the general procedure of ref. [4] and apply it to the present situation. A shortcut is to start from what has been already proved in ref. [19] and derive the required formulae by performing the chiral change of fermionic variables that brings from the standard tm-LQCD action to the action (4.12).

Our formulae are written in terms of (bare) local currents and quark density operators. To make easy contact with the existing literature the relevant renormalization coefficients are expressed in terms of the (r-even) renormalization constants, Z_V, Z_A, Z_P and Z_{S^0}, of the local operators of the standard Wilson theory (see appendix A for notations and definitions).

The renormalized vector and axial currents can be taken to be

$$\hat{V}^1_\mu = Z_{VV}(\omega_r,\omega)\,\bar\psi\gamma_\mu\frac{\tau_1}{2}\psi + Z_{VA}(\omega_r,\omega)\,\bar\psi\gamma_\mu\gamma_5\frac{\tau_2}{2}\psi \tag{4.22}$$

$$\hat{V}^2_\mu = Z_{VV}(\omega_r,\omega)\,\bar\psi\gamma_\mu\frac{\tau_2}{2}\psi - Z_{VA}(\omega_r,\omega)\,\bar\psi\gamma_\mu\gamma_5\frac{\tau_1}{2}\psi \tag{4.23}$$

$$\hat{V}^3_\mu = Z_V\,\bar\psi\gamma_\mu\frac{\tau_3}{2}\psi \tag{4.24}$$

$$\hat{A}^1_\mu = Z_{AA}(\omega_r,\omega)\,\bar\psi\gamma_\mu\gamma_5\frac{\tau_1}{2}\psi + Z_{AV}(\omega_r,\omega)\,\bar\psi\gamma_\mu\frac{\tau_2}{2}\psi \tag{4.25}$$

$$\hat{A}^2_\mu = Z_{AA}(\omega_r,\omega)\,\bar\psi\gamma_\mu\gamma_5\frac{\tau_2}{2}\psi - Z_{AV}(\omega_r,\omega)\,\bar\psi\gamma_\mu\frac{\tau_1}{2}\psi \tag{4.26}$$

$$\hat{A}^3_\mu = Z_A\,\bar\psi\gamma_\mu\gamma_5\frac{\tau_3}{2}\psi\,, \tag{4.27}$$

where Z_{VV}, Z_{VA}, Z_{AV}, Z_{AA} are finite functions of g_0^2, r, ω_r and ω, given by the formulae

$$Z_{VV}(\omega_r,\omega) = \frac{1}{Z_M(\omega)}\Big[Z_V z_m\cos\omega_r\cos\omega + Z_A\sin\omega_r\sin\omega\Big] \tag{4.28}$$

$$Z_{VA}(\omega_r,\omega) = \frac{1}{Z_M(\omega)}\Big[-Z_V z_m\sin\omega_r\cos\omega + Z_A\cos\omega_r\sin\omega\Big] \tag{4.29}$$

$$Z_{AA}(\omega_r,\omega) = \frac{1}{Z_M(\omega)}\Big[Z_A z_m\cos\omega_r\cos\omega + Z_V\sin\omega_r\sin\omega\Big] \tag{4.30}$$

$$Z_{AV}(\omega_r,\omega) = \frac{1}{Z_M(\omega)}\Big[-Z_A z_m\sin\omega_r\cos\omega + Z_V\cos\omega_r\sin\omega\Big]\,. \tag{4.31}$$

In eqs. (4.28) to (4.31) we used the definitions (4.19) and (A.10) and we set

$$Z_M(\omega) = \left[z_m^2 \cos^2\omega + \sin^2\omega\right]^{1/2} . \tag{4.32}$$

With reference to the currents (4.22) to (4.27), the WTI's with the insertion of the renormalized (multi-local) operator $\hat{O}(y)$ $(y \neq x)$ take the expected form $(b = 1, 2, 3)$

$$\langle \partial^\star_\mu \hat{V}^b_\mu(x)\hat{O}(y)\rangle\Big|^{(\omega_r,\omega_m)}_{(r,m_q)} = \mathrm{O}(a) \tag{4.33}$$

$$\langle \partial^\star_\mu \hat{A}^b_\mu(x)\hat{O}(y)\rangle\Big|^{(\omega_r,\omega_m)}_{(r,m_q)} = 2\hat{m}_q \langle \hat{P}^b(x)\hat{O}(y)\rangle\Big|^{(\omega_r,\omega_m)}_{(r,m_q)} + \mathrm{O}(a) \tag{4.34}$$

with

$$\hat{m}_q = Z_M(\omega) Z_P^{-1} m_q\,, \tag{4.35}$$

provided we define in terms of bare quantities the renormalized pseudo-scalar operators, $\hat{P}^b$, to be

$$\hat{P}^b = Z_P\, \bar{\psi}\frac{\tau_b}{2}\gamma_5\psi \qquad b = 1, 2 \tag{4.36}$$

$$\hat{P}^3 = Z_P\left[Z_{PP}(\omega_r,\omega)\bar{\psi}\frac{\tau_3}{2}\gamma_5\psi + Z_{PS^0}(\omega_r,\omega)\frac{i}{2}\bar{\psi}\psi + Z_{P\mathbb{1}}(\omega)\mathbb{1}\frac{i}{a^3}\right] \tag{4.37}$$

with

$$Z_{PP}(\omega_r,\omega) = \frac{1}{Z_M(\omega)}\left[z_m \cos\omega_r \cos\omega + z_m^{-1}\sin\omega_r \sin\omega\right] \tag{4.38}$$

$$Z_{PS^0}(\omega_r,\omega) = \frac{1}{Z_M(\omega)}\left[-z_m \sin\omega_r \cos\omega + z_m^{-1}\cos\omega_r \sin\omega\right] \tag{4.39}$$

$$Z_{P\mathbb{1}}(\omega) = \frac{\sin\omega}{Z_M(\omega)}\rho_P(am_q,\omega)\,. \tag{4.40}$$

Equations from (4.33) to (4.40) need a number of qualifications. First of all, the set of labels $(\omega_r, \omega_m, r, m_q)$ in eqs. (4.33) and (4.34) is there to remind that, if the general lattice action (4.12) is used, the formulae (4.22) to (4.27) for the currents and (4.36), (4.37) for the pseudo-scalar quark densities have to be consequently employed. Secondly, the unusual mixing of $\bar{\psi}\frac{\tau_3}{2}\gamma_5\psi$ with $\bar{\psi}\psi$ and the identity operator is due to the breaking of parity and isospin induced in the action (4.12) by the twisting of the Wilson and mass term. Finally $\rho_P(am_q,\omega)$ is a coefficient function even in ω (and odd in r) which admits a simple polynomial expansion in am_q. Details about the structure of the power divergent subtraction in eq. (4.37) can be found in ref. [46].

In conclusion in this section we have recollected for completeness the general formulae (equations from (4.22) to (4.40)), that can be used to smoothly interpolate between the situation in which the whole twist is carried by the Wilson term (physical quark basis with $\omega_r = \omega$, $\omega_m = 0$, eq. (4.18)) and the tm-LQCD formulation of ref. [19], where $\omega_r = 0$, $\omega_m = \omega$ (eq. (4.15)).

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5. Improved physics from tm-LQCD

To make the discussion of improvement transparent it is convenient to use the form (4.18) of the tm-LQCD action.

With the help of the formalism developed in section 3 it is straightforward to show that WA's of pairs of tm-LQCD correlators computed with opposite values of r and a common value of m_q are free of $O(a)$ corrections at fixed value of ω. Exactly as in the case of the standard Wilson formulation, an identical result is obtained if correlators computed with a fixed value of r but mass terms of opposite sign are combined (mass average, MA) with a relative sign equal to the $\mathcal{R}_5$-parity of the operator O whose expectation value is being computed. Moreover, an analysis of the properties of the (unimproved) lattice correlators and derived quantities under $\omega \to -\omega$ leads to a deeper understanding of the practical consequences of the parity and isospin breaking that occurs at $\omega \neq 0$. From this analysis it turns out that the tm-LQCD action (4.18) with $\omega = \pm\pi/2$ is particularly convenient for physical applications.

5.1 Improving correlators: the general argument

The proof of improvement of WA's (or MA's) of correlators in tm-LQCD exactly parallels the argument presented in section 3, observing that tm-LQCD action (4.18) is invariant under the spurionic transformation (3.1). We only remark for future use that changing the sign of the Wilson term is equivalent to shifting the twisting angle by π. In other words the combined transformation $[r \to -r] \times [\omega \to \omega + \pi]$ leaves the action (4.18) invariant.

The proof proceeds by showing that all the steps we went through in the untwisted, Wilson case remain valid also here. One starts with the Symanzik expansion

$$\langle O\rangle\Big|_{(r,m_q)}^{(\omega)} = [\zeta_O^O(\omega,r) + am_q\xi_O^O(\omega,r)]\langle O\rangle\Big|_{(m_q)}^{\mathrm{cont}} + a\sum_\ell (m_q)^{n_\ell}\eta_{O_\ell}^O(\omega,r)\langle O_\ell\rangle\Big|_{(m_q)}^{\mathrm{cont}} + \mathrm{O}(a^2)\,, \tag{5.1}$$

where, as in section 3, O is a multi-local, m.r. operator. Lattice expectation values in eq. (5.1) are characterized by r, m_q and ω. The parameter ω is kept fixed in all the arguments of this section and the dependence on g_0^2 is always understood. As in the standard Wilson case we are concerned with the r-dependence of the Symanzik coefficients ζ, ξ and η. It should be noted that for generic values of ω more operators, O_ℓ, contribute to the expansion (5.1), as compared to the standard Wilson case. The new operators arise due to the breaking of parity and isospin induced by the chiral twist of the Wilson term in eq. (4.18). This fact, however, does not harm the argument that follows. In fact, as we prove in appendix C, the relation

$$P_{\mathcal{R}_5}[O] + P_{\mathcal{R}_5}[O_\ell] + n_\ell = 1 \bmod (2) \tag{5.2}$$

also holds in the tm-LQCD case, because the symmetry considerations upon which it is based remain valid for the whole set of operators O_ℓ entering the expansion (5.1). Thus all the formulae we proved in section 3 maintain their validity also here at any fixed value of ω. In particular all the results concerning the WA improvement of correlators (eq. (3.9)) and derived quantities (eqs. (3.26), (3.28) and (3.31)), as well as the property of renormalization constants of being even in r and the formula for the $O(a)$ improvement of their determination (section 3.3) remain true in the framework of tm-LQCD.

As in the case of standard Wilson fermions, $O(a)$ improvement via WA is equivalent to the observation that the Symanzik coefficients ζ, ξ and η appearing in the r.h.s. of eq. (5.1) have definite r-parity properties

$$\begin{aligned} \zeta_O^O(\omega,r) &= \zeta_O^O(\omega,-r) = \zeta_O^O(\omega+\pi,r) \\ \xi_O^O(\omega,r) &= -\xi_O^O(\omega,-r) = -\xi_O^O(\omega+\pi,r) \\ \eta_{O_\ell}^O(\omega,r) &= -\eta_{O_\ell}^O(\omega,-r) = -\eta_{O_\ell}^O(\omega+\pi,r)\,. \end{aligned} \tag{5.3}$$

In eqs. (5.3) the second equality of each line follows from the invariance of the action (4.18) under $[r \to -r] \times [\omega \to \omega + \pi]$.

5.2 The ω-dependence of lattice correlators

While working with $\omega \neq 0$ in the action (4.18) solves all the problems related to spurious modes of the WD operator, it implies, as we repeatedly said, a breaking of the parity (and isospin) symmetry. It should be noted, however, that if the parity operation is accompanied by a change of sign of ω, the action remains invariant.

It is, in fact, immediate to verify that under the combined transformation $\mathcal{P} \times (\omega \to -\omega)$, where (remember the definition $x_P = (-\mathbf{x}, t)$)

$$\mathcal{P} : \begin{cases} U_0(x) \to U_0(x_P)\,, \qquad U_k(x) \to U_k^\dagger(x_P - a\hat{k})\,, \qquad k = 1,2,3 \\ \psi_{\rm ph}(x) \to \gamma_0 \psi_{\rm ph}(x_P) \\ \bar{\psi}_{\rm ph}(x) \to \bar{\psi}_{\rm ph}(x_P)\gamma_0 \end{cases} \tag{5.4}$$

is the physical parity of the theory, the action (4.18) goes into itself. In the spirit of spurion analysis this invariance and the further property $[\mathcal{P} \times (\omega \to -\omega)]^2 = \mathbb{1}$ imply that a definite parity label, p, can be attributed to any multi-local operator on the basis of the relation (see also appendix F)

$$\langle O^{(p)}(x_1, x_2, \ldots, x_n)\rangle\Big|_{(r,m_q)}^{(\omega)} = (-1)^p \, \langle O^{(p)}(x_{1P}, x_{2P}, \ldots, x_{nP})\rangle\Big|_{(r,m_q)}^{(-\omega)}\,. \tag{5.5}$$

We remark that the renormalization of tm-LQCD is such as to respect eq. (5.5). In particular, this means that, whenever two bare local operators with opposite transformation properties under (5.4) mix, the relative mixing coefficient must be odd in ω. Examples of this phenomenon are found in eqs. (4.22), (4.23), (4.25), (4.26) and (4.37). Clearly the situation for $\mathcal{P}$ here is identical to the one we had before for $\mathcal{R}_5$. From now on, for short, we will call $(-1)^p$ the formal parity of the operator $O^{(p)}$. Notice that what we are calling formal parity coincides with the parity of the operator when parity invariance is restored ($\omega = 0$ and continuum limit).

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Inserting the appropriate form of Symanzik expansion (5.1) in the two sides of the relation (5.5), one can prove the following parity properties of the Symanzik coefficients under $\omega \to -\omega$

$$\begin{aligned} \zeta_{O^{(p)}}^{O^{(p)}}(\omega, r) &= \zeta_{O^{(p)}}^{O^{(p)}}(-\omega, r) \\ \xi_{O^{(p)}}^{O^{(p)}}(\omega, r) &= \xi_{O^{(p)}}^{O^{(p)}}(-\omega, r) \\ \eta_{O_\ell}^{O^{(p)}}(\omega, r) &= (-1)^{p+p_\ell} \eta_{O_\ell}^{O^{(p)}}(-\omega, r) \,. \end{aligned} \tag{5.6}$$

In the last of the eqs. (5.6) $(-1)^{p_\ell}$ is the physical parity of the operator O_ℓ in the formal continuum theory, defined by the formula (analogous to (5.5))

$$\langle O_\ell(x_1, x_2, \ldots, x_n)\rangle\Big|_{(m_q)}^{\text{cont}} = (-1)^{p_\ell} \langle O_\ell(x_{1P}, x_{2P}, \ldots, x_{nP})\rangle\Big|_{(m_q)}^{\text{cont}} . \tag{5.7}$$

From eqs. (5.6) one can derive a number of interesting consequences concerning the nature and the magnitude of parity violating terms in lattice correlators.

First of all, we observe that at $\omega = 0$ (no twisting), where the physical parity (5.4) is an exact symmetry of the lattice theory, the last of the relations (5.6) implies

$$\eta_{O_\ell}^{O^{(p)}}(0, r) = (-1)^{p+p_\ell} \eta_{O_\ell}^{O^{(p)}}(0, r) \,. \tag{5.8}$$

As expected, we find that only operators, O_ℓ, with the same parity as $O^{(p)}$ ($p_\ell = p \bmod (2)$) can contribute to the Symanzik expansion of the latter, because $p+p_\ell = 1 \bmod (2)$ implies $\eta_{O_\ell}^{O^{(p)}}(0, r) = 0$.

If $\omega \neq 0$, parity is broken and also operators, O_ℓ, with $p_\ell = p + 1 \bmod (2)$ may contribute. These terms are odd in ω and, consistently with universality (they vanish at $\omega = 0$), appear in the Symanzik expansion multiplied by an explicit factor of a.

The results of the whole analysis can be summarized by saying that

1. all physically relevant quantities are contained in the ω-even parts of lattice correlators (see the first of eqs. (5.6)),

2. ω-odd parts of lattice correlators are $O(a)$,

3. contributions from continuum operators with $p_\ell = p + 1 \bmod (2)$ enter lattice correlators only at $O(a)$ or higher.

5.3 The ω-parity of energies and matrix elements

Exploiting the invariance of the tm-LQCD action (4.18) under the $\mathcal{P} \times (\omega \to -\omega)$, it is possible to study the transformation properties under $\omega \to -\omega$ of energy eigenvalues and matrix elements of m.r. local operators between pairs of eigenstates of the transfer matrix. From this analysis it follows that hadron masses and matrix elements between zero momentum eigenstates have definite parity under $\omega \to -\omega$.

Furthermore we show that one can introduce a parity label for the eigenstates of the transfer matrix that turns out to coincide with the usual parity quantum number when parity is restored as a symmetry of the theory, i.e. either at $\omega = 0$ or in the continuum limit.

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This notion is interesting in itself as it allows to control the magnitude of parity violating contributions in lattice correlators and proves to be useful in discussing $O(a)$ improvement in the special case $\omega = \pm\pi/2$.

5.3.1 Matrix elements, energy eigenvalues and masses

It is not difficult to analyse the transformation properties of energy eigenvalues and matrix elements under $\omega \to -\omega$ and prove that masses are ω-even quantities.

Let us start by considering the two-point correlation function

$$G_{hh}(\mathbf{x},t;\omega,r,m_q) = \langle \Phi_h(\mathbf{x},t)\, \Phi_h^\dagger(\mathbf{0},0)\rangle\Big|_{(r,m_q)}^{(\omega)}, \tag{5.9}$$

where Φ_h is a m.r. local operator with definite formal parity, $(-1)^{p_{\Phi_h}}$. The spatial FT of (5.9)

$$G_{hh}(\mathbf{k},t;\omega,r,m_q) = a^3 \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle \Phi_h(\mathbf{x},t)\, \Phi_h^\dagger(\mathbf{0},0)\rangle\Big|_{(r,m_q)}^{(\omega)} \tag{5.10}$$

admits the spectral representation $(t > 0)$

$$G_{hh}(\mathbf{k},t;\omega,r,m_q) = \sum_n \frac{e^{-E_{h,n}(\mathbf{k};\omega,r,m_q)t}}{2E_{h,n}(\mathbf{k};\omega,r,m_q)} |R_{h,n}(\mathbf{k};\omega,r,m_q)|^2\,, \tag{5.11}$$

where

$$R_{h,n}(\mathbf{k};\omega,r,m_q) = \langle\Omega|\Phi_h(\mathbf{0},0)|h,n,\mathbf{k}\rangle\Big|_{(r,m_q)}^{(\omega)} \tag{5.12}$$

and $|h,n,\mathbf{k}\rangle|_{(r,m_q)}^{(\omega)}$ is the eigenstate of the transfer matrix, $\widehat{T}(\omega,r,m_q)$, that belongs to the eigenvalue $E_{h,n}(\mathbf{k};\omega,r,m_q)$, according to the relation [15]

$$\widehat{T}(\omega,r,m_q)|h,n,\mathbf{k}\rangle\Big|_{(r,m_q)}^{(\omega)} = e^{-aE_{h,n}(\mathbf{k};\omega,r,m_q)}|h,n,\mathbf{k}\rangle\Big|_{(r,m_q)}^{(\omega)}. \tag{5.13}$$

The key formula is the relation

$$G_{hh}(\mathbf{k},t;\omega,r,m_q) = G_{hh}(-\mathbf{k},t;-\omega,r,m_q)\,, \tag{5.14}$$

which follows by performing in the functional integral defining the expectation value in (5.10) the change of integration variables induced by the parity transformation (5.4). Eq. (5.14) implies similar relations for energy eigenvalues and the modulus of matrix elements, namely

$$E_{h,n}(\mathbf{k};\omega,r,m_q) \;=\; E_{h,n}(-\mathbf{k};-\omega,r,m_q)\,. \tag{5.15}$$

$$|R_{h,n}(\mathbf{k};\omega,r,m_q)| \;=\; |R_{h,n}(-\mathbf{k};-\omega,r,m_q)|\,, \tag{5.16}$$

At $\mathbf{k} = \mathbf{0}$ eq. (5.15) becomes the announced result about the invariance of masses under a sign change of ω, i.e.

$$M_{h,n}(\omega,r,m_q) = M_{h,n}(-\omega,r,m_q)\,. \tag{5.17}$$

In appendix E we sketch how this result can be extended to the baryonic sector of the theory.

[15] Actually a transfer matrix has been constructed only for $|r| = 1$. For $|r| < 1$ one should make reference to the transfer matrix over two lattice spacings (see appendix B). For simplicity we shall ignore this subtlety in the following.

5.3.2 The parity of the transfer matrix eigenstates

As we already remarked, the symmetry under parity of the (continuum and) standard Wilson theory is replaced in tm-LQCD by the invariance of the action under the transformation $\mathcal{P}^{\rm sp} \equiv \mathcal{P} \times (\omega \to -\omega)$.

Since at $\omega \neq 0$ parity is broken, a natural question to ask is how the parity operator, $\widehat{\mathcal{P}}$, acts on the eigenstates of the transfer matrix. The answer is surprisingly simple and it is contained in the formula

$$\widehat{\mathcal{P}}\,|h,n,\mathbf{k}\rangle\Big|^{(\omega)}_{(r,m_q)} = \eta_{h,n}|h,n,-\mathbf{k}\rangle\Big|^{(-\omega)}_{(r,m_q)}\,, \qquad \eta^2_{h,n} = 1\,. \tag{5.18}$$

This equation, which is proved in a costructive way in appendix F, allows us to uniquely associate a sign, $\eta_{h,n} = \pm 1$, to each eigenstate of the transfer matrix. With a little abuse of language we will simply call it the "parity" of the state, in view of the fact that at $\omega = 0$ the above formula precisely yields the usual definition of parity. Eq. (5.18) implies for the matrix elements of a m.r. operator B with definite formal parity $(-1)^{p_B}$ the important relation

$$\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|^{(\omega)}_{(r,m_q)} = \eta^B_{hn,h'n'}\langle h,n,-\mathbf{k}|B|h',n',-\mathbf{k}'\rangle\Big|^{(-\omega)}_{(r,m_q)}\,, \tag{5.19}$$

where

$$\eta^B_{hn,h'n'} = \eta_{h,n}(-1)^{p_B}\eta_{h',n'}\,. \tag{5.20}$$

Eq. (5.19) confirms that the label we have introduced coincides in value with the usual parity quantum number of the continuum states. In fact, at zero spatial momenta, $\mathbf{k} = \mathbf{k}' = \mathbf{0}$, the matrix element $\langle h,n,\mathbf{0}|B|h',n',\mathbf{0}\rangle|^{(\omega)}_{(r,m_q)}$ is odd in ω if the product $\eta_{h,n}\eta_{h',n'}$ does not match the formal parity of B, thus it vanishes at $\omega = 0$ and by universality it must also do so as $a \to 0$ for generic ω. This means that for sufficiently small a it is $O(a)$ or higher. If instead $\eta^B_{hn,h'n'} = +1$, eq. (5.19) at vanishing three-momenta simply tells us that the matrix elements of B are even in ω, thus not necessarily vanishing in the continuum limit.

5.3.3 Deciding the parity of transfer matrix eigenstates

We want to schematically describe how one can in practice decide what is the parity label, as defined by eq. (5.18), of a given transfer matrix eigenstate.

Let Φ_1 and Φ_2 be two local, m.r. operators with the same unbroken lattice quantum numbers and definite opposite formal parities, $\eta_1 = (-1)^{p_1}$ and $\eta_2 = (-1)^{p_2}$ ($\eta_1 = -\eta_2$) under $\mathcal{P}$. As a concrete example one may think of the currents in eqs. (4.23) and (4.25). Consider the four correlators ($t > 0$)

$$G_{ij}(t;\omega,r,m_q) = a^3\sum_{\mathbf{x}}\langle\Phi_i(\mathbf{x},t)\Phi^\dagger_j(\mathbf{0},0)\rangle\Big|^{(\omega)}_{(r,m_q)} \qquad i,j = 1,2\,. \tag{5.21}$$

Performing the change of fermionic integration variables induced by the transformation (5.4), it is easily proved that the correlators with $i = j$ are even in ω, hence of $O(1)$ in a, while the correlators with $i \neq j$ are odd and by universality of $O(a)$. The spectral decomposition of the correlators G_{ij} reads

$$G_{ij}(t;\omega,r,m_q) = \sum_n \frac{e^{-M_{h,n}(\omega,r,m_q)t}}{2M_{h,n}(\omega,r,m_q)} \langle\Omega|\Phi_i|h,n\rangle\langle h,n|\Phi_j^\dagger|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)}, \tag{5.22}$$

where the states $|h,n\rangle|^{(\omega)}_{(r,m_q)}$ [16] are characterized by the set of conserved quantum numbers h and the integer n which labels them in order of increasing mass.

Consider now the state lying at level n and compare the quantities

$$\Big|\langle h,n|\Phi_1|\Omega\rangle|^{(\omega)}_{(r,m_q)}\Big|^2 \qquad \text{and} \qquad \Big|\langle h,n|\Phi_2|\Omega\rangle|^{(\omega)}_{(r,m_q)}\Big|^2, \tag{5.23}$$

that appear in the spectral expansions (5.22) with $i = j$. Since the cross product $\langle\Omega|\Phi_1|h, n\rangle\langle h,n|\Phi_2^\dagger|\Omega\rangle|^{(\omega)}_{(r,m_q)}$ is necessarily of $O(a)$, as this quantity (or its c.c.) is the n^{th} coefficient in the expansions (5.22) with $i \neq j$, we find that for each eigenstate one must have either

$$\Big|\langle h,n|\Phi_1|\Omega\rangle|^{(\omega)}_{(r,m_q)}\Big|^2 \gg \Big|\langle h,n|\Phi_2|\Omega\rangle|^{(\omega)}_{(r,m_q)}\Big|^2, \tag{5.24}$$

or

$$\Big|\langle h,n|\Phi_2|\Omega\rangle|^{(\omega)}_{(r,m_q)}\Big|^2 \gg \Big|\langle h,n|\Phi_1|\Omega\rangle|^{(\omega)}_{(r,m_q)}\Big|^2. \tag{5.25}$$

The reason is simply that in order for the four correlators (5.21) to have the right "order of magnitude" in a, one has to have either

$$\langle h,n|\Phi_1|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)} = \mathrm{O}(1) \qquad \text{and} \qquad \langle h,n|\Phi_2|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)} = \mathrm{O}(a), \tag{5.26}$$

or

$$\langle h,n|\Phi_1|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)} = \mathrm{O}(a) \qquad \text{and} \qquad \langle h,n|\Phi_2|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)} = \mathrm{O}(1). \tag{5.27}$$

In case the inequality (5.24) holds, with $\eta_{h,n}$ the parity of the state $|h,n\rangle$, we will set

$$\eta_{h,n} = (-1)^{p_1}. \tag{5.28}$$

If viceversa the inequality (5.25) is satisfied, we will set

$$\eta_{h,n} = (-1)^{p_2}. \tag{5.29}$$

Notice that the conditions (5.24) and (5.25) are not difficult to analyze numerically in the scaling region, as one is comparing $O(1)$ with $O(a^2)$ quantities. For the same reason, sufficiently close to the continuum limit the value assigned to $\eta_{h,n}$ will be independent from the choice of the operators Φ_1 and Φ_2 and the details of their lattice discretization. This must be so, if $\eta_{h,n}$ has to be interpreted as the parity label for the state $|h,n\rangle^{(\omega)}_{(r,m_q)}$.

We end with an observation about isospin. Although tm-LQCD breaks isospin, "partial" isospin labels that become conserved quantum numbers in the continuum limit can be attached to transfer matrix eigenstates. This possibility results from the fact that the

[16] We drop the momentum label $\mathbf{k} = \mathbf{0}$ as it is of no relevance for the present argument.

transformations $\mathcal{P}_F^{1,2}$ can be written in the form

$$\mathcal{P}_F^{1,2} = \mathcal{P} \times \mathcal{T}^{1,2}\,, \tag{5.30}$$

where

$$\mathcal{T}^{1,2}: \begin{cases} \psi_{\rm ph} \rightarrow\; e^{i\pi\tau_{1,2}/2}\,\psi_{\rm ph} \\ \\ \bar\psi_{\rm ph} \rightarrow\; \bar\psi_{\rm ph}\,e^{-i\pi\tau_{1,2}/2} \end{cases} \tag{5.31}$$

are discrete isospin transformations.[17] We remark that the combined transformation $\mathcal{T}^{1,2}\times(\omega\to-\omega)$ sends the action (4.18) into itself, just like the product $\mathcal{P}\times(\omega\to-\omega)$ does.

Eq. (5.30) proves our statement. In fact, as soon as a parity has been attributed to a state, definite values for the isospin labels associated to the discrete transformations $\mathcal{T}^{1,2}$ are in turn uniquely determined, as the transformations $\mathcal{P}_F^{1,2}$ are exact symmetries of the action (4.18).

5.4 Some observations about the practical use of tm-LQCD

In this section we want to address two important issues concerning the practical feasibility of numerical simulations within a lattice regularization which, like tm-LQCD, besides chiral symmetry, also breaks parity. The first has to do with the problem of taking the limit $m_q \to 0$ and the second with the question of the scaling behaviour and the numerical importance of contributions with "wrong parity" to lattice correlators.

5.4.1 The limit $m_q \to 0$

The subtleties of the limit $m_q \to 0$ we have emphasized in the case of Wilson fermions show up also in the case of tm-LQCD. Their discussion does not reveal any new feature here and we refer the reader to section 3.1.3. In particular (in the presence of SχSB) to ensure that the chiral phase of the vacuum is determined by the quark mass term proportional to m_q, and not by the twisted Wilson term, it is necessary to work with lattice parameters satisfying the bound (3.13) in the unimproved case, or possibly under the weaker condition (3.14) if one is dealing with $O(a)$ improved correlators. When these order of magnitude conditions are violated, cutoff effects on lattice observables may become numerically large. As discussed in section 3.1.3, it remains the fact that the continuum limit should in principle be taken before the chiral limit.

5.4.2 "Wrong parity" contributions

The discussion of section 5.3 is relevant for the analysis of actual simulation data, where energy eigenvalues and operator matrix elements are evaluated (at finite lattice spacing a, usually for $m_q \neq 0$) by parameterizing lattice expectation values in terms of a spectral representation. As a consequence of the breaking of parity at $\omega \neq 0$, contributions from states with both values of the parity label we have introduced above will appear in the spectral representation.

[17] While the transformations $\mathcal{P}_F^{1,2}$ have the form (4.11) in all the quark bases we have considered, $\mathcal{P}$ and $\mathcal{T}^{1,2}$ have only been reported in the text in the physical basis.

To illustrate the situation in a simple instance and show how one can possibly control these effects, let us consider the typical case of a two-point correlator with operators inserted at zero three-momentum

$$G_{\Phi\Xi}(t;\omega,r,m_q) = a^3 \sum_{\mathbf{x}} \langle \Phi(\mathbf{x},t)\Xi^\dagger(\mathbf{0},0)\rangle\Big|^{(\omega)}_{(r,m_q)} \tag{5.32}$$

with Φ and Ξ m.r. local operators having equal formal parity. From all we said in section 5.3 it should be clear that $G_{\Phi\Xi}$ is even in ω. As for the matrix elements of the local operators between the vacuum and the eigenstates of the transfer matrix, there are two possibilities: 1) if the intermediate state in consideration has the same parity as the operators Φ and Ξ, both matrix elements are ω-even and $O(1)$ in the continuum limit; 2) if the intermediate state has the opposite parity, the two matrix elements are ω-odd and vanish in the continuum limit at least as a. Thus "wrong parity" contributions, necessarily appearing in pairs, lead to $O(a^2)$ (or higher) effects.

Arguments of this kind can be constructed for more complicated ω-even correlators, as for instance the three-point correlators with two of the operators inserted at zero three-momentum. As intermediate state projectors occur in pairs in the spectral representation, contributions from states of "wrong parity" (compared to the naively expected one), necessarily contain an even number of ω-odd matrix elements. Thus again states with "wrong parity" lead to contributions of $O(a^2)$ or higher. When operators are inserted at non-vanishing three-momentum, the situation is governed by eq. (5.19). No new special problems arise due to the breaking of parity. Though a number of specific results could be derived on the subject, we will not pursue any further their discussion in this paper.

Notwithstanding all the control we have on "wrong parity" contributions, one should not forget that, if intermediate states with naively unexpected parity come into play, they cannot be ignored altogether, because some of them may have masses smaller, or not much larger, than the state(s) of interest for the problem under study. Thus, for some range of values of the relevant time separations, the contributions from states with "wrong parity" can be numerically non-negligible. In this situation, if one does not want to end up with intolerably large lattice discretization errors on the final result,[18] a disentangling procedure of the type one is used to in the case of mixings among low-lying and excited states has to be carried out. This task requires the evaluation of several correlators differing among each other by the formal parity of the interpolating operators.

6. A special case: $\omega = \pm\pi/2$

The choice $\omega = \pm\pi/2$ (full twist) in the tm-LQCD action (4.18) is especially worth mentioning, because all quantities that are even under $\omega \to -\omega$ are $O(a)$ improved with no need of any averaging. This result is a consequence of the fact that for the particular value $\omega = \pi/2$ (or $\omega = -\pi/2$) of the twisting angle a sign inversion of the latter is equivalent $(\mathrm{mod}\,(2\pi))$ to a shift by π. This operation is in turn the same as inverting the sign of

[18] Non-large $O(a^2)$ errors on physical quantities extracted from ω-even correlators are however perfectly tolerable.

r. The quantities that are even in ω are hence also even in r. In this situation the two terms entering the Wilson average are just identical, therefore performing the average is unnecessary to get up $O(a)$ improved lattice quantities.

The list of physical quantities that are automatically $O(a)$ improved includes among others the following important physical quantities (see section 5.3)

1. hadronic masses
2. matrix elements $\langle h, n, \mathbf{0}|B|h', n', \mathbf{0}\rangle|^{(\pm\pi/2)}_{(r,m_q)}$, of operators whose formal parity is equal to the product of the parities of the external states.

Actually one can prove more than that. One can prove that taking appropriate linear combinations of quantities computed with opposite values of the external momenta leads to $O(a)$ improved lattice data. This observation is very important as it shows that $O(a)$ improved energies and matrix elements can be obtained from simulations carried out within a single lattice regularization, i.e. without the need to consider averaging over simulations performed with opposite values of r.

6.1 $O(a)$ improvement of energy eigenvalues and matrix elements

The $O(a)$ improvement of averages of energy eigenvalues with opposite momenta at, say, $\omega = \pi/2$ follows from the chain of equalities

$$E_{h,n}\left(\mathbf{k}; \frac{\pi}{2}, r, m_q\right) = E_{h,n}\left(\mathbf{k}; -\frac{\pi}{2}, -r, m_q\right) = E_{h,n}\left(-\mathbf{k}; \frac{\pi}{2}, -r, m_q\right), \tag{6.1}$$

where the first equality is a consequence of the fact that $(\omega \to \omega + \pi) \times (r \to -r) = \mathbb{1}$ and the second of eq. (5.15). The same result could be obtained by using the spurionic symmetry (only valid at $\omega = \pm\pi/2$) $\mathcal{P} \times (r \to -r)$.

At this point it is enough to observe that the WA formula for energy eigenvalues (analogous to the eq. (3.26) valid in the Wilson case)

$$\frac{1}{2}\left[E_{h,n}\left(\mathbf{k}; \frac{\pi}{2}, r, m_q\right) + [r \to -r]\right] = E^{\rm cont}_{h,n}(\mathbf{k}, m_q) + \mathrm{O}(a^2), \tag{6.2}$$

becomes

$$\frac{1}{2}\left[E_{h,n}\left(\mathbf{k}; \frac{\pi}{2}, r, m_q\right) + [\mathbf{k} \to -\mathbf{k}]\right] = E^{\rm cont}_{h,n}(\mathbf{k}, m_q) + \mathrm{O}(a^2). \tag{6.3}$$

Concerning the matrix elements of local operators between pairs of transfer matrix eigenstates at non-zero spatial momenta, we recall that we only have the relation (5.19) from which automatic $O(a)$ improvement does not follow. Although improvement can always be achieved via WA, at the particular value of the twisting angle we are considering in this section there is the possibility of getting $O(a)$ improved lattice matrix elements without the need of carrying out two separate computations. Consider, in fact, the linear combination

$$\langle h, n, \mathbf{k}|B|h', n', \mathbf{k}'\rangle\Big|^{(\omega)\,{\rm sym}}_{(r,m_q)} =$$
$$= \frac{1}{2}\left[\langle h, n, \mathbf{k}|B|h', n', \mathbf{k}'\rangle\Big|^{(\omega)}_{(r,m_q)} + \eta^B_{hn,h'n'}\langle h, n, -\mathbf{k}|B|h', n', -\mathbf{k}'\rangle\Big|^{(\omega)}_{(r,m_q)}\right]. \tag{6.4}$$

Thanks to eq. (5.19), this particular quantity is symmetric in ω, thus $O(a)$ improved at $\omega = \pm\pi/2$. From the extension of eq. (3.31) to the tm-LQCD case with, say, $\omega = \pi/2$ one can make contact with the continuum, obtaining

$$\begin{aligned}\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|^{(\frac{\pi}{2})\,\mathrm{sym}}_{(r,m_q)} &= \frac{1}{2}\Big[\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|^{(\frac{\pi}{2})}_{(r,m_q)} + \langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|^{(\frac{\pi}{2})}_{(-r,m_q)}\Big] \\ &= \zeta_B^B\left(\frac{\pi}{2},r\right)\langle h,n,\mathbf{k}|B|h',n',\mathbf{k}'\rangle\Big|^{\mathrm{cont}}_{(m_q)} + \mathrm{O}(a^2)\,, \end{aligned} \tag{6.5}$$

where in the first equality the spurionic symmetry $\mathcal{P}\times(r\to -r)$ has been used again.

Symanzik expansions too simplify noticeably at $\omega = \pm\pi/2$. Combining eqs. (5.3) with (5.6), one obtains for an operator of formal parity $(-1)^p$ (eq. (5.5)) the set of relations

$$\begin{aligned}\zeta^{O^{(p)}}_{O^{(p)}}\left(\frac{\pi}{2},r\right) &\overset{\text{eq.(5.6)}}{=} \zeta^{O^{(p)}}_{O^{(p)}}\left(-\frac{\pi}{2},r\right) \overset{\text{eq.(5.3)}}{=} \zeta^{O^{(p)}}_{O^{(p)}}\left(\frac{\pi}{2},r\right) \\ \xi^{O^{(p)}}_{O^{(p)}}\left(\frac{\pi}{2},r\right) &\overset{\text{eq.(5.6)}}{=} \xi^{O^{(p)}}_{O^{(p)}}\left(-\frac{\pi}{2},r\right) \overset{\text{eq.(5.3)}}{=} -\xi^{O^{(p)}}_{O^{(p)}}\left(\frac{\pi}{2},r\right) \\ \eta^{O^{(p)}}_{O_\ell}\left(\frac{\pi}{2},r\right) &\overset{\text{eq.(5.6)}}{=} (-1)^{p+p_\ell}\eta^{O^{(p)}}_{O_\ell}\left(-\frac{\pi}{2},r\right) \overset{\text{eq.(5.3)}}{=} -(-1)^{p+p_\ell}\eta^{O^{(p)}}_{O_\ell}\left(\frac{\pi}{2},r\right). \end{aligned} \tag{6.6}$$

From the above equations one concludes that the coefficients $\xi^{O^{(p)}}_{O^{(p)}}(\pm\pi/2)$ are vanishing and that the only operators, O_ℓ, which can contribute to the Symanzik expansion of $\langle O^{(p)}\rangle|_{(\pm\pi/2,m_q)}$ have $p_\ell = p+1$ mod (2), i.e. are those which are multiplied by Symanzik coefficients odd under a sign inversion of the twisting angle. This analysis confirms that the whole mass spectrum and all the matrix elements of local operators that are even under sign inversion of the twisting angle are automatically $O(a)$ improved.

The same results could be obtained by noticing that the action (4.18) with $\omega = \pm\pi/2$ is invariant under the combined transformation[19]

$$\mathcal{R}_5\,\times\,\mathcal{P}\,\times\,(m_q\to -m_q)\,. \tag{6.7}$$

Analogously to what we did in sects. 3 and 5.1, to get eqs. (6.6) it is enough to equate the Symanzik expansions of the two sides of the equation

$$\langle O^{(p)}(x_1,x_2,\ldots,x_n)\rangle\Big|^{(\frac{\pi}{2})}_{(r,m_q)} = (-1)^{P_{\mathcal{R}_5}[O]+p}\langle O^{(p)}(x_{P1},x_{P2},\ldots,x_{Pn})\rangle\Big|^{(\frac{\pi}{2})}_{(r,-m_q)}\,, \tag{6.8}$$

which is obtained performing in the functional integral the change of integration variables induced by the transformation $\mathcal{R}_5\,\times\,\mathcal{P}$. At this point one has to make use of the parity and chirality properties of the continuum theory as well as the relation (3.11).

We wish to end this section by explicitly noting that, remarkably, the critical WD operator appearing in the fermion action (4.18) at $\omega = \pm\pi/2$

$$D^{(\pm\pi/2)}_{\mathrm{cr}} = \frac{1}{2}\sum_\mu\gamma_\mu(\nabla^\star_\mu + \nabla_\mu) \pm i\gamma_5\tau_3\Big(a\frac{r}{2}\sum_\mu\nabla^\star_\mu\nabla_\mu - M_{\mathrm{cr}}(r)\Big) \tag{6.9}$$

is anti-hermitean, so its spectrum is purely imaginary. Consequently the full WD operator cannot have any vanishing eigenvalue as soon as $m_q \neq 0$ (see eq. (4.20) at $\omega = \pm\pi/2$).

[19]This transformation is the product of $\mathcal{R}_5^{\mathrm{sp}}$ (which is valid for any ω) times $\mathcal{P}\times(r\to -r)$ (which only holds at $\omega = \pm\pi/2$).

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6.2 An application: the computation of F_π

As an example of the peculiarity of the choice $\omega = \pm\pi/2$, we wish to discuss the computation of the pion decay constant, F_π. It was already pointed out in refs. [22, 19] that within the fully twisted formulation of LQCD F_π can be obtained from a conserved lattice current (i.e. one with trivial renormalization properties) and without $O(a)$ cutoff effects, provided the lattice action is improved à la Symanzik. Here we restate this result in our notation and show that, in fact, in tm-LQCD with $\omega = \pm\pi/2$, there is no need to improve the action.

In the formal continuum theory F_π is defined by the equation[20]

$$\langle\Omega|\hat{A}_0^1|\pi\rangle\Big|_{(m_q)}^{\rm cont} = m_\pi\sqrt{2}F_\pi\,, \tag{6.10}$$

with $\hat{A}_0^1$ the temporal component of the renormalized axial current, and can be extracted by evaluating at large times, e.g., the ratio ($t > 0$)

$$\frac{e^{m_\pi t/2}}{\sqrt{m_\pi}}\frac{a^3\sum_{\mathbf{x}}\langle\hat{A}_0^1(\mathbf{x},t)P^1(0)\rangle\Big|_{(\frac{\pi}{2},m_q)}}{\sqrt{a^3\sum_{\mathbf{x}}\langle P^1(\mathbf{x},t)P^1(0)\rangle\Big|_{(\frac{\pi}{2},m_q)}}} \stackrel{t\to\infty}{\to} F_\pi\,, \tag{6.11}$$

where P^1 is the pseudo-scalar quark density operator. In (6.11) we did not multiply P^1 by its renormalization constant, because all Z_P factors would anyway drop out in the ratio. The isospin index has been set equal to 1, which corresponds to a charged pion. The reason for this choice is that in this way other contributing intermediate states are substantially heavier than the charged pion, including states with "wrong parity" (see the concluding remark in section 5.4.2).

Among the possible choices for the lattice (discretization of the) axial current to be used in eq. (6.11), the most naive one is to take the current $\hat{A}_\mu^1$ of eq. (4.25), which at $\omega_r = \omega = \pi/2$ simply becomes

$$\hat{A}_\mu^1(x) = Z_V\bar{\psi}_{\rm ph}(x)\frac{\tau_1}{2}\gamma_\mu\gamma_5\psi_{\rm ph}(x)\,. \tag{6.12}$$

The operator $\hat{A}_\mu^1$ has a definite (positive) $\mathcal{R}_5$-parity (in the sense of the definitions (2.6) or (3.2)). At the cost of a preliminary determination of Z_V, an $O(a)$ improved estimate of F_π is then obtained with no need of averaging. We are, in fact, dealing with zero three-momentum correlators, which are even under a sign inversion of the twisting angle (section 5.3.2)).

A remarkable fact about the choice $\pm\pi/2$ is that it is possible to get an $O(a)$ improved estimate of F_π which requires neither Wilson averaging nor the computation of any

[20] Strictly speaking eq. (6.10) is not written in a completely correct way. To comply with eq. (3.5) (and always taking $F_\pi > 0$) a factor equal to the sign of m_q should appear in the r.h.s. As it is, eq. (6.10) is valid for $m_q > 0$, given our conventions concerning the relative sign of the kinetic and mass terms in the fermionic action.

renormalization factor. Let us, in fact, consider the 1-point split current [22, 19]

$$\begin{aligned}\hat{A}^1_\mu(x)\Big|^{1-\mathrm{pt}} &= \frac{1}{2}\Big[\bar\psi_{\rm ph}(x)\frac{\tau_1}{2}\gamma_\mu\gamma_5 U_\mu(x)\psi_{\rm ph}(x+a\hat\mu) + \\ &\quad + \bar\psi_{\rm ph}(x+a\hat\mu)\frac{\tau_1}{2}\gamma_\mu\gamma_5 U^\dagger_\mu(x)\psi_{\rm ph}(x)\Big] + \\ &\quad -\frac{r}{2}\left[\bar\psi_{\rm ph}(x)\frac{\tau_2}{2}U_\mu(x)\psi_{\rm ph}(x+a\hat\mu) - \bar\psi_{\rm ph}(x+a\hat\mu)\frac{\tau_2}{2}U^\dagger_\mu(x)\psi_{\rm ph}(x)\right]. \end{aligned} \tag{6.13}$$

The current (6.13) has similarly to the current (6.12) a definite (positive) $\mathcal{R}_5$-parity. It is obtained from the eq. (4.8) with $b = 2$ by setting $\omega_r = \pi/2$. With this choice the transformation (4.7) is an axial transformation with isospin index equal to 1. Since, as we remarked in section 4.1, this current is exactly conserved at $m_q = 0$, its renormalization constant is equal to 1.

The net result is that with the choice $\omega = \pm\pi/2$ of the twisting angle in the action (4.18) and the use of the (conserved) 1-point split current (6.13) one can get an automatically $O(a)$ improved determination of F_π which furthermore does not require the computation of any renormalization constant. This is certainly a remarkable result, especially if one observes that no problems can occur with spurious fermionic modes, while the required computational effort is minimal.

7. Conclusions and outlook

In this paper we have shown that in LQCD with Wilson fermions it is possible to improve the approach to the continuum limit and the chiral behaviour of correlation functions of gauge invariant m.r. operators by taking arithmetic averages of pairs of correlators computed in theories regularized with Wilson terms of opposite sign and identical values of m_q (Wilson average), or equivalently the appropriate linear combination of the correlators computed in a given regularization but with opposite values of m_q (mass average). Improved hadronic masses and matrix elements can be similarly obtained by taking the Wilson average of the corresponding quantities computed in the two different regularizations, or the appropriate linear combination of quantities computed with opposite values of m_q.

To avoid the problems related to the nature of the spectrum of the WD operator we advocate the use of tm-LQCD for the actual computation of the correlators taking part to the averages. We have shown that all the nice cancellations of $O(a)$ terms that we find in the standard Wilson case extend to tm-LQCD with mass degenerate quark doublets. Moreover, it turns out that, if the tm-LQCD formulation with $|\omega| = \pi/2$ is employed, all hadronic energies and operator matrix elements can be evaluated with no $O(a)$ lattice artifacts and without making recourse to WA's, but taking (appropriate) linear combinations of quantities evaluated with opposite external momenta.

A striking, though still partial, confirmation of the validity of the approach outlined above and of the remarkable properties of tm-LQCD at $|\omega| = \pi/2$ comes from the recent work of ref. [44], where a (quenched) study of the scaling behaviour of the pseudoscalar meson decay constant and the vector meson mass was carried out down to small values of

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β. Lattice results for these quantities at fixed pseudoscalar meson mass ($\sim 700\,\mathrm{MeV}$) show surprisingly small cutoff effects from $\beta = 6.2$ to $\beta = 5.85$. Furthermore a nice analytic check of automatic $O(a)$ improvement of the pseudoscalar meson mass and decay constant in tm-LQCD at $|\omega| = \pi/2$ has been obtained in lattice chiral perturbation theory by the authors of ref. [45].

Our presentation of tm-LQCD, which follows a perspective complementary to that of ref. [19], provides a simple understanding of the many simplifications that have been previously observed to occur at $|\omega| = \pi/2$ [19]–[22], in the renormalization and $O(a)$ improvement of the matrix elements of certain local operators, such as the isotriplet axial current or the isosinglet scalar density.

All the results we have obtained are based on the observation that $M_{\rm cr}(r)$ is odd under $r \to -r$, the property (C.8) enjoyed by lattice and continuum correlators (see appendix C), as well as the behaviour of $O(a)$ terms under the spurionic symmetry $\mathcal{R}_5^{\rm sp}$ (eq. (3.1)). Considerations of this kind can be generalized without any essential modification to the case of mass non-degenerate quark doublets [28]. The point will be further discussed in a forthcoming paper [29], where we deal with the strategy for computing the matrix elements of the (CP-conserving) effective weak Hamiltonian.

Before briefly illustrating the potential of the method we have presented in this paper for further physical applications, we wish to comment on two important, related aspects of our approach, namely its computational cost compared to other schemes and the problem of how to most effectively perform the statistical analysis of available simulation data.

7.1 Computational cost

The computational cost of the approach we propose is in the worst case (i.e. if averaging is required) twice the typical one for simulations with unimproved standard Wilson fermions or tm-LQCD [20], and [46]–[49].

The gain offered by our strategy is, however, quite significant in practical terms, because the systematic removal of $O(a)$ lattice artifacts, allowing a better control of cutoff effects, gives the possibility of working with coarser lattices than in the absence of improvement. This may lead to a dramatic reduction of the computational cost especially in the unquenched case, where CPU times have been estimated to increase like a^{-k} with $k \simeq 7$ [50]. In the quenched case, assuming "ideal" critical slowing down, one finds a similar behaviour with $k = 5$. It should be also mentioned that the efficiency of algorithms for simulations with dynamical fermions of the multi-boson type [51] is expected to significantly benefit from the absence of the SW term (1.1) in the lattice action.

7.2 Statistical analysis of simulation data

A little thinking reveals that the most useful way to make use of simulation data depends on whether the fermionic determinant (4.20) (and hence the partition function) is invariant under $r \to -r$ (or equivalently under the shift $\omega \to \omega + \pi$) or not.

If the determinant is not invariant under $r \to -r$, the computation of Wilson averages requires to carry out two independent simulations leading to two different Markov chains of gauge configurations. The statistical analysis of the corresponding two sets of estimators,

$\{X_{j,r}\}$ and $\{X_{j,-r}\}$ ($j = 1, \ldots, N_{\rm meas}$), of the physical quantity X must be carried out separately. Only after this step has been completed, the Wilson average of the two mean values and the associated statistical error can be computed.

When the determinant is invariant, the whole functional measure is invariant too and only one Markov chain of configurations needs to be generated. In this situation the optimal procedure is to perform the Wilson average at the level of the individual (possibly "jackknived") statistical estimators, $X_{j,r}$. This is done by first computing the averages

$$X_j^{WA} = \frac{1}{2}\left(X_{j,r} + X_{j,-r}\right) , \qquad j = 1, \ldots, N_{\rm meas} , \tag{7.1}$$

and then going on with the standard statistical analysis of the $N_{\rm meas}$ Wilson averaged quantities X_j^{WA}.

As we already noticed, in all cases the extra computational effort necessary when averaging is required is not larger than a factor ~ 2 as compared to the case of simulations with unimproved fermions. Most interestingly, this factor reduces essentially to 1 in the case of simulations with $|\omega| = \pi/2$, because Wilson averaging is unnecessary.

From this discussion it emerges that the best strategy to deal with the unquenched theory is to "decouple" sea and valence quarks, by having all the sea quarks assembled in flavour doublets and regularized with twisting angles equal to $\pm\pi/2$, while for valence quarks each flavour is introduced with the chiral phase of the Wilson term chosen so as to minimize the complexity of the mixing pattern of (valence) quark composite operators. Unlike what is usually done, here we are proposing to regularize sea and valence quarks with Wilson terms of not necessarily identical structure [29].

7.3 Outlook

The last considerations bring about the question of the computation of the matrix elements of the various (valence) quark operators that are of interest for physical applications, like, for instance, the chiral order parameter and the matrix elements of the effective weak hamiltonian, $\mathcal{H}_{\rm eff}$. In particular for the CP-conserving sector of $\mathcal{H}_{\rm eff}$ we will show in [29] that, with a clever choice of the twisting angle entering the Wilson term of the different valence quarks, it is possible at the same time to have $O(a)$ improvement and to get rid of all the "wrong chirality" mixings. The virtue of tm-LQCD in simplifying the mixing pattern of CP-conserving four fermion operators in both the $\Delta S = 2$ and the $\Delta S = 1$ sector was already observed in refs. [19] and [24], respectively. Besides achieving $O(a)$ improvement, we will prove [28, 29] that mass non-degenerate sea quarks can be regularized so as to also have the resulting fermionic determinant real and positive.

We would like to close this list of applications by mentioning another important case, where the strategy advocated in this work can be of help. This is the computation of the decay constants, semi-leptonic form factors and masses of heavy-light mesons, which has been recently shown to be feasible with relativistic $O(a)$ improved c [52] and, even, b [53] quark, by making recourse in the last case to a clever use of finite size scaling techniques to bridge the gap between the largely different scales present in the problem.

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A. Improving axial Ward-Takahashi identities

In this appendix for illustrative purposes we discuss in full detail the improvement of the flavour non-singlet axial WTI's in the framework of the standard Wilson formulation.

From the action (2.2) one derives the lattice identity

$$\langle \partial^\star_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(r,M_0)} = 2M_0 \langle P^b(x)P^b(0)\rangle\Big|_{(r,M_0)} + \langle X^b(x) P^b(0)\rangle\Big|_{(r,M_0)} \quad x \neq 0\,, \tag{A.1}$$

where $\partial^\star_\mu$ is the discretized backward derivative.[21]. The lattice expressions of $\partial^\star_\mu A^b_\mu$ and X^b, whose explicit form we do not need here, can be found in ref. [4]. A^b_μ and P^b are the axial current and the pseudo-scalar quark density (eq. (2.15)), respectively. To be concrete the inserted operator in (A.1) was taken to be the pseudo-scalar quark density. It would not be difficult to generalize the arguments that follow by considering the insertion of a more general m.r. operator with definite γ_5-chirality.

In ref. [4] it is shown how one can recover from (A.1) the continuum WTI. Indeed, (A.1) can be renormalized to yield

$$Z_A(r)\langle \partial^\star_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(r,M_0)} = 2[M_0 - \bar{M}(r,M_0)]\langle P^b(x)P^b(0)\rangle\Big|_{(r,M_0)} + \mathrm{O}(a) \quad x \neq 0\,. \tag{A.2}$$

The two sides of eq. (A.2) possess a well defined continuum limit, as soon as they are multiplied by a suitable (logarithmically divergent) renormalization constant (i.e. the renormalization constant of the pseudo-scalar quark density), if the quantities Z_A and $\bar{M}$ are set to their appropriate values. Comparing the expression (A.2) with the form of the continuum WTI

$$\langle \partial_\mu \hat{A}^b_\mu(x)\hat{P}^b(0)\rangle = 2\hat{m}_q \langle \hat{P}^b(x)\hat{P}^b(0)\rangle\,, \tag{A.3}$$

one concludes that Z_A is the renormalization constant of the lattice axial current and the critical mass is the value of M_0 which solves the equation $M_0 = \bar{M}(r,M_0)$. We note incidentally that from the transformation properties of the various terms in eqs. (A.1) and (A.2) under $\mathcal{R}_5$, one can infer the relations

$$Z_A(r) = Z_A(-r)\,, \tag{A.4}$$

$$\bar{M}(r,M_0) = -\bar{M}(-r,-M_0)\,. \tag{A.5}$$

[21]For notational simplicity we write formulae with derivatives inside expectation values. It is, however, always understood that derivatives have to be thought as acting outside. As in the main text, we indicate nowhere the dependence upon the bare coupling constant, g_0^2, unless necessary to remove possible ambiguities.

Eqs. (A.4) and (A.5) confirm the result that the renormalization constant of a multiplicative renormalizable operator is generally even under $r \to -r$ (see section 3.3), while the critical mass is odd (eq. (2.7)).

The relations between the renormalized continuum quantities indicated with the symbol ˆ in eq. (A.3) and the corresponding bare lattice ones are

$$\hat{A}^b_\mu = Z_A A^b_\mu \tag{A.6}$$
$$\hat{P}^b = Z_P P^b \tag{A.7}$$
$$\hat{m}_q = z_m Z_P^{-1}(M_0 - M_{\rm cr}) = Z_{S^0}^{-1} m_q \,, \tag{A.8}$$

where Z_{S^0} is the multiplicative renormalization constant of the (subtracted) isosinglet scalar quark density and

$$z_m(r) = 1 - \frac{\partial \bar{M}(r, M_0)}{\partial M_0}\Big|_{M_0 = M_{\rm cr}(r)} \,. \tag{A.9}$$

The last equality in eq. (A.8) follows from the identity

$$z_m = \frac{Z_P}{Z_{S^0}} \,, \tag{A.10}$$

proved in ref. [39].

As we argued in the text, in order to discuss the issue of improvement one has to make reference to the notion of effective theory introduced by Symanzik and use the related Symanzik expansion of lattice correlators in terms of correlators of the continuum theory. Recalling the analysis carried out in ref. [8], one gets up to $O(a)$ corrections the explicit expansions ($x \neq 0$)

$$\begin{aligned}
\langle P^b(x) P^b(0)\rangle\Big|_{(r,m_q)} &= [\zeta^{PP}_{PP}(r) + am_q \xi^{PP}_{PP}(r)]\langle P^b(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ a\,\eta^{PP}_{\rm SW}(r)\langle P^b(x) P^b(0) \int d^4y\, \mathcal{L}_{\rm SW}(y)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ am_q\,\eta^{PP}_{FF}(r)\langle P^b(x) P^b(0) \int d^4y\, FF(y)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ am_q^2\,\eta^{PP}_{\bar\psi\psi}(r)\langle P^b(x) P^b(0) \int d^4y\, \bar\psi\psi(y)\rangle\Big|^{\rm cont}_{(m_q)} + {\rm O}(a^2)\,,
\end{aligned} \tag{A.11}$$

$$\begin{aligned}
\langle \tilde\partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(r,m_q)} &= [\zeta^{AP}_{AP}(r) + am_q \xi^{AP}_{AP}(r)]\langle \partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ a\,\eta^{AP}_{PP}(r)\langle \partial_\mu\partial_\mu P^b(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ a\,\eta^{AP}_{\rm SW}(r)\langle \partial_\mu A^b_\mu(x) P^b(0) \int d^4y\, \mathcal{L}_{\rm SW}(y)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ am_q\,\eta^{AP}_{FF}(r)\langle \partial_\mu A^b_\mu(x) P^b(0) \int d^4y\, FF(y)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+ am_q^2\,\eta^{AP}_{\bar\psi\psi}(r)\langle \partial_\mu A^b_\mu(x) P^b(0) \int d^4y\, \bar\psi\psi(y)\rangle\Big|^{\rm cont}_{(m_q)} + {\rm O}(a^2)\,,
\end{aligned} \tag{A.12}$$

where FF is a shorthand for $\mathrm{Tr}[F_{\mu\nu}F_{\mu\nu}]$ and

$$\mathcal{L}_{\rm SW}(x) = \bar{\psi}\frac{i}{4}\sigma_{\mu\nu}F_{\mu\nu}\psi(x)\,. \tag{A.13}$$

To avoid trivial $O(a)$ effects we have replaced the backward lattice derivative of eq. (A.1) with the symmetric one, $\tilde{\partial}_\mu \equiv (\partial_\mu + \partial^\star_\mu)/2$. As in the text, by slightly changing the notation employed in eqs. (A.1) and (A.2), we have indicated the parameters that specify the fermionic action using, besides r, the excess quark mass, $m_q = M_0 - M_{\rm cr}$, instead of M_0. In order to get the Symanzik expansions in the form given above, use has been made of the equations of motion and the continuum WTI (A.3) in the r.h.s. of eqs. (A.11) and (A.12).

As explained in the text (section 3), the coefficients ζ, ξ and η are all finite functions of r and g_0^2 and are necessary to match the lattice correlators on the l.h.s. to the continuum Green functions on the r.h.s. of eqs. (A.11) and (A.12). There is an obvious correspondence between the appearance of the terms with the coefficients ξ and η in front in the above Symanzik expansions and the need to introduce the coefficients $c_{\rm SW}$, b_m, b_g and c_A, b_A, b_P to improve the action and the operators A^b_μ, P^b.

Even in the limit of vanishing lattice spacing, eqs. (A.11) and (A.12) have a logarithmically divergent a-dependence which can be easily disposed of by multiplying the two sides of the equations by the appropriate renormalization constants.

We remark that in the expansions (A.11) and (A.12), besides correlators of genuine multi-local operators ("fully localized operators" in the following), one has also to include terms where the multi-local operator under consideration (be it $P^b(x)P^b(0)$ or $\tilde{\partial}_\mu A^b_\mu(x)P^b(0)$) is inserted together with space-time integrated local densities. The former are related to the improvement of the various local factors making up the operator in the l.h.s., while the latter owe their origin from the need to improve the action [8]. Integrated terms require a little discussion, as the integration variable, y, will inevitably hit the points where the bi-local (in the present instance) operator in consideration is localized (i.e. x and 0). To analyze the situation one may imagine to split the space-time integral in three different regions: one around x, a second one around 0 plus the rest. Terms coming from integration regions concentrated around the points x and 0 can be shown, by an analysis based on the O.P.E., to lead to $O(a)$ contributions of the same form as those of the fully localized multi-local operators already present in the expansion. They only have the effect of redefining the corresponding Symanzik coefficients. The integration over the remaining portion of the space-time is finite and gives rise to genuine $O(a)$ contributions.

Starting from the expansions (A.11) and (A.12), there are two equivalent ways to construct $O(a)$ improved lattice quantities, which we now want to make fully explicit: the Wilson average and the mass average method.

A.1 The Wilson average method

Under the change of variables (1.3), we obtain the lattice formulae (valid for any value of a)

$$\langle P^b(x)P^b(0)\rangle\Big|_{(r,M_0)} = \langle P^b(x)P^b(0)\rangle\Big|_{(-r,-M_0)} \tag{A.14}$$

$$\langle \tilde\partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(r,M_0)} = -\langle \tilde\partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(-r,-M_0)} . \tag{A.15}$$

Using (2.7), these relations can be rewritten, with the same little abuse of notation as before, in the more expressive form

$$\langle P^b(x) P^b(0)\rangle\Big|_{(r,m_q)} = \langle P^b(x) P^b(0)\rangle\Big|_{(-r,-m_q)} \tag{A.16}$$

$$\langle \tilde\partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(r,m_q)} = -\langle \tilde\partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|_{(-r,-m_q)} . \tag{A.17}$$

To write down the equations that are obtained from the expansions (A.11) and (A.12) when both r and m_q change sign we refer to the analysis presented after eq. (3.4) in section 3.

For completeness we list below the obvious parities of the continuum correlators appearing in the r.h.s. of eqs. (A.11) and (A.12) under $m_q \to -m_q$, which are implied by the transformation (1.3):

$$\langle P^b(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{even} \tag{A.18}$$

$$\langle P^b(x) P^b(0) \int d^4y\, \mathcal{L}_{\rm SW}(y)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{odd} \tag{A.19}$$

$$\langle P^b(x) P^b(0) \int d^4y\, F\tilde F(y)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{even} \tag{A.20}$$

$$\langle P^b(x) P^b(0) \int d^4y\, \bar\psi\psi(y)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{odd} \tag{A.21}$$

$$\langle \partial_\mu A^b_\mu(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{odd} \tag{A.22}$$

$$\langle \partial_\mu \partial_\mu P^b(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{even} \tag{A.23}$$

$$\langle \partial_\mu A^b_\mu(x) P^b(0) \int d^4y\, \mathcal{L}_{\rm SW}(y)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{even} \tag{A.24}$$

$$\langle \partial_\mu A^b_\mu(x) P^b(0) \int d^4y\, F\tilde F(y)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{odd} \tag{A.25}$$

$$\langle \partial_\mu A^b_\mu(x) P^b(0) \int d^4y\, \bar\psi\psi(y)\rangle\Big|^{\rm cont}_{(m_q)} \qquad \text{even} \tag{A.26}$$

Using equations from (A.18) to (A.21), the identity (A.16) leads to the relations

$$\zeta^{PP}_{PP}(r) = \zeta^{PP}_{PP}(-r) , \tag{A.27}$$

$$\begin{aligned}
&am_q\,[\xi^{PP}_{PP}(r) + \xi^{PP}_{PP}(-r)]\langle P^b(x) P^b(0)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+a\,[\eta^{PP}_{\rm SW}(r) + \eta^{PP}_{\rm SW}(-r)]\langle P^b(x) P^b(0) \int d^4y\, \mathcal{L}_{\rm SW}(y)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+am_q\,[\eta^{PP}_{F\tilde F}(r) + \eta^{PP}_{F\tilde F}(-r)]\langle P^b(x) P^b(0) \int d^4y\, F\tilde F(y)\rangle\Big|^{\rm cont}_{(m_q)} + \\
&+am_q^2\,[\eta^{PP}_{\bar\psi\psi}(r) + \eta^{PP}_{\bar\psi\psi}(-r)]\langle P^b(x) P^b(0) \int d^4y\, \bar\psi\psi(y)\rangle\Big|^{\rm cont}_{(m_q)} = 0
\end{aligned} \tag{A.28}$$

from terms of $O(a^0)$ and $O(a)$, respectively. Similarly, using equations from (A.22) to (A.26), the identity (A.17) leads to the relations

$$\zeta_{AP}^{AP}(r) = \zeta_{AP}^{AP}(-r)\,, \tag{A.29}$$

$$\begin{aligned}
&am_q\,[\xi_{AP}^{AP}(r)+\xi_{AP}^{AP}(-r)]\langle\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(m_q)}^{\rm cont}+\\
&+a\,[\eta_{PP}^{AP}(r)+\eta_{PP}^{AP}(-r)]\langle\partial_\mu\partial_\mu P^b(x)P^b(0)\rangle\Big|_{(m_q)}^{\rm cont}+\\
&+a\,[\eta_{\rm SW}^{AP}(r)+\eta_{\rm SW}^{AP}(-r)]\langle\partial_\mu A_\mu^b(x)P^b(0)\int d^4y\,\mathcal{L}_{\rm SW}(y)\rangle\Big|_{(m_q)}^{\rm cont}+\\
&+am_q\,[\eta_{FF}^{AP}(r)+\eta_{FF}^{AP}(-r)]\langle\partial_\mu A_\mu^b(x)P^b(0)\int d^4y\,FF(y)\rangle\Big|_{(m_q)}^{\rm cont}+\\
&+am_q^2\,[\eta_{\bar\psi\psi}^{AP}(r)+\eta_{\bar\psi\psi}^{AP}(-r)]\langle\partial_\mu A_\mu^b(x)P^b(0)\int d^4y\,\bar\psi\psi(y)\rangle\Big|_{(m_q)}^{\rm cont}=0\,.
\end{aligned} \tag{A.30}$$

From the above four equations one immediately comes to the conclusion that the average of correlators computed with lattice actions having Wilson terms of opposite signs and the same value of $m_q = M_0 - M_{\rm cr}$ are free of $O(a)$ discretization effects. In formulae one gets, in fact

$$\frac{1}{2}\Big[\langle P^b(x)P^b(0)\rangle\Big|_{(r,m_q)}+\langle P^b(x)P^b(0)\rangle\Big|_{(-r,m_q)}\Big] = \zeta_{PP}^{PP}(r)\langle P^b(x)P^b(0)\rangle\Big|_{(m_q)}^{\rm cont}+{\rm O}(a^2)\,, \tag{A.31}$$

$$\frac{1}{2}\Big[\langle\tilde\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(r,m_q)}+\langle\tilde\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(-r,m_q)}\Big] = \zeta_{AP}^{AP}(r)\langle\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(m_q)}^{\rm cont}+{\rm O}(a^2)\,. \tag{A.32}$$

Though unnecessary to obtain the improved formulae (A.31) and (A.32), we observe that the vanishing of the sum of terms in eqs. (A.28) and (A.30) for arbitrary values of x implies that all the Symanzik coefficients η and ξ are odd functions of r.

A.2 The mass average method

An equivalent way of getting $O(a)$ improved lattice data from standard Wilson simulations consists in comparing the two sets of formulae that are obtained by only changing sign to m_q in eqs. (A.11) and (A.12). Taking into account the γ_5-chirality properties of the continuum correlators listed in eqs. (A.18) to (A.21) and (A.22) to (A.26), it is immediate to verify that lattice correlators computed with fixed value of r and opposite excess quark mass, $m_q = M_0 - M_{\rm cr}$, if linearly combined with a relative sign equal to the $\mathcal{R}_5$-parity of the multi-local lattice operator under consideration, yield quantities that are free of $O(a)$ discretization effects. In the case at hand one gets

$$\frac{1}{2}\Big[\langle P^b(x)P^b(0)\rangle\Big|_{(r,m_q)}+\langle P^b(x)P^b(0)\rangle\Big|_{(r,-m_q)}\Big] = \zeta_{PP}^{PP}(r)\langle P^b(x)P^b(0)\rangle\Big|_{(m_q)}^{\rm cont}+{\rm O}(a^2)\,, \tag{A.33}$$

$$\frac{1}{2}\Big[\langle\tilde\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(r,m_q)}-\langle\tilde\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(r,-m_q)}\Big] = \zeta_{AP}^{AP}(r)\langle\partial_\mu A_\mu^b(x)P^b(0)\rangle\Big|_{(m_q)}^{\rm cont}+{\rm O}(a^2)\,. \tag{A.34}$$

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Eqs. (A.33) and (A.34) are perfectly equivalent to eqs. (A.31) and (A.32), respectively, as it is immediately seen by using the lattice identities

$$\langle P^b(x)P^b(0)\rangle\Big|_{(r,-m_q)} = \langle P^b(x)P^b(0)\rangle\Big|_{(-r,m_q)} \tag{A.35}$$

$$-\langle\tilde{\partial}_\mu A^b_\mu(x)P^b(0)\rangle\Big|_{(r,-m_q)} = \langle\tilde{\partial}_\mu A^b_\mu(x)P^b(0)\rangle\Big|_{(-r,m_q)}, \tag{A.36}$$

which are direct consequences of (A.16) and (A.17).

B. Reflection positivity and transfer matrix

In the continuum euclidean theory the Wightman reconstruction theorem is based on the axiom of reflection positivity [34], i.e. on the existence of an anti-linear operator, Θ, which transforms an arbitrary functional of the fields, F_+, with support in a region, R, of the half-space $t>0$ into a functional, ΘF_+, with support in the reflected region, θR (with the definition $\theta x = \theta(\mathbf{x},t) = (\mathbf{x},-t)$), such that

$$\langle F_+\,\Theta F_+\rangle \geq 0\,. \tag{B.1}$$

This condition implies the existence of a positive definite, self-adjoint hamiltonian. For a gauge theory the theorem is proved by choosing the gauge $A_0=0$ (temporal gauge).

A similar theorem holds on the lattice [35, 36, 37]. However, one has to distinguish between link and site reflection positivity. The associated reflection operations act differently on lattice points: the former, θ_ℓ, refers to reflection across a hyperplane which cuts time links in half (e.g. the links $(\mathbf{x},0)-(\mathbf{x},a)$), while the latter, θ_s, to reflection across a time hyperplane which passes through sites (e.g. the sites $(\mathbf{x},0)$). Explicitly in the above examples one has

$$\theta_\ell(\mathbf{x},t) = (\mathbf{x},-t+a) \qquad \theta_s(\mathbf{x},t) = (\mathbf{x},-t)\,. \tag{B.2}$$

The validity of both site reflection positivity (eq. (B.1) with $\Theta=\Theta_s$) and link reflection positivity (eq. (B.1) with $\Theta=\Theta_\ell$) is a sufficient condition for the existence of an hermitean positive lattice (single-link) transfer matrix. Viceversa, if such a transfer matrix exists, one can prove that both types of reflection positivity hold. If only one kind of reflection positivity is valid (e.g. link reflection positivity, which typically holds under weaker conditions on the action parameters than site reflection positivity) one can still prove the existence of a positive transfer matrix acting over a time translation of two lattice sites (to be interpreted as the square of the single-link transfer matrix). Naturally in the limit $a\to 0$ the condition of link (or site) reflection positivity alone is perfectly sufficient to extract continuum physics from lattice data.

As in the continuum theory all these statements are proved in the temporal gauge, which in the lattice corresponds to set all the link variables associated to temporal links equal to the identity element of the gauge group (except at one set of links, which can be conveniently chosen to be $(\mathbf{x},0)-(\mathbf{x},a)$).

For completeness we report the explicit action of the anti-linear reflection operation on the fundamental fields of the theory. Θ_s and Θ_ℓ act on $\bar\psi(x)$, $\psi(x)$ and $U_\mu(x)$ in the same way, the only difference is how the arguments they depend on get reflected. With the subscript $_s$ or $_\ell$ understood one has[22]

$$\Theta[U_0(x)] = U_0^T(\theta x - a\hat{0}) \,, \qquad \Theta[U_k(x)] = U_k^*(\theta x) \,,\; k = 1,2,3 \tag{B.3}$$

$$\Theta[\psi(x)] = \bar{\psi}(\theta x)\gamma_0 \,, \qquad \Theta[\bar{\psi}(x)] = \gamma_0 \psi(\theta x) \tag{B.4}$$

and on monomials of fermionic fields

$$\Theta[f(U)\psi(x_1)\cdots\bar{\psi}(x_n)] = f^\star(\Theta[U])\Theta[\bar{\psi}(x_n)]\cdots\Theta[\psi(x_1)] \,, \tag{B.5}$$

$f(U)$ being a functional of link variables only. As usual the definition

$$\Phi^\dagger(\theta x) \equiv \Theta[\Phi(x)] \tag{B.6}$$

is employed in this work.

B.1 Site reflection positivity for Wilson fermions

In ref. [38] it was proved that site reflection positivity holds for Wilson fermions, provided

$$|8r + 2aM_0| > 6 \,, \qquad r = 1 \,. \tag{B.7}$$

The explicit construction of the transfer matrix of the lattice theory was carried out in ref. [54].

The proof of site reflection positivity given in [38] for $r = 1$ can be extended to $r = -1$ by noting that Θ_s commutes with $\mathcal{R}_5$. In fact, let $F_+(\bar{\psi}, \psi, U)$ be a functional of the field variables defined at positive euclidean times. Consider the expectation value $\langle F_+ \, \Theta_s F_+ \rangle$. The change of integration variables induced by the transformation (1.3) leads to the relation

$$\begin{aligned} &\langle F_+(\bar{\psi}, \psi, U) \, \Theta_s F_+(\bar{\psi}, \psi, U) \rangle \Big|_{(-1, M_0)} = \\ &\quad = \langle F_+(-\bar{\psi}\gamma_5, \gamma_5\psi, U) \, \Theta_s F_+(-\bar{\psi}\gamma_5, \gamma_5\psi, U) \rangle \Big|_{(1, -M_0)} \,. \end{aligned} \tag{B.8}$$

Thanks to reflection positivity which holds for $r = 1$, one concludes that the r.h.s. of eq. (B.8) is non-negative, provided (eq. (B.7) with $M_0 \to -M_0$)

$$|8 - 2aM_0| > 6 \,. \tag{B.9}$$

The inequality (B.9) is precisely the condition (B.7), only written for $r = -1$. This shows that Wilson fermions obey site reflection positivity for both $r = 1$ and $r = -1$ under the condition $|8r + 2aM_0| > 6 \,, r = \pm 1$. Link reflection positivity was discussed in section 2.3.

[22] In the two argument notation $U_\mu(x) \equiv U(x, x + a\hat{\mu})$ the action of Θ reads $\Theta[U(x,y)] = U^*(\theta x, \theta y)$, $y = x + a\hat{\mu}$.

B.2 Site reflection positivity for tm-LQCD

The situation for tm-LQCD is similar to that of the standard Wilson theory summarized above. The validity of site reflection positivity was indirectly proved in [21], where along the lines of the work of ref. [54] the transfer matrix for the action (4.15) was constructed under the condition ($\omega = \omega_m + \omega_r$)

$$|8r + 2aM_{\rm cr}(r) + 2am_q \cos\omega| > 6\,, \qquad r = 1\,. \tag{B.10}$$

From this result the validity of site reflection positivity for the form (4.18) of the tm-LQCD action can be proved by noting that Θ_s commutes with the chiral fermion field transformation (4.3). One finds, in fact, under the condition (B.10)

$$\begin{aligned}\langle F_+(\bar\psi_{\rm ph},\psi_{\rm ph},U)\,\Theta_s F_+(\bar\psi_{\rm ph},\psi_{\rm ph},U)\rangle\Big|^{(\omega_r=\omega,\,\omega_m=0)}_{(r,m_q)} &= \\ = \langle F_+(\bar\psi,\psi,U)\,\Theta_s F_+(\bar\psi,\psi,U)\rangle\Big|^{(\omega_r=0,\,\omega_m=\omega)}_{(r,m_q)} &\geq 0\end{aligned} \tag{B.11}$$

with

$$\psi = e^{-i\omega\gamma_5\tau_3/2}\psi_{\rm ph} \quad \bar\psi = \bar\psi_{\rm ph}e^{-i\omega\gamma_5\tau_3/2}\,, \tag{B.12}$$

where the last inequality follows from the validity of site reflection positivity for the action (4.15).

C. Proof of eq. (3.11)

In this Appendix we want to show that the γ_5-chiralities of the operators appearing in the Symanzik expansion (3.3), or in the analogous expansion (5.1) if tm-LQCD is employed, satisfy the equation

$$P_{\mathcal{R}_5}[O] + P_{\mathcal{R}_5}[O_\ell] + n_\ell = 1 \bmod (2)\,. \tag{C.1}$$

Eq. (C.1) is an immediate consequence of the dimensional relation (3.4) and the formula

$$P_{\mathcal{R}_5}[O] + d[O] = P_{\mathcal{R}_5}[O_\ell] + d[O_\ell] \bmod (2)\,, \tag{C.2}$$

which we prove below. From these equations one gets, in fact, successively

$$\begin{aligned}P_{\mathcal{R}_5}[O] + P_{\mathcal{R}_5}[O_\ell] + n_\ell &= P_{\mathcal{R}_5}[O] + d[O] + P_{\mathcal{R}_5}[O_\ell] - d[O_\ell] + 1 \\ &= P_{\mathcal{R}_5}[O] + d[O] - P_{\mathcal{R}_5}[O_\ell] - d[O_\ell] + 1 \bmod (2) = 1 \bmod (2)\,.\end{aligned} \tag{C.3}$$

In order to prove eq. (C.2) we note that with the definition

$$\Delta_5[O] = P_{\mathcal{R}_5}[O] + d[O] \tag{C.4}$$

eq. (C.2) becomes

$$\Delta_5[O] - \Delta_5[O_\ell] = 0 \bmod (2)\,. \tag{C.5}$$

Eq. (C.5) is a direct consequence of the following symmetry considerations.

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1. The Wilson and tm-LQCD actions (eqs. (2.2) and (4.18), respectively), and *a fortiori* the formal continuum action, are invariant under the combined transformation $\mathcal{R}_5 \times \mathcal{D}_d$, where [23]

$$\mathcal{D}_d : \begin{cases} U_\mu(x) \to U_\mu^\dagger(-x - a\hat{\mu}) \\ \psi(x) \quad \to e^{3i\pi/2}\psi(-x) \\ \bar{\psi}(x) \quad \to e^{3i\pi/2}\bar{\psi}(-x) \,. \end{cases} \tag{C.6}$$

The invariance of the pure gauge part of the action is obvious. For the fermionic part invariance follows by first noting that under $\mathcal{D}_d$ (recall the definitions (2.3))

$$\begin{aligned} &\bar{\psi}(x)\sum_\mu \gamma_\mu(\nabla_\mu + \nabla_\mu^*)\psi(x) \;\to\; \bar{\psi}(-x)\sum_\mu \gamma_\mu(\nabla_\mu + \nabla_\mu^*)\psi(-x) \\ &\bar{\psi}(x)\sum_\mu \nabla_\mu^*\nabla_\mu\psi(x) \;\to\; -\bar{\psi}(-x)\sum_\mu \nabla_\mu^*\nabla_\mu\psi(-x) \\ &\bar{\psi}(x)\psi(x) \;\to\; -\bar{\psi}(-x)\psi(-x) \,. \end{aligned} \tag{C.7}$$

The minus sign in front of the chirally non-invariant terms is compensated by the transformation $\mathcal{R}_5$. Finally the space-time arguments are brought back to their initial values by the trivial change of space-time integration variables $-x \to x$ in the action. In the formal continuum theory an analogous argument goes through. In fact, the continuum version of the transformation $\mathcal{D}_d$, besides changing the sign of all the space-time coordinates, has simply the effect of multiplying each local term $\mathcal{L}_i$ in the action density by the factor $(-1)^{d[\mathcal{L}_i]}$, where $d[\mathcal{L}_i]$ is the naive dimension of $\mathcal{L}_i$.

2. Performing the change of functional integration variables induced by the transformation $\mathcal{R}_5 \times \mathcal{D}_d$, one can prove that the lattice correlators of the type we are interested in obey the formula

$$\langle O(x_1, x_2, \ldots, x_n)\rangle\Big|_{(r,m_q)}^{(\omega)} = (-1)^{\Delta_5[O]}\langle O(-x_1, -x_2, \ldots, -x_n)\rangle\Big|_{(r,m_q)}^{(\omega)} \tag{C.8}$$

with $\omega = 0$ in the case of the standard Wilson action (2.2). The relation (C.8) directly follows from our definition of Δ_5 (eq. (C.4)) and the way $\mathcal{D}_d$ (eq. (C.6)) acts on the fundamental fields in O.

Similarly, all continuum operators contributing to the Symanzik expansions (3.3) or (5.1) of the expectation value of $O(x_1, x_2, \ldots, x_n)$ must obey eq. (C.8) with a value of Δ_5 equal (mod (2)) to that of O. In other words all terms in the Symanzik expansion of O must have the same $(-1)^{\Delta_5}$-parity as O. This is just our thesis, eq. (C.5).

D. Discretization effects in the determination of $M_{\rm cr}$

In this appendix we want to show that $O(a)$ discretization effects in the determination of $M_{\rm cr}(r)$ do not jeopardize the proof of $O(a)$ improvement of averaged correlators given in the text. We give the proof in the case of standard Wilson fermions. The generalization to tm-LQCD is straightforward.

[23] In this appendix, for notational uniformity, we will always denote the quark fields by ψ and $\bar{\psi}$ (as in eq. (2.2)), even when we refer to the tm-LQCD action (4.18).

D.1 The problem

In PT the analytic dependence of lattice correlators on a is completely and explicitly computable. Thus an unambiguous expression of $M_{\rm cr}(r)$ can be given to any order in g_0^2. The situation is different non-perturbatively. An estimate of $M_{\rm cr}(r)$ can be obtained by using, for instance, PCAC or the observation that (in the presence of SχSB) the pion mass is expected to vanishes at the chiral point (modulo cutoff effects, see section 2.2). If the the pion mass is employed to determine $M_{\rm cr}(r)$, one has to proceed by extracting from the large t behaviour of the two-point correlator[24]

$$G_\pi(t;r,M_0) = a^3 \sum_{\mathbf{x}} \langle P^b(\mathbf{x},t) P^b(0)\rangle\Big|_{(r,M_0)}\,, \tag{D.1}$$

a lattice measurement of the pion mass, $m_\pi(r,M_0)$. A sensible estimate of the critical mass, which will be referred to as $M_{\rm cr}^{e_1}(r)$ and obeys

$$M_{\rm cr}^{e_1}(r) = -M_{\rm cr}^{e_1}(-r)\,, \tag{D.2}$$

can thus be obtained as discussed in section 2.2.

If PCAC (see e.g. eq. (A.2)) is employed to measure $M_{\rm cr}(r)$, one would get another, equally good, non-perturbative estimate of it, say $M_{\rm cr}^{e_2}$, given by the solution of the equation

$$\bar{M}(r, M_{\rm cr}^{e_2}(r)) - M_{\rm cr}^{e_2}(r) = 0\,. \tag{D.3}$$

The new estimate is again odd in r (see eq. (A.5)).

For the sake of this argument we may summarize the situation by formally writing for any such estimate

$$M_{\rm cr}^{e}(r) = M_{\rm cr}(r) + \delta^e(r)\,, \tag{D.4}$$

with

$$\delta^e(r) = -\delta^e(-r) = \mathrm{O}(a)\,. \tag{D.5}$$

The difference $M_{\rm cr}(r) - M_{\rm cr}^{e}(r)$ is obviously odd under $r \to -r$, because $M_{\rm cr}(r)$ as well as anyone of its estimates is odd in r (see section 2).

The problem we want to address is whether $O(a)$ ambiguities in the knowledge of the critical mass can invalidate the argument for $O(a)$ improvement developed in section 3 leading to eqs. (3.9) and (3.12) (or to the similar ones valid in the case of tm-LQCD). We show below that eqs. (D.4) and (D.5) are indeed all is needed for eqs. (3.9) and (3.12) to be valid.

This result should not come as a surprise, since effectively we are here merely claiming that all the $O(a)$ cutoff effects, which generically are present before averaging, get canceled in WA's of correlators and derived quantities. Among these cutoff effects there are, indeed, also those arising from $O(a)$ errors on $M_{\rm cr}(r)$. They are not in any sense special and actually stem from the presence of $O(a)$ cutoff effects in the correlators employed to estimate the value of the critical mass.

[24] In this appendix we label lattice expectation values by using, besides r, the bare quark mass. As in the rest of the paper, the ubiquitous g_0^2 dependence is understood.

D.2 The proof

Once the values of r (> 0), g_0^2 and the bare lattice mass $M_0 = M_0^+$ are chosen, the Symanzik expansion of the expectation value of the operator O takes the form (see eq. (3.3) in section 3)

$$\langle O\rangle\Big|_{(r,M_0^+)} = [\zeta_O^O(r) + am_q^+\xi_O^O(r)]\langle O\rangle\Big|_{(m_q^+)}^{\mathrm{cont}} + a\sum_\ell (m_q^+)^{n_\ell}\eta_{O_\ell}^O(r)\langle O_\ell\rangle\Big|_{(m_q^+)}^{\mathrm{cont}} + \mathrm{O}(a^2)\,, \quad \text{(D.6)}$$

where

$$m_q^+ \equiv M_0^+ - M_{\mathrm{cr}}(r) \quad \text{(D.7)}$$

is the continuum mass at the subtraction point a^{-1}. m_q^+ is defined in terms of the (unknown) value of the critical mass, $M_{\mathrm{cr}}(r)$.

We want to average this expectation value with the similar expression obtained by changing sign to r and adjusting M_0 to a suitable value, $M_0 \to M_0^-$, such that all $O(a)$ terms cancel in the sum. We have shown in section 3 that this is indeed possible with the choice

$$M_0^- - M_{\mathrm{cr}}(-r) = M_0^+ - M_{\mathrm{cr}}(r) = m_q^+\,. \quad \text{(D.8)}$$

The "practical" problem with this prescription is that, as we just recalled, one can only get an "estimate", $M_{\mathrm{cr}}^e(r)$, of the critical mass with the properties summarized in eqs. (D.4) and (D.5).

Now the question is: given M_0^+, which value of the bare lattice mass do we have to take in practice, when we go over to $-r$, in order to get rid of $O(a)$ terms?

Clearly the only possible answer (and, as we shall see, the right one) is to consider the expectation value of O computed with $-r$ and a bare mass, ${M'}_0^-$, given by

$${M'}_0^- \equiv M_0^+ - M_{\mathrm{cr}}^e(r) + M_{\mathrm{cr}}^e(-r) = M_0^+ - 2M_{\mathrm{cr}}^e(r)\,, \quad \text{(D.9)}$$

where the last equality follows from the r-parity properties of $M_{\mathrm{cr}}^e(r)$. The Symanzik expansion of $\langle O\rangle|_{(-r,{M'}_0^-)}$ takes the form

$$\langle O\rangle\Big|_{(-r,{M'}_0^-)} = [\zeta_O^O(-r) + am_q^-\xi_O^O(-r)]\langle O\rangle\Big|_{(m_q^-)}^{\mathrm{cont}} + a\sum_\ell (m_q^-)^{n_\ell}\eta_{O_\ell}^O(-r)\langle O_\ell\rangle\Big|_{(m_q^-)}^{\mathrm{cont}} + \mathrm{O}(a^2)\,, \quad \text{(D.10)}$$

with the definition

$$m_q^- = {M'}_0^- - M_{\mathrm{cr}}(-r)\,. \quad \text{(D.11)}$$

For future use we note the chain of equalities

$$\begin{aligned} m_q^- &= {M'}_0^- - M_{\mathrm{cr}}(-r) = M_0^+ - 2M_{\mathrm{cr}}^e(r) - M_{\mathrm{cr}}(-r) \\ &= M_0^+ - 2M_{\mathrm{cr}}^e(r) + M_{\mathrm{cr}}(r) = M_0^+ - M_{\mathrm{cr}}(r) - 2\delta^e(r) \\ &= m_q^+ - 2\delta^e(r)\,, \end{aligned} \quad \text{(D.12)}$$

where eqs. (D.9), (D.4) and (D.5) have been employed.

Clearly the $O(a)$ mismatch between M_0^- (eq. (D.8)) and M'^-_0 (eq. (D.9)), as well as that between m_q^+ and m_q^- matters only for the first term of the expansions (D.6) and (D.10), because all the other terms have an explicit factor of a in front of them. Thus summing (D.6) and (D.10) all $O(a)$ contributions that are multiplied by the (r odd) Symanzik coefficients ξ and η cancel and we get (see eq. (3.7))

$$\langle O\rangle\Big|_{(r,M_0^+)} + \langle O\rangle\Big|_{(-r,M'^-_0)} = \zeta_O^O(r)\Big[\langle O\rangle\Big|^{\rm cont}_{(m_q^+)} + \langle O\rangle\Big|^{\rm cont}_{(m_q^-)}\Big] + \mathrm{O}(a^2)\,. \tag{D.13}$$

At this point, recalling the expressions (D.7) of m_q^+ and (D.12) of m_q^-, we can put the r.h.s. of the previous equation in the form

$$\begin{aligned}\zeta_O^O(r)\Big[\langle O\rangle\Big|^{\rm cont}_{(m_q^+)} + \langle O\rangle\Big|^{\rm cont}_{(m_q^-)}\Big] + \mathrm{O}(a^2) = \\ = \zeta_O^O(r)\Big[\langle O\rangle\Big|^{\rm cont}_{(M_0^+-M_{\rm cr}(r))} + \langle O\rangle\Big|^{\rm cont}_{(M_0^+-M_{\rm cr}(r)-2\delta^e(r))}\Big] + \mathrm{O}(a^2)\,.\end{aligned} \tag{D.14}$$

In this expression the two continuum correlators are evaluated at "slightly" different values of the excess quark mass, namely $M_0^+ - M_{\rm cr}(r)$ and $M_0^+ - M_{\rm cr}(r) - 2\delta^e(r)$. Neglecting $O(a^2)$ terms, they can be immediately brought to the common value of the mass parameter

$$m_q = M_0^+ - M_{\rm cr}(r) - \delta^e(r) = M_0^+ - M^e_{\rm cr}(r) = M'^-_0 - M^e_{\rm cr}(-r) \tag{D.15}$$

by a simple Taylor expansion of the continuum correlators in powers of $\delta^e(r)$. The terms with the mass derivative of continuum correlators cancel out and one gets

$$\frac{1}{2}\Big[\langle O\rangle\Big|_{(r,m_q+M^e_{\rm cr}(r))} + \langle O\rangle\Big|_{(-r,m_q-M^e_{\rm cr}(r))}\Big] = \zeta_O^O(r)\langle O\rangle\Big|^{\rm cont}_{(m_q)} + \mathrm{O}(a^2)\,, \tag{D.16}$$

where only well defined, numerically accessible inputs, like $M^e_{\rm cr}(r)$ and the excess quark mass, m_q, appear.

We end by noticing that, had we used the excess quark mass to label lattice correlators (as we did in the text after section 3), the formula (D.16) would have actually read

$$\frac{1}{2}\Big[\langle O\rangle\Big|_{(r,m_q)} + \langle O\rangle\Big|_{(-r,m_q)}\Big] = \zeta_O^O(r)\langle O\rangle\Big|^{\rm cont}_{(m_q)} + \mathrm{O}(a^2)\,. \tag{D.17}$$

The result of this elaborated discussion is that $O(a)$ improved correlators are obtained using the formula (D.17) — which is identical to the WA prescription (3.9) — with m_q given by eq. (D.15).

E. Improvement of the baryonic spectrum

In this appendix we want to give a quick argument to show that the procedure for $O(a)$ improvement proposed in this paper (eq. (3.26) and its tm-LQCD counterpart) works also for the baryonic sector of the hadronic spectrum. For concreteness we will concentrate on the spin 1/2 and 3/2 states that can be formed with an $\mathrm{SU}(2)_\mathrm{f}$ flavour doublet of quarks.

First of all we note that all baryonic energies can be extracted from spin averaged two-point correlators of the type (3.18) and (5.10), for the untwisted and twisted Wilson formulations, respectively. The (bare) interpolating operators for spin 1/2 and 3/2 baryonic states are of the form

$$[\Phi^f_{h,\alpha}](x) = [\epsilon_{ijl}\psi^f_{\alpha,i}\mathcal{M}^{jl}_h](x)\,, \tag{E.1}$$

where f and α are free flavour and Dirac indices, i, j, l represent (contracted) color indices and $\mathcal{M}^{jl}_h$ is a bosonic operator with definite transformation properties under $\mathcal{R}_5$. For instance, for proton ($f = 1$, $\psi^1 \equiv u$) or neutron ($f = 2$, $\psi^2 \equiv d$) states we can take

$$\mathcal{M}^{jl}_{p,n} = i\bar{\psi}^{\rm c}_j\,\gamma_5\tau_2\,\psi_l \tag{E.2}$$

with $\bar{\psi}^{\rm c}$ denoting the charge conjugated of $\bar{\psi}$. Similarly, the (bare) interpolating operator for the spin 3/2 baryon Δ^{++} is of the form (E.1) with $f = 1$ and

$$\mathcal{M}^{jl}_{\Delta,k} \;=\; \bar{\psi}^{\rm c}_j\,\frac{1}{2}(1+\tau_3)\gamma_k\,\psi_l\,, \qquad k = 1, 2, 3\,. \tag{E.3}$$

In all cases the bi-local operator $\Phi_h(x)\Phi^\dagger_h(0)$ (with all Dirac indices contracted) has definite (positive) $\mathcal{R}_5$-parity. Since this property is preserved also in presence of mixing, we can apply the considerations of section 3.2 (or the analogous ones valid for tm-LQCD) and conclude that also baryonic masses are improved by the usual WA procedure.

Moreover, in the tm-LQCD formulation with action (4.18) the masses of the baryonic states (E.1) are even functions of the twisting angle ω, hence automatically free of $O(a)$ corrections if $\omega = \pm\pi/2$. To prove this result it is sufficient to check that the argument presented in section 5.3.1 for the ω-parity of masses applies to the states under consideration here. This is actually so, because the interpolating operators (E.1) are such that the spin averaged product $\Phi_h(x)\Phi^\dagger_h(0)$ has obviously a definite positive formal parity (eq. (5.5)) and this property is preserved under renormalization. Incidentally, Φ_h itself could be chosen to have definite formal parity, if one decides to multiply the operator in the r.h.s. of (E.1) by the projectors $(1 \pm \gamma_0)/2$.

F. Proof of eq. (5.18)

A detailed proof of eq. (5.18) requires repeating in the case of tm-LQCD the line of arguments that in a parity invariant theory leads from the way $\mathcal{P}$ acts on the elementary fields entering the lagrangian density (see eq. (5.4)) to the notion of parity for the eigenstates of the hamiltonian. Observing that in the case at hand (action (4.18)) the spurionic symmetry $\mathcal{P}^{\rm sp} \equiv \mathcal{P} \times (\omega \to -\omega)$ ($(\mathcal{P}^{\rm sp})^2 = \mathbb{1}$) replaces $\mathcal{P}$, one can proceed as follows.

1. To composite bare operators formal parity labels are attributed according to the naive prescription induced by the field transformation (5.4).

2. A basis of m.r. operators can always be constructed, consisting of operators endowed with a definite parity label. In fact, to comply with the symmetry $\mathcal{P}^{\rm sp}$ the mixing pattern will have to be such that (bare) operators with opposite formal parity get mixed with coefficients whose relative ω-parity is negative. This procedure is equivalent to assign a parity label via eq. (5.5). If one wishes to employ this method, one should

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start by assigning parity to local operators (e.g. quark bilinears) or simple products of local operators with non-zero (for suitable choices of the space-time arguments) vacuum expectation value and then move on to progressively more complicated cases.

The situation here is exactly analogous to what happens with the spurionic symmetry $\mathcal{R}_5^{\rm sp}$, where eq. (3.2) is exploited to attribute a definite γ_5-chirality, $P_{\mathcal{R}_5}[O]$, actually the naive one, to any (gauge invariant) m.r. composite operator, O.

3. For the vacuum state we have in general

$$\widehat{\mathcal{P}}|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)} = \eta_\Omega(\omega)|\Omega\rangle\Big|^{(-\omega)}_{(r,m_q)}\,, \tag{F.1}$$

with $\eta_\Omega(\omega)\eta_\Omega(-\omega) = 1$ (from $\widehat{\mathcal{P}}^2 = 1\!\!1$ [55]) and $|\eta_\Omega(\omega)|^2 = 1$ (from the vacuum normalization condition). In view of these results one can always decide to simply take the phase of the vacuum state such that $\eta_\Omega(\omega) = 1$ for any value of ω. If one does not want to do so, one will have to keep track of the vacuum phase in all the forthcoming formulae.

4. A basis for the states of the Fock space is constructed by applying creation operators to the vacuum (cyclic vector). The elements of the basis are highly non-trivial and schematically can be written in the form

$$|h,\mathbf{k};\alpha\rangle^{(\omega)}_{(r,m_q)} = a^\dagger_{h\alpha}(\mathbf{k})|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)}\,, \tag{F.2}$$

where, according to 1) and 2), the creation operators $a^\dagger_{h\alpha}(\mathbf{k})$ (α is an index which labels the states with the same unbroken quantum numbers h and three-momenta $\mathbf{k}$) will satisfy the relation

$$\widehat{\mathcal{P}} a^\dagger_{h\alpha}(\mathbf{k})\widehat{\mathcal{P}} = \eta_{h\alpha} a^\dagger_{h\alpha}(-\mathbf{k})\,. \tag{F.3}$$

where $\eta_{h\alpha}$ ($=\pm 1$) is by construction an ω- and $\mathbf{k}$-independent label.

5. The eigenstates of the transfer matrix $\widehat{T}(\omega,r,m_q)$ (see eq. (5.13)) will be expressed as linear combinations of the states (F.2) of the kind

$$|h,n,\mathbf{k}\rangle\Big|^{(\omega)}_{(r,m_q)} = \sum_\alpha c_{n\alpha}(\omega,r,m_q)|h,\mathbf{k};\alpha\rangle^{(\omega)}_{(r,m_q)} = \sum_\alpha c_{n\alpha}(\omega,r,m_q)a^\dagger_{h\alpha}(\mathbf{k})|\Omega\rangle\Big|^{(\omega)}_{(r,m_q)}\,, \tag{F.4}$$

with appropriate coefficients, $c_{n\alpha}(\omega,r,m_q)$, to ensure normalizability of the state and consistency with the spurionic invariance $\mathcal{P}^{\rm sp}$.

In particular, consistency with the spurionic symmetry $\mathcal{P}^{\rm sp}$ implies the operator relation

$$\widehat{\mathcal{P}}\left[|h,n,\mathbf{k}\rangle\langle h,n,\mathbf{k}|\right]^{(\omega)}_{(r,m_q)}\widehat{\mathcal{P}} = \left[|h,n,-\mathbf{k}\rangle\langle h,n,-\mathbf{k}|\right]^{(-\omega)}_{(r,m_q)}\,, \tag{F.5}$$

which is proved below in subsection F.1. This relation can only hold if the coefficients $c_{n\alpha}(\omega,r,m_q)$ have (up to an irrelevant α-independent phase, which we set equal to unity[25]) a definite parity, $s_{n\alpha} = \pm 1$, under $\omega \to -\omega$, i.e. only if they satisfy the relation

$$c_{n\alpha}(\omega, r, m_q) = s_{n\alpha} c_{n\alpha}(-\omega, r, m_q) \tag{F.6}$$

with

$$\eta_{h,n} \equiv \eta_{h\alpha} s_{n\alpha} \tag{F.7}$$

an α-independent label.

6. For the states (F.4) the relation

$$\widehat{\mathcal{P}} |h, n, \mathbf{k}\rangle^{(\omega)}_{(r,m_q)} = \eta_{h,n} |h, n, -\mathbf{k}\rangle^{(-\omega)}_{(r,m_q)}, \tag{F.8}$$

is immediately seen to be a consequence of eqs. (F.3), (F.6) and (F.7). By construction (see eq. (F.7)) $\eta_{h,n}$ can only take the values ± 1. The relation (F.8) is nothing but eq. (5.18) of section 5.3.2.

Whether the parity label $\eta_{h,n}$ is 1 or -1 can be decided numerically by the method discussed in section 5.3.3. The resulting value of $\eta_{h,n}$ — at least for values of the bare parameters for which quantities of $O(a^2)$ and $O(a^0)$ can be unambiguously distinguished — is to be identified with the parity quantum number of the state corresponding to $|h, n, \mathbf{k}\rangle_{(r,m_q)}$ in the continuum limit. By construction $\eta_{h,n}$ is independent of the three-momentum of the state, but does depend on the excitation level n because $\mathcal{P}$ is not an exact symmetry of tm-LQCD. There may exist, in fact, states with opposite parities but the same unbroken tm-LQCD quantum numbers. For instance in the vacuum sector one encounters the vacuum itself (with $\eta_\Omega = 1$), the neutral pion (with $\eta_{\pi^0} = -1$), etc.

We observe in conclusion that one could decide to separately alter the phases of the states $|h, n, \mathbf{k}\rangle^{(\omega)}_{(r,m_q)}$ and $|h, n, -\mathbf{k}\rangle^{(-\omega)}_{(r,m_q)}$ with respect to what one gets from the above construction. If one does so, then track of this modification should be kept in all the relevant equations, in particular in eq. (F.8). The only consequence of this choice is that all lattice formulae relating quantities with opposite values of ω, or with values of ω differing by π, become unnaturally and unnecessarily cumbersome.

F.1 Proving eq. (F.5)

Let us finally come to the proof of eq. (F.5). For this purpose it is convenient to consider the general two-point correlator

$$G_{\Phi_h \Xi_h}(\mathbf{k}, t; \omega, r, m_q) = a^3 \sum_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} \langle \Phi_h(\mathbf{x}, t)\, \Xi_h^\dagger(\mathbf{0}, 0)\rangle\Big|^{(\omega)}_{(r,m_q)}, \tag{F.9}$$

where Φ_h and Ξ_h are two arbitrary local operators with formal parities η_{Φ_h} and η_{Ξ_h} and equal unnbroken quantum numbers h. Performing the change of variables induced by (5.4), one obtains

$$G_{\Phi_h \Xi_h}(\mathbf{k}, t; \omega, r, m_q) = \eta_{\Phi_h} \eta_{\Xi_h} G_{\Phi_h \Xi_h}(-\mathbf{k}, t; -\omega, r, m_q)\,. \tag{F.10}$$

[25]This phase can always be readsorbed in a physically unconsequential redefinition of the overall phase of the state $|h, n, \mathbf{k}\rangle|^{(\omega)}_{(r,m_q)}$. See also the comment at the end of this section.

By comparing the spectral representations of the two sides of eq. (F.10) and using eq. (5.15), we can get the set of relations

$$\langle\Omega|\Phi_h(\mathbf{0},0)|h,n,\mathbf{k}\rangle\langle h,n,\mathbf{k}|\Xi_h^\dagger(\mathbf{0},0)|\Omega\rangle\Big|_{(r,m_q)}^{(\omega)} = \\ = \eta_{\Phi_h}\eta_{\Xi_h}\langle\Omega|\Phi_h(\mathbf{0},0)|h,n,-\mathbf{k}\rangle\langle h,n,-\mathbf{k}|\Xi_h^\dagger(\mathbf{0},0)|\Omega\rangle\Big|_{(r,m_q)}^{(-\omega)}, \tag{F.11}$$

thanks to the leverage we have from the dependence of $G_{\Phi_h\Xi_h}$ on t. Inserting factors $\widehat{\mathcal{P}}^2 = \mathbb{1}$ on the l.h.s. of eq. (F.11) yields

$$\langle\Omega|\widehat{\mathcal{P}}\,\Phi_h(\mathbf{0},0)\widehat{\mathcal{P}}|h,n,\mathbf{k}\rangle\langle h,n,\mathbf{k}|\widehat{\mathcal{P}}\,\Xi_h^\dagger(\mathbf{0},0)\widehat{\mathcal{P}}|\Omega\rangle\Big|_{(r,m_q)}^{(\omega)} = \\ = \langle\Omega|\Phi_h(\mathbf{0},0)|h,n,-\mathbf{k}\rangle\langle h,n,-\mathbf{k}|\Xi_h^\dagger(\mathbf{0},0)|\Omega\rangle\Big|_{(r,m_q)}^{(-\omega)}. \tag{F.12}$$

If we now combine eq. (F.1) with eq. (F.12) and exploit the arbitrariness of the operators Φ_h and Ξ_h, we arrive at the relation (F.5).

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