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O(a) improved twisted mass lattice QCD

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Abstract: Lattice QCD with Wilson quarks and a chirally twisted mass term (tmQCD) has been introduced in refs. [1, 2]. We here apply Symanzik's improvement programme to this theory and list the counterterms which arise at first order in the lattice spacing a. Based on the generalised transfer matrix, we define the tmQCD Schrödinger functional and use it to derive renormalized on-shell correlation functions. By studying their continuum approach in perturbation theory we then determine the new O(a) counterterms of the action and of a few quark bilinear operators to one-loop order.

Keywords: Lattice Gauge Field Theories, Lattice QCD.

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Contents

1. Introduction

In ref. [2] twisted mass lattice QCD (tmQCD) has been introduced as a solution to the problem of unphysical fermion zero modes which plague standard lattice QCD with quarks of the Wilson type. We will assume that the reader is familiar with the motivation of this approach, and refer to [1] for an introduction. The main topic of the present paper is the application of Symanizik's improvement programme to tmQCD. We introduce the set-up in the simplest case of two mass-degenerate quarks, and study the improved action and the improved composite fields which appear in the PCAC and PCVC relations.

Our strategy follows closely refs. [3, 4, 5]: in section 2 we go through the structure of the O(a) improved theory. We then define the Schrödinger functional for tmQCD, and use it to derive suitable on-shell correlation functions (section 3). The perturbation expansion is then carried out along the lines of ref. [5], and the new O(a) improvement coefficients are obtained at the tree-level in section 4 and to one-loop order in section 5. A few details have been delegated to appendices. Appendix A describes how the twisted mass term can be incorporated in Lüscher's construction of the transfer matrix [6], and appendix B contains the analytic expressions for the coefficients used in the analysis of the one-loop calculation.

2. Renormalized and O(a) improved tmQCD

The renormalization procedure for twisted mass lattice QCD with Wilson quarks has already been discussed in ref. [2]. Here we apply Symanzik's improvement programme to first order in the lattice spacing a. The procedure is standard and the details of its application to lattice QCD with N_f mass degenerate Wilson quarks can be found in ref. [3].

Our starting point is the unimproved tmQCD lattice action for a doublet of mass degenerate quarks,

$$S[U,\bar{\psi},\psi] = S_\mathrm{G}[U] + S_\mathrm{F}[U,\bar{\psi},\psi]\,, \qquad (2.1)$$

with the standard Wilson gauge action and the fermionic part

$$S_\mathrm{F}[U,\bar{\psi},\psi] = a^4 \sum_x \bar{\psi}(x)\left(D + m_0 + i\mu_\mathrm{q}\gamma_5\tau^3\right)\psi(x)\,. \qquad (2.2)$$

The massless Wilson-Dirac operator is given by

$$D = \frac{1}{2}\sum_\mu \left\{(\nabla_\mu + \nabla_\mu^*)\gamma_\mu - a\nabla_\mu^*\nabla_\mu\right\}, \qquad (2.3)$$

where the forward and backward covariant lattice derivatives in direction μ are denoted by ∇_μ and ∇_μ^*, respectively. As tmQCD with vanishing twisted mass parameter μ_q reduces to standard lattice QCD we expect that improvement is achieved by using the standard O(a) improved theory and adding the appropriate O(a) counterterms which are proportional to (powers of) μ_q, and which are allowed by the lattice symmetries. The procedure hence consists in a straightforward extension of ref. [3], and we take over notation and conventions from this reference without further notice.

2.1 Renormalized $\mathrm{O}(a)$ improved parameters

Following ref. [3] we assume that a mass-independent renormalization scheme has been chosen, and we take the same steps as done there for standard lattice QCD. At $\mu_\mathrm{q} = 0$ the Sheikholeslami-Wohlert term [7] suffices to improve the action, up to a rescaling of the bare parameters by terms proportional to the subtracted bare mass $m_\mathrm{q} = m_0 - m_\mathrm{c}$ [3]. At non-vanishing μ_q we find that improved bare parameters are of the form

$$\begin{aligned} \tilde{g}_0^2 &= g_0^2(1 + b_\mathrm{g} a m_\mathrm{q}) \,, \\ \widetilde{m}_\mathrm{q} &= m_\mathrm{q}(1 + b_\mathrm{m} a m_\mathrm{q}) + \tilde{b}_\mathrm{m} a \mu_\mathrm{q}^2 \,, \\ \widetilde{\mu}_\mathrm{q} &= \mu_\mathrm{q}(1 + b_\mu a m_\mathrm{q}) \,, \end{aligned} \tag{2.4}$$

i.e. there exist two new counterterms with coefficients b_μ and $\tilde{b}_\mathrm{m}$. The renormalized $\mathrm{O}(a)$ improved mass and coupling constant are then proportional to these parameters, viz.

$$g_\mathrm{R}^2 = \tilde{g}_0^2 Z_\mathrm{g}(\tilde{g}_0^2, a\mu) \,, \qquad m_\mathrm{R} = \widetilde{m}_\mathrm{q} Z_\mathrm{m}(\tilde{g}_0^2, a\mu) \,, \qquad \mu_\mathrm{R} = \widetilde{\mu}_\mathrm{q} Z_\mu(\tilde{g}_0^2, a\mu) \,. \tag{2.5}$$

The ratio of the appropriately renormalized mass parameters determines the angle α which is involved in the physical interpretation of the theory [2]. We will discuss below the general $\mathrm{O}(a)$ improved definition of α. Here we note that the case of particular interest, $\alpha = \pi/2$, corresponds to $m_\mathrm{R} = 0$, which implies $m_\mathrm{q} = \mathrm{O}(a)$ [2]. In this case all the usual b-coefficients multiply terms of $\mathrm{O}(a^2)$ and are thus negligible in the spirit of $\mathrm{O}(a)$ improvement. One then remains with a single coefficient $\tilde{b}_\mathrm{m}$, which compares favorably to the situation in standard lattice QCD where two coefficients, b_m and b_g, are required.

2.2 Renormalized $\mathrm{O}(a)$ improved composite fields

We assume that composite fields are renormalized in a mass-independent scheme, and such that the tmQCD Ward identities are respected [2]. Attention will be restricted to the quark bilinear operators which appear in the PCAC and PCVC relations. Moreover, we only consider the first two flavour components, and thus avoid the renormalization of power divergent operators such as the iso-singlet scalar density [2]. As explained in ref. [2], the third flavour component of the PCAC and PCVC relations can be inferred in the continuum limit, by assuming the restoration of the physical isospin symmetry. The $\mathrm{O}(a)$ improved currents and pseudo-scalar density with indices $a, b \in \{1, 2\}$ are then parameterised as follows,

$$(A_\mathrm{R})_\mu^a = Z_\mathrm{A}(1 + b_\mathrm{A} a m_\mathrm{q}) \left[A_\mu^a + c_\mathrm{A} a \tilde{\partial}_\mu P^a + a\mu_\mathrm{q} \, \tilde{b}_\mathrm{A} \, \varepsilon^{3ab} V_\mu^b \right] , \tag{2.6}$$

$$(V_\mathrm{R})_\mu^a = Z_\mathrm{V}(1 + b_\mathrm{V} a m_\mathrm{q}) \left[V_\mu^a + c_\mathrm{V} a \tilde{\partial}_\nu T_{\mu\nu}^a + a\mu_\mathrm{q} \, \tilde{b}_\mathrm{V} \, \varepsilon^{3ab} A_\mu^b \right] , \tag{2.7}$$

$$(P_\mathrm{R})^a = Z_\mathrm{P}(1 + b_\mathrm{P} a m_\mathrm{q}) \, P^a \,. \tag{2.8}$$

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Here we have chosen the bare operators which are local on the lattice, with the conventions of ref. [3]. While this is the simplest choice, we also recall the definition of the point-split vector current,

$$\widetilde{V}_\mu^a(x) = \frac{1}{2}\left\{\bar\psi(x)(\gamma_\mu - 1)\frac{\tau^a}{2}U(x,\mu)\psi(x+a\hat\mu) + \right.$$
$$\left. + \bar\psi(x+a\hat\mu)(\gamma_\mu + 1)\frac{\tau^a}{2}U(x,\mu)^{-1}\psi(x)\right\}, \tag{2.9}$$

which is obtained through a vector variation of the action. This current is protected against renormalization, and the PCVC relation

$$\partial_\mu^* \tilde{V}_\mu^a(x) = -2\mu_{\rm q}\varepsilon^{3ab}P^b(x)\,, \tag{2.10}$$

is an *exact* lattice identity, with the local pseudo-scalar density and the backward derivative ∂_μ^* in μ-direction [2]. This implies the identity $Z_\mu Z_{\rm P} = 1$ in any renormalization scheme which respects the PCVC relation.

2.3 An alternative definition of the improved vector current

An alternative renormalized improved current can be obtained from the point-split current (2.9). For this it is convenient to start from the symmetrized version

$$\bar{V}_\mu^a(x) = \frac{1}{2}\left(\widetilde{V}_\mu^a(x) + \widetilde{V}_\mu^a(x - a\hat\mu)\right), \tag{2.11}$$

which behaves under space-time reflections in the same way as the local vector current. The counterterm structure then is the same as in eq. (2.7), i.e. one finds

$$(\bar{V}_{\rm R})_\mu^a = Z_{\bar{\rm V}}(1 + b_{\bar{\rm V}}am_{\rm q})\left[\bar{V}_\mu^a + c_{\bar{\rm V}}a\tilde\partial_\nu T_{\mu\nu}^a + \tilde{b}_{\bar{\rm V}}a\mu_{\rm q}\varepsilon^{3ab}A_\mu^b\right], \tag{2.12}$$

where we have again restricted the indices a, b to the first two components. One may now easily show that

$$Z_{\bar{\rm V}} = 1\,, \qquad b_{\bar{\rm V}} = 0\,. \tag{2.13}$$

To see this we first note that at $\mu_{\rm q} = 0$ the vector charge of this current is given by

$$Q_{\bar{\rm V}}^a(t) = \frac{1}{2}Z_{\bar{\rm V}}(1 + b_{\bar{\rm V}}am_{\rm q})\left[Q_{\rm V}^a(t) + Q_{\rm V}^a(t-a)\right], \tag{2.14}$$

with

$$Q_{\rm V}^a(x_0) = a^3\sum_{\mathbf{x}}\widetilde{V}_0^a(x)\,. \tag{2.15}$$

At $\mu_{\rm q} = 0$, correlation functions of the charge are x_0-independent,[1] and the O(a) improved charge algebra for $Q_{\bar{\rm V}}^a$ and the exact charge algebra for $Q_{\rm V}^a$ together imply that the whole renormalization factor in eq. (2.14) must be unity. As this holds independently of $m_{\rm q}$, one arrives at the conclusion (2.13).

[1] i.e. as long as the time ordering of the space-time arguments in the given correlation function remains unchanged.

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A further relation is obtained by noting that the PCVC relation between the renormalized O(a) improved fields,

$$\tilde{\partial}_\mu (\bar{V}_{\rm R})^a_\mu = -2\mu_{\rm R}\varepsilon^{3ab}(P_{\rm R})^b\,, \tag{2.16}$$

with the symmetric derivative $\tilde{\partial}_\mu = \frac{1}{2}(\partial_\mu + \partial^*_\mu)$ must hold up to O(a^2) corrections. Then, using the identity

$$\tilde{\partial}_\mu \bar{V}^a_\mu(x) = \partial^*_\mu \left(\widetilde{V}^a_\mu(x) + \frac{1}{4}a^2\partial^*_\mu\partial_\mu \widetilde{V}^a_\mu(x)\right)\,, \tag{2.17}$$

one obtains the relation

$$Z_{\rm P}Z_{\rm m}Z_{\rm A}^{-1}\tilde{b}_{\bar{\rm V}} = -(b_\mu + b_{\rm P})\,. \tag{2.18}$$

The scale-independent combination of renormalization constants multiplying $\tilde{b}_{\bar{\rm V}}$ is determined by axial Ward identities [8], so that eq. (2.18) can be considered a relation between improvement coefficients.

2.4 O(a) improved definition of the angle α

The physical interpretation of the correlation functions in tmQCD depends on the angle α, which is defined through

$$\tan\alpha = \frac{\mu_{\rm R}}{m_{\rm R}}\,. \tag{2.19}$$

In this equation $\mu_{\rm R}$ and $m_{\rm R}$ are the O(a) improved renormalized mass parameters which appear in the PCAC and PCVC relations [2]. Up to terms of O(a^2) we then find

$$\frac{\mu_{\rm R}}{m_{\rm R}} = \frac{\mu_{\rm q}[1+(b_\mu - b_{\rm m})am_{\rm q}]}{Z_{\rm P}Z_{\rm m}[m_{\rm q} + \tilde{b}_{\rm m}a\mu_{\rm q}^2]} = \frac{\mu_{\rm q}[1+(b_\mu + b_{\rm P} - b_{\rm A})am_{\rm q}]}{Z_{\rm A}[m + \tilde{b}_{\rm A}a\mu_{\rm q}^2 Z_{\rm V}^{-1}]}\,. \tag{2.20}$$

Here, m denotes a bare mass which is obtained from some matrix element of the PCAC relation involving the unrenormalized axial current $A^1_\mu + c_{\rm A}\partial_\mu P^1$ and the local density P^1. Given m, the critical mass $m_{\rm c}$, and the finite renormalization constants $Z_{\rm A}$, $Z_{\rm V}$ and $Z_{\rm P}Z_{\rm m}$, the determination of the O(a) improved angle requires the knowledge of two (combinations of) improvement coefficients, which may be chosen to be $b_\mu - b_{\rm m}$ and $\tilde{b}_{\rm m}$, or $b_\mu + b_{\rm P} - b_{\rm A}$ and $\tilde{b}_{\rm A}$. A special case is again $\alpha = \pi/2$, which is obtained for vanishing denominators in eq. (2.20). For this it is sufficient to know either $\tilde{b}_{\rm A}$ or $\tilde{b}_{\rm m}$, and the finite renormalization constants $Z_{\rm A}$ or $Z_{\rm P}Z_{\rm m}$ are then not needed.

2.5 Redundancy of improvement coefficients

Having introduced all O(a) counterterms allowed by the lattice symmetries, it is guaranteed that there exists a choice for the improvement coefficients such that O(a) lattice artefacts in on-shell correlation functions are completely eliminated. We now want to show that there is in fact a redundancy in the set of the new counterterms introduced so far, i.e. the counterterms are not unambiguously determined by the requirement of on-shell improvement alone. To see this we consider the renormalized 2-point functions

$$\begin{aligned} G_{\rm A}(x-y) &= \left\langle (A_{\rm R})^1_0(x)(P_{\rm R})^1(y)\right\rangle , \\ G_{\rm V}(x-y) &= \left\langle (V_{\rm R})^2_0(x)(P_{\rm R})^1(y)\right\rangle , \end{aligned} \tag{2.21}$$

of the renormalized O(a) improved fields defined in subsection 2.2. We assume that a quark mass independent renormalization scheme has been chosen, and with the proper choice for the improvement coefficients one finds,

$$G_{\rm X}(x) = \lim_{a\to 0} G_{\rm X}(x) + {\rm O}(a^2)\,, \qquad {\rm X} = {\rm A}, {\rm V}\,, \tag{2.22}$$

provided that x is kept non zero in physical units. If the new improvement coefficients $\tilde{b}_{\rm m}$, b_μ, $\tilde{b}_{\rm A}$ and $\tilde{b}_{\rm V}$ were all necessary any change of O(1) in these coefficients would introduce uncancelled O(a) artefacts in eq. (2.22). Varying the coefficients $\tilde{b}_{\rm m} \to \tilde{b}_{\rm m} + \Delta\tilde{b}_{\rm m}$, $b_\mu \to b_\mu + \Delta b_\mu$ and $\tilde{b}_{\rm A} \to \tilde{b}_{\rm A} + \Delta\tilde{b}_{\rm A}$ in the correlation function $G_{\rm A}(x)$, we find that the correlation function itself changes according to

$$\begin{aligned} \Delta G_{\rm A}(x) = -a\mu_{\rm R} Z_{\rm P} \Big[& \Delta\tilde{b}_{\rm m} Z_{\rm P} Z_{\rm m}\, \mu_{\rm R} \frac{\partial}{\partial m_{\rm R}} G_{\rm A}(x) + \Delta b_\mu (Z_{\rm P} Z_{\rm m})^{-1} m_{\rm R} \frac{\partial}{\partial \mu_{\rm R}} G_{\rm A}(x) - \\ & - \Delta\tilde{b}_{\rm A} Z_{\rm A} Z_{\rm V}^{-1} G_{\rm V}(x) \Big]\,, \end{aligned} \tag{2.23}$$

where terms of O(a^2) have been neglected. In the derivation of this equation one has to be careful to correctly take into account the counterterms proportional to b_μ and $\tilde{b}_{\rm m}$. First of all we notice that changing an O(a) counterterm can only induce changes of O(a) in the correlation function. For instance, the equation

$$G_{\rm A}(x)|_{b_\mu \to b_\mu + \Delta b_\mu} = G_{\rm A}(x) + \Delta b_\mu \frac{\partial}{\partial b_\mu} G_{\rm A}(x) + {\rm O}(a^2)\,, \tag{2.24}$$

holds even for finite changes Δb_μ. Second, when taking the continuum limit the bare mass parameters become functions of the improvement coefficients such that the renormalized O(a) improved masses are fixed. For instance one has

$$\mu_{\rm q} = Z_{\rm P} \mu_{\rm R} (1 - b_\mu Z_{\rm m}^{-1} a m_{\rm R}) + {\rm O}(a^2)\,, \tag{2.25}$$

and a straightforward application of the chain rule leads to

$$\frac{\partial}{\partial b_\mu} G_{\rm A}(x) = \left(\frac{\partial \mu_{\rm q}}{\partial b_\mu}\right) \frac{\partial}{\partial \mu_{\rm q}} G_{\rm A}(x) = -a\mu_{\rm R} m_{\rm R} Z_{\rm P} Z_{\rm m}^{-1} \frac{\partial}{\partial \mu_{\rm q}} G_{\rm A}(x)\,, \tag{2.26}$$

where we have used eq. (2.25) and neglected terms of O(a^2). Proceeding in the same way for the variation with respect to $\tilde{b}_{\rm m}$, and changing to renormalized parameters $\mu_{\rm q} = Z_{\rm P}\mu_{\rm R} + {\rm O}(a)$, $m_{\rm q} = Z_m^{-1} m_{\rm R} + {\rm O}(a)$ eventually leads to eq. (2.23).

At this point we recall ref. [2, eq. (3.13)], which expresses the reparameterization invariance with respect to changes of the angle α. In terms of the above correlation functions one finds, up to cutoff effects,

$$\frac{\partial}{\partial\alpha}G_{\rm A}(x) \equiv \left(m_{\rm R}\frac{\partial}{\partial\mu_{\rm R}} - \mu_{\rm R}\frac{\partial}{\partial m_{\rm R}}\right) G_{\rm A}(x) = -G_{\rm V}(x)\,. \tag{2.27}$$

As a consequence not all the terms in eq. (2.23) are independent, and the requirement that $\Delta G_{\rm A}(x)$ be of order a^2 entails only two conditions,

$$\begin{aligned}\Delta\tilde{b}_{\rm m} + \Delta b_\mu(Z_{\rm P}Z_{\rm m})^{-2} &= 0\,,\\ \Delta\tilde{b}_{\rm m} - \Delta\tilde{b}_{\rm A}(Z_{\rm P}Z_{\rm m}Z_{\rm V})^{-1}Z_{\rm A} &= 0\,.\end{aligned} \tag{2.28}$$

This makes precise the redundancy or over-completeness of the counterterms alluded to above. The same procedure applies to $G_{\rm V}(x)$, and we conclude that the requirement of on-shell O(a) improvement only determines the combinations of improvement coefficients $\tilde{b}_{\rm m} + b_\mu(Z_{\rm P}Z_{\rm m})^{-2}$, $\tilde{b}_{\rm m} - \tilde{b}_{\rm V}(Z_{\rm P}Z_{\rm m}Z_{\rm A})^{-1}Z_{\rm V}$, and $\tilde{b}_{\rm m} - \tilde{b}_{\rm A}(Z_{\rm P}Z_{\rm m}Z_{\rm V})^{-1}Z_{\rm A}$. We emphasize that this redundancy is a generic feature of tmQCD, and not linked to special choices for the fields or correlation functions. In particular we note that the third component of the axial variation of any composite field ϕ has the correct quantum numbers to appear as an O($a\mu_{\rm q}$) counterterm to ϕ itself.

In conclusion, O(a) improved tmQCD as defined here constitutes a one-parameter family of improved theories. In view of practical applications it is most convenient to choose $\tilde{b}_{\rm m}$ as the free parameter and set it to some numerical value. For reasons to become clear in section 4 our preferred choice is $\tilde{b}_{\rm m} = -1/2$. However, in the following we will keep all coefficients as unknowns and only make a choice at the very end. In order to define on-shell correlation functions which are readily accessible to perturbation theory we will first define the Schrödinger functional for tmQCD. It is then straightforward to extend the techniques of refs. [4, 5] to tmQCD and study the continuum approach of correlation functions derived from the Schrödinger functional.

3. The Schrödinger functional for tmQCD

This section follows closely ref. [3, section 5] and ref. [4]. The reader will be assumed familiar with these references, and we will refer to equations there by using the prefix I and II, respectively.

3.1 Definition of the Schrödinger functional

To define the Schrödinger functional for twisted mass lattice QCD, it is convenient to follow refs. [9, 10]. The Schrödinger functional is thus obtained as the integral kernel of some integer power T/a of the transfer matrix. Its euclidean representation is given by

$$\mathcal{Z}[\rho', \bar{\rho}', C'; \rho, \bar{\rho}, C] = \int \mathrm{D}[U]\mathrm{D}[\psi]\mathrm{D}[\bar{\psi}]\ \mathrm{e}^{-S[U,\bar{\psi},\psi]}\,, \tag{3.1}$$

and is thus considered as a functional of the fields at euclidean times 0 and T. From the structure of the transfer matrix it follows that the boundary conditions for all fields are the same as in the standard framework. In particular, the quark fields satisfy,

$$\begin{aligned} P_+\psi|_{x_0=0} &= \rho\,, \qquad & P_-\psi|_{x_0=T} &= \rho'\,, \\ \bar{\psi}P_-|_{x_0=0} &= \bar{\rho}\,, \qquad & \bar{\psi}P_+|_{x_0=T} &= \bar{\rho}'\,, \end{aligned} \tag{3.2}$$

with the usual projectors $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$. The gauge field boundary conditions are as in eqs. (I.4.1) and (I.4.2) and will not be repeated here.

The action in eq. (3.1),

$$S[U, \bar{\psi}, \psi] = S_{\mathrm{G}}[U] + S_{\mathrm{F}}[U, \bar{\psi}, \psi]\,, \tag{3.3}$$

splits into the gauge part (I.4.5) and the quark action, which assumes the same form as on the infinite lattice (2.2). Note that we adopt the same conventions as in [3, subsection 4.2], in particular the quark and antiquark fields are extended to all times by "padding" with zeros, and the covariant derivatives in the finite space-time volume now contain the additional phase factors related to θ_k, ($k = 1, 2, 3$).

3.2 Renormalization and O(a) improvement

Renormalizability of the tmQCD Schrödinger functional could be verified along the lines of ref. [11]. However, this is not necessary as any new counterterm is expected to be proportional to the twisted mass parameter and is therefore at least of mass dimension 4. One therefore expects the Schrödinger functional to be finite after renormalization of the mass parameters and the gauge coupling as in infinite volume [2], and by scaling the quark and anti-quark boundary fields with a common renormalization constant [11]. This expectation will be confirmed in the course of the perturbative calculation.

The structure of the new counterterms at O(a) is again determined by the symmetries. These are the same as in infinite space-time volume, except for those which exchange spatial and temporal directions. The improved action,

$$S_{\mathrm{impr}}[U, \bar{\psi}, \psi] = S[U, \bar{\psi}, \psi] + \delta S_{\mathrm{v}}[U, \bar{\psi}, \psi] + \delta S_{\mathrm{G,b}}[U] + \delta S_{\mathrm{F,b}}[U, \bar{\psi}, \psi]\,, \tag{3.4}$$

has the same structure as in the standard framework, in particular, δS_{v} and $\delta S_{\mathrm{G,b}}$ are as given in eqs. (I.5.3) and (I.5.6). The symmetries allow for two new fermionic boundary counterterms,

$$\mathcal{O}_\pm = i\mu_{\mathrm{q}}\bar{\psi}\gamma_5\tau^3 P_\pm\psi\,. \tag{3.5}$$

The equations of motion do not lead to a further reduction and the action with the fermionic boundary counterterms at $\mathrm{O}(a)$ is then given by

$$\begin{aligned}\delta S_{\mathrm{F,b}}[U,\bar{\psi},\psi] = a^4\sum_{\mathbf{x}}\Big\{&(\tilde{c}_\mathrm{s}-1)\Big[\widehat{\mathcal{O}}_\mathrm{s}(\mathbf{x})+\widehat{\mathcal{O}}'_\mathrm{s}(\mathbf{x})\Big]+(\tilde{c}_\mathrm{t}-1)\Big[\widehat{\mathcal{O}}_\mathrm{t}(\mathbf{x})-\widehat{\mathcal{O}}'_\mathrm{t}(\mathbf{x})\Big]+\\ &+(\tilde{b}_1-1)\Big[\widehat{Q}_1(\mathbf{x})+\widehat{Q}'_1(\mathbf{x})\Big]+\\ &+(\tilde{b}_2-1)\Big[\widehat{Q}_2(\mathbf{x})+\widehat{Q}'_2(\mathbf{x})\Big]\Big\}\,. \end{aligned}\tag{3.6}$$

Here, we have chosen lattice operators as follows,

$$\begin{aligned}\widehat{Q}_1(\mathbf{x}) &= i\mu_\mathrm{q}\bar{\psi}(x)\gamma_5\tau^3\psi(x)\big|_{x_0=a}\,,\\ \widehat{Q}'_1(\mathbf{x}) &= i\mu_\mathrm{q}\bar{\psi}(x)\gamma_5\tau^3\psi(x)\big|_{x_0=T-a}\,,\\ \widehat{Q}_2(\mathbf{x}) &= i\mu_\mathrm{q}\bar{\rho}(\mathbf{x})\gamma_5\tau^3\rho(\mathbf{x})\,,\\ \widehat{Q}'_2(\mathbf{x}) &= i\mu_\mathrm{q}\bar{\rho}'(\mathbf{x})\gamma_5\tau^3\rho'(\mathbf{x})\,,\end{aligned}\tag{3.7}$$

and the expressions for the lattice operators $\widehat{\mathcal{O}}_{\mathrm{s,t}}$ and $\widehat{\mathcal{O}}'_{\mathrm{s,t}}$ are given in eqs. (I.5.21)–(I.5.24). Note that the improvement coefficients are the same for both boundaries, as the counterterms are related by a time reflection combined with a flavour exchange.

3.3 Dirac equation and classical solutions

For euclidean times $0 < x_0 < T$ the lattice Dirac operator and its adjoint are formally defined through

$$\begin{aligned}\frac{\delta S_\mathrm{impr}}{\delta\bar{\psi}(x)} &= (D+\delta D+m_0+i\mu_\mathrm{q}\gamma_5\tau^3)\psi(x)\,,\\ -\frac{\delta S_\mathrm{impr}}{\delta\psi(x)} &= \bar{\psi}(x)(\overleftarrow{D}^\dagger+\delta\overleftarrow{D}^\dagger+m_0+i\mu_\mathrm{q}\gamma_5\tau^3)\,,\end{aligned}\tag{3.8}$$

where $\delta D = \delta D_\mathrm{v} + \delta D_\mathrm{b}$ is the sum of the volume and the boundary $\mathrm{O}(a)$ counterterms. Equation (II.2.3) for the volume counterterms remains valid, whereas for the boundary counterterms one obtains

$$\begin{aligned}\delta D_\mathrm{b}\psi(x) = (\tilde{c}_\mathrm{t}-1)\frac{1}{a}\big\{&\delta_{x_0,a}\left[\psi(x)-U(x-a\hat{0},0)^{-1}P_+\psi(x-a\hat{0})\right]+\\ &+\delta_{x_0,T-a}\left[\psi(x)-U(x,0)P_-\psi(x+a\hat{0})\right]\big\}+\\ +(\tilde{b}_1-1)&\left[\delta_{x_0,a}+\delta_{x_0,T-a}\right]i\mu_\mathrm{q}\gamma_5\tau^3\psi(x)\,.\end{aligned}\tag{3.9}$$

We observe that the net effect of the additional counterterm consists in the replacement $\mu_\mathrm{q}\to\tilde{b}_1\mu_\mathrm{q}$ close to the boundaries. Although a boundary $\mathrm{O}(a)$ effect is unlikely to have a major impact, we note that the presence of this counterterm with a general coefficient $\tilde{b}_1$ invalidates the argument by which zero modes of the Wilson-Dirac operator are absent in twisted mass lattice QCD. To circumvent this problem we remark that the counterterm may also be implemented by explicit insertions into the correlation functions. As every insertion comes with a power of a, a single insertion will be sufficient in most cases, yielding a result that is equivalent up to terms of $\mathrm{O}(a^2)$.

Given the Dirac operator, the propagator is now defined through

$$(D + \delta D + m_0 + i\mu_{\mathrm{q}}\gamma_5\tau^3)S(x,y) = a^{-4}\delta_{xy}\,, \qquad 0 < x_0 < T\,, \tag{3.10}$$

and the boundary conditions

$$P_+ S(x,y)|_{x_0=0} = P_- S(x,y)|_{x_0=T} = 0\,. \tag{3.11}$$

Boundary conditions in the second argument follow from the conjugation property,

$$S(x,y)^\dagger = \gamma_5\tau^1 S(y,x)\gamma_5\tau^1\,, \tag{3.12}$$

which is the usual one up to an exchange of the flavour components.

As in the standard framework [4, 11], it is useful to consider the classical solutions of the Dirac equation,

$$\begin{aligned} \left(D + \delta D + m_0 + i\mu_{\mathrm{q}}\gamma_5\tau^3\right)\psi_{\mathrm{cl}}(x) &= 0\,, \\ \bar{\psi}_{\mathrm{cl}}(x)\left(\overleftarrow{D}^\dagger + \delta\overleftarrow{D}^\dagger + m_0 + i\mu_{\mathrm{q}}\gamma_5\tau^3\right) &= 0\,. \end{aligned} \tag{3.13}$$

Here, the time argument is restricted to $0 < x_0 < T$, while at the boundaries the classical solutions are required to satisfy the inhomogeneous boundary conditions (3.2). It is not difficult to obtain the explicit expressions,

$$\begin{aligned} \psi_{\mathrm{cl}}(x) &= \tilde{c}_{\mathrm{t}} a^3 \sum_{\mathbf{y}} \Big\{ S(x,y)U\,(y-a\hat{0},0)^{-1}P_+\rho(\mathbf{y})\big|_{y_0=a} + \\ &\qquad + \; S(x,y)U(y,0)P_-\;\rho'(\mathbf{y})\big|_{y_0=T-a}\Big\}\,, \\ \bar{\psi}_{\mathrm{cl}}(x) &= \tilde{c}_{\mathrm{t}} a^3 \sum_{\mathbf{y}} \Big\{ \bar{\rho}(\mathbf{y})P_-\;U(y-a\hat{0},0)S(y,x)\big|_{y_0=a} + \\ &\qquad + \bar{\rho}'(\mathbf{y})P_+\;U(y,0)^{-1}S(y,x)\big|_{y_0=T-a}\Big\}\,, \end{aligned} \tag{3.14}$$

which are again valid for $0 < x_0 < T$. Note that these expressions are exactly the same as in ref. [4], except that the quark propagator here is the solution of eq. (3.10).

3.4 Quark functional integral and basic 2-point functions

We shall use the same formalism for the quark functional integral as described in subsection II.2.3. Most of the equations can be taken over literally, in particular, eq. (II.2.21) holds again. The presence of the twisted mass term merely leads to a

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modification of the improved action of the classical fields, [eq. (II.2.22)], which is now given by

$$
\begin{aligned}
S_{\mathrm{F,impr}}[U,\bar\psi_{\mathrm{cl}},\psi_{\mathrm{cl}}] = a^3\sum_{\mathbf{x}}\Big\{ & \tilde b_2 a\mu_{\mathrm{q}}\left[\bar\rho(\mathbf{x})i\gamma_5\tau^3\rho(\mathbf{x})+\bar\rho'(\mathbf{x})i\gamma_5\tau^3\rho'(\mathbf{x})\right]+\\
&+\tilde c_{\mathrm{s}}a\Big[\bar\rho(\mathbf{x})\gamma_k\frac{1}{2}(\nabla_k+\nabla_k^*)\rho(\mathbf{x})+\\
&\qquad+\bar\rho'(\mathbf{x})\gamma_k\frac{1}{2}(\nabla_k+\nabla_k^*)\rho'(\mathbf{x})\Big]-\\
&-\tilde c_{\mathrm{t}}\left[\bar\rho(\mathbf{x})U(x-a\hat 0,0)\psi_{\mathrm{cl}}(x)\big|_{x_0=a}+\right.\\
&\left.+\bar\rho'(\mathbf{x})U(x,0)^{-1}\psi_{\mathrm{cl}}(x)\,|_{x_0=T-a}\right]\Big\}\,.
\end{aligned} \tag{3.15}
$$

The quark action is a quadratic form in the Grassmann fields, and the functional integral can be solved explicitly. Therefore, in a fixed gauge field background any fermionic correlation function can be expressed in terms of the basic two-point functions. Besides the propagator already introduced above,

$$
\left[\psi(x)\bar\psi(y)\right]_{\mathrm{F}} = S(x,y)\,, \tag{3.16}
$$

we note that the boundary-to-volume correlators can be written in a convenient way using the classical solutions,

$$
\begin{aligned}
\left[\zeta(\mathbf{x})\bar\psi(y)\right]_{\mathrm{F}} &= \frac{\delta\bar\psi_{\mathrm{cl}}(y)}{\delta\bar\rho(\mathbf{x})}\,, \qquad & \left[\psi(x)\bar\zeta(\mathbf{y})\right]_{\mathrm{F}} &= \frac{\delta\psi_{\mathrm{cl}}(x)}{\delta\rho(\mathbf{y})}\,,\\
\left[\zeta'(\mathbf{x})\bar\psi(y)\right]_{\mathrm{F}} &= \frac{\delta\bar\psi_{\mathrm{cl}}(y)}{\delta\bar\rho'(\mathbf{x})}\,, \qquad & \left[\psi(x)\bar\zeta'(\mathbf{y})\right]_{\mathrm{F}} &= \frac{\delta\psi_{\mathrm{cl}}(x)}{\delta\rho'(\mathbf{y})}\,.
\end{aligned} \tag{3.17}
$$

The explicit expressions in terms of the quark propagator can be easily obtained from eqs. (3.14), and coincide with those given in ref. [4]. The boundary-to-boundary correlators can be written as follows,

$$
\begin{aligned}
\left[\zeta(\mathbf{x})\bar\zeta'(\mathbf{y})\right]_{\mathrm{F}} &= \tilde c_{\mathrm{t}}P_-U(x-a\hat 0,0)\left[\psi(x)\bar\zeta'(\mathbf{y})\right]_{\mathrm{F}}\big|_{x_0=a}\,,\\
\left[\zeta'(\mathbf{x})\bar\zeta(\mathbf{y})\right]_{\mathrm{F}} &= \tilde c_{\mathrm{t}}P_+U(x,0)^{-1}\left[\psi(x)\bar\zeta(\mathbf{y})\right]_{\mathrm{F}}\big|_{x_0=T-a}\,.
\end{aligned} \tag{3.18}
$$

The correlators of two boundary quark fields at the same boundary receive additional contributions due to the new boundary counterterms, viz.

$$
\begin{aligned}
\left[\zeta(\mathbf{x})\bar\zeta(\mathbf{y})\right]_{\mathrm{F}} &= \tilde c_{\mathrm{t}}^2\,P_-U(x-a\hat 0,0)S(x,y)U(y-a\hat 0,0)^{-1}P_+\big|_{x_0=y_0=a}-\\
&\quad-P_-\left[\tilde c_{\mathrm{s}}\gamma_k\frac{1}{2}(\nabla_k^*+\nabla_k)+\tilde b_2 i\mu_{\mathrm{q}}\gamma_5\tau^3\right]a^{-2}\delta_{\mathbf{xy}}\,,\\
\left[\zeta'(\mathbf{x})\bar\zeta'(\mathbf{y})\right]_{\mathrm{F}} &= \tilde c_{\mathrm{t}}^2\,P_+U(x,0)^{-1}S(x,y)U(y,0)P_-\big|_{x_0=y_0=T-a}-\\
&\quad-P_+\left[\tilde c_{\mathrm{s}}\gamma_k\frac{1}{2}(\nabla_k^*+\nabla_k)+\tilde b_2 i\mu_{\mathrm{q}}\gamma_5\tau^3\right]a^{-2}\delta_{\mathbf{xy}}\,.
\end{aligned} \tag{3.19}
$$

We finally note that the conjugation property (3.12) implies,

$$\begin{aligned}
\left[\psi(x)\bar{\zeta}(\mathbf{y})\right]_{\mathrm{F}}^{\dagger} &= \gamma_5\tau^1\left[\zeta(\mathbf{y})\bar{\psi}(x)\right]_{\mathrm{F}}\gamma_5\tau^1\,,\\
\left[\zeta(\mathbf{x})\bar{\zeta}'(\mathbf{y})\right]_{\mathrm{F}}^{\dagger} &= \gamma_5\tau^1\left[\zeta'(\mathbf{y})\bar{\zeta}(\mathbf{x})\right]_{\mathrm{F}}\gamma_5\tau^1\,,\\
\left[\zeta(\mathbf{x})\bar{\zeta}(\mathbf{y})\right]_{\mathrm{F}}^{\dagger} &= \gamma_5\tau^1\left[\zeta(\mathbf{y})\bar{\zeta}(\mathbf{x})\right]_{\mathrm{F}}\gamma_5\tau^1\,,
\end{aligned} \tag{3.20}$$

and analogous equations for the remaining 2-point functions.

3.5 SF Correlation functions

With this set-up of the SF we now define a few on-shell correlation functions involving the composite fields of section 2. With the boundary source

$$\mathcal{O}^a = a^6\sum_{\mathbf{y},\mathbf{z}}\bar{\zeta}(\mathbf{y})\gamma_5\frac{1}{2}\tau^a\zeta(\mathbf{z})\,, \tag{3.21}$$

we define the correlation functions

$$\begin{aligned}
f_{\mathrm{A}}^{ab}(x_0) &= -\langle A_0^a(x)\mathcal{O}^b\rangle\,,\\
f_{\mathrm{P}}^{ab}(x_0) &= -\langle P^a(x)\mathcal{O}^b\rangle\,,\\
f_{\mathrm{V}}^{ab}(x_0) &= -\langle V_0^a(x)\mathcal{O}^b\rangle\,.
\end{aligned} \tag{3.22}$$

In the following we restrict the isospin indices to $a,b\in\{1,2\}$. It is convenient to define the matrix [12, 13],

$$H(x) = a^3\sum_{\mathbf{y}}\frac{\delta\psi_{\mathrm{cl}}(x)}{\delta\rho(\mathbf{y})}\,. \tag{3.23}$$

Its hermitean conjugate matrix is given by

$$H(x)^{\dagger} = a^3\sum_{\mathbf{y}}\gamma_5\tau^1\frac{\delta\bar{\psi}_{\mathrm{cl}}(x)}{\delta\bar{\rho}(\mathbf{y})}\gamma_5\tau^1\,, \tag{3.24}$$

and the correlation functions can be expressed in terms of $H(x)$, viz.

$$f_{\mathrm{X}}^{ab}(x_0) = \left\langle\frac{1}{4}\,\mathrm{tr}\left\{H(x)^{\dagger}\gamma_5\Gamma_{\mathrm{X}}\tau^1\tau^a H(x)\tau^b\tau^1\right\}\right\rangle_{\mathrm{G}}\,. \tag{3.25}$$

As in ref. [4] the bracket $\langle\cdots\rangle_{\mathrm{G}}$ means an average over the gauge fields with the effective gauge action,

$$S_{\mathrm{eff}}[U] = S_{\mathrm{G}}[U] + \delta S_{\mathrm{G,b}}[U] - \ln\det\left(D+\delta D+m_0+i\mu_{\mathrm{q}}\gamma_5\tau^3\right), \tag{3.26}$$

and the trace is over flavour, Dirac and colour indices. The gamma structures are $\Gamma_{\mathrm{X}} = \gamma_0\gamma_5,\gamma_5,\gamma_0$, where X stands for A,P and V, respectively.

3.6 Reducing the flavour structure

In order to carry out the flavour traces we introduce the flavour projectors

$$Q_{\pm} = \frac{1}{2}(1 \pm \tau^3)\,. \tag{3.27}$$

Inserting the flavour decomposition,

$$H(x) = H_{+}(x)Q_{+} + H_{-}(x)Q_{-}\,, \tag{3.28}$$

into the expression eq. (3.25) leads to

$$f_{\rm X}^{ab}(x_0) = \sum_{i,j=\pm} {\rm tr}\{Q_i\tau^1\tau^a Q_j\tau^b\tau^1\} \left\langle \frac{1}{4}\,{\rm tr}\left\{H_i(x)^\dagger\gamma_5\Gamma_{\rm X}H_j(x)\right\}\right\rangle_{\rm G}\,. \tag{3.29}$$

Since we restrict the indices a and b to values in $\{1,2\}$ this expression further simplifies leading to

$$f_{\rm X}^{ab}(x_0) = \sum_{i=\pm} {\rm tr}\{Q_i\tau^b\tau^a\} \left\langle \frac{1}{4}\,{\rm tr}\left\{H_i(x)^\dagger\gamma_5\Gamma_{\rm X}H_i(x)\right\}\right\rangle_{\rm G}\,. \tag{3.30}$$

In order to simplify the expressions further, we now study the behaviour under a parity transformation combined with the exchange $\mu_{\rm q} \to -\mu_{\rm q}$. Notice that the parity transformation also transforms the background fields, in particular it implies $\theta_k \to -\theta_k$ $(k = 1,2,3)$. On the matrices $H_{\pm}(x)$ this transformation acts according to

$$H_{\pm}(x) \longrightarrow \gamma_0 H_{\mp}(\tilde{x})\,, \tag{3.31}$$

where $\tilde{x} = (x_0, -\mathbf{x})$ is the parity transformed space-time argument, and we recall that $H_{\pm}(x)$ depend implicitly on the background gauge field. After averaging over the gauge fields and due to parity invariance of the effective gauge action (3.26) one then finds

$$\left\langle {\rm tr}\left\{H_{\pm}(x)^\dagger\gamma_5\Gamma_{\rm X}H_{\pm}(x)\right\}\right\rangle_{\rm G} = \eta({\rm X})\left\langle {\rm tr}\left\{H_{\mp}(x)^\dagger\gamma_5\Gamma_{\rm X}H_{\mp}(x)\right\}\right\rangle_{\rm G}\,, \tag{3.32}$$

where the sign factor depends on whether $\Gamma_{\rm X}$ commutes $(\eta({\rm X}) = -1)$ or anti-commutes $(\eta({\rm X}) = 1)$ with γ_0. Using this result in eq. (3.30) it follows that

$$f_{\rm A}^{12}(x_0) = f_{\rm P}^{12}(x_0) = f_{\rm V}^{11}(x_0) = 0\,. \tag{3.33}$$

Furthermore, the exact U(1) flavour symmetry implies that

$$f_{\rm X}^{22}(x_0) = f_{\rm X}^{11}(x_0)\,, \qquad f_{\rm X}^{21}(x_0) = -f_{\rm X}^{12}(x_0)\,, \tag{3.34}$$

so that we may restrict attention to the following non-vanishing correlation functions:

$$\begin{aligned} f_{\rm A}^{11}(x_0) &= -\frac{1}{2}\left\langle {\rm tr}\left\{H_{+}(x)^\dagger\gamma_0 H_{+}(x)\right\}\right\rangle_G\,, \\ f_{\rm P}^{11}(x_0) &= \frac{1}{2}\left\langle {\rm tr}\left\{H_{+}(x)^\dagger H_{+}(x)\right\}\right\rangle_G\,, \\ f_{\rm V}^{12}(x_0) &= \frac{i}{2}\left\langle {\rm tr}\left\{H_{+}(x)^\dagger\gamma_0\gamma_5 H_{+}(x)\right\}\right\rangle_G\,. \end{aligned} \tag{3.35}$$

Note that eq. (3.32) has allowed to eliminate the dependence upon the second flavour component $H_-(x)$. This is convenient both for perturbative calculations and in the framework of numerical simulations.

4. O(a) improvement of the free theory

We determine the improvement coefficients in the free theory, which is obtained by setting all gauge links to unity. In this context correlation functions of quark and antiquark fields are suitable on-shell quantities which ought to be improved. We may therefore consider the improvement of the one-particle energies, the quark propagator and basic 2-point functions in the Schrödinger functional, in addition to the SF correlation functions introduced in section 3.

4.1 The free quark propagator

All correlation functions in the SF are obtainable from the quark propagator, which can be computed using standard methods [4]. We set the standard improvement coefficients to their known values [4],

$$\tilde{c}_\mathrm{t} = \tilde{c}_\mathrm{s} = 1\,, \tag{4.1}$$

and compute the propagator assuming $\tilde{b}_1 = 1$. As discussed in section 3, any other value can be obtained by insertion of the corresponding boundary counterterm. The propagator can be written in the form

$$S(x,y) = \left(D^\dagger + m_0 - i\mu_\mathrm{q}\gamma_5\tau^3\right) G(x,y)\,, \tag{4.2}$$

where $G(x,y)$ is given by

$$G(x,y) = L^{-3}\sum_{\mathbf{p}} \mathrm{e}^{i\mathbf{p}(\mathbf{x}-\mathbf{y})}\left[G_+(\mathbf{p},x_0,y_0)P_+ + G_-(\mathbf{p},x_0,y_0)P_-\right], \tag{4.3}$$

with the functions

$$\begin{aligned} G_+(\mathbf{p};x_0,y_0) &= \mathcal{N}(p^+)\left\{M_-(p^+)\left[\mathrm{e}^{-\omega(\mathbf{p}^+)(|x_0-y_0|-T)} - \mathrm{e}^{\omega(\mathbf{p}^+)(x_0+y_0-T)}\right] + \right.\\ &\quad \left. + M_+(p^+)\left[\mathrm{e}^{\omega(\mathbf{p}^+)(|x_0-y_0|-T)} - \mathrm{e}^{-\omega(\mathbf{p}^+)(x_0+y_0-T)}\right]\right\},\\ G_-(\mathbf{p};x_0,y_0) &= G_+(\mathbf{p};T-x_0,T-y_0)\,. \end{aligned} \tag{4.4}$$

Here, $M_\pm(p^+) = M(p^+) \pm i\mathring{p}_0^+$ (II.3.17), with $M(p)$ as defined in eq. (II.3.6) and $p_\mu^+ = p_\mu + \theta_\mu/L$. Furthermore, we recall that in the above formulae it is understood that $p_0 = p_0^+ = i\omega(\mathbf{p}^+)$, where for given spatial momentum $\mathbf{q}$ the energy $\omega(\mathbf{q})$ is obtained as the solution of the equation

$$\sinh\left[\frac{a}{2}\,\omega(\mathbf{q})\right] = \frac{a}{2}\left\{\frac{\mathring{\mathbf{q}}^2 + \mu_\mathrm{q}^2 + (m_0 + \frac{1}{2}a\hat{\mathbf{q}}^2)^2}{1 + a(m_0 + \frac{1}{2}a\hat{\mathbf{q}}^2)}\right\}^{1/2}. \tag{4.5}$$

Finally, using again the notation of ref. [4], the normalization factor is given by

$$\mathcal{N}(p^+) = \left\{-2i\mathring{p}_0^+ A(\mathbf{p}^+) R(p^+) \mathrm{e}^{\omega(\mathbf{p}^+)T}\right\}^{-1}. \tag{4.6}$$

4.2 Improvement conditions and results

In the free quark theory, the quark energy ω is a suitable on-shell quantity. At zero spatial momentum it coincides with the pole mass, which is related to the bare masses through

$$\cosh am_{\rm p} = 1 + \frac{\frac{1}{2}a^2(m_0^2+\mu_{\rm q}^2)}{(1+am_0)}\,. \tag{4.7}$$

Up to terms of $\mathrm{O}(a^2)$ one then finds ($m_{\rm c}=0$ at tree level)

$$m_{\rm p}^2 = \left(m_{\rm q}^2+\mu_{\rm q}^2\right)(1-am_{\rm q}) + \mathrm{O}(a^2)\,. \tag{4.8}$$

Replacing the bare masses by the renormalized $\mathrm{O}(a)$ improved mass parameters and requiring the absence of $\mathrm{O}(a)$ artifacts one obtains

$$b_{\rm m} = -\frac{1}{2}\,, \qquad b_\mu + \tilde{b}_{\rm m} + \frac{1}{2} = 0\,, \tag{4.9}$$

and the same condition is obtained from the $\mathrm{O}(a)$ improved energy at finite spatial momentum. One may wonder whether it is possible to get an additional condition by considering the improvement of the quark propagator itself. This is not so, for the reasons given in subsection 2.5. As an illustration we consider the quark propagator (4.2) in the limit of infinite time extent T with the limit taken at fixed $x_0-T/2$ and $y_0-T/2$. This eliminates the boundaries both at $x_0=0$ and $x_0=T$, so that one is left with the improvement of the mass parameters, and of the quark and antiquark fields, viz.

$$\begin{aligned}\psi_{\rm R} &= \left(1+b_\psi am_0+\tilde{b}_\psi ia\mu_{\rm q}\gamma_5\tau^3\right)\psi\,,\\ \bar{\psi}_{\rm R} &= \bar{\psi}\left(1+b_{\bar{\psi}}am_0+\tilde{b}_{\bar{\psi}}ia\mu_{\rm q}\gamma_5\tau^3\right).\end{aligned} \tag{4.10}$$

Requiring the quark propagator to be $\mathrm{O}(a)$ improved we find the usual result of the untwisted theory, $b_\psi = b_{\bar{\psi}} = 1/2$, and

$$\tilde{b}_{\bar{\psi}} = \tilde{b}_\psi\,, \qquad 2\tilde{b}_\psi - \tilde{b}_{\rm m} - \frac{1}{2} = 0\,, \qquad 2\tilde{b}_\psi + b_\mu = 0\,, \tag{4.11}$$

i.e. 3 equations for 4 coefficients. Similarly, by studying the SF correlation functions of the improved quark bilinear fields we find the standard results of the untwisted theory, $c_{\rm A}=c_{\rm V}=0$ and $2\,b_\zeta = b_{\rm A} = b_{\rm V} = b_{\rm P} = 1$, and the following conditions involving the new coefficients,

$$\begin{aligned}\tilde{b}_1 - \frac{1}{2}\left(\tilde{b}_{\rm m}+\frac{1}{2}\right) &= 1\,,\\ b_\mu + \tilde{b}_{\rm m} + \frac{1}{2} &= 0\,,\\ \tilde{b}_{\rm A} - \left(\tilde{b}_{\rm m}+\frac{1}{2}\right) &= 0\,,\\ \tilde{b}_{\rm V} - \left(\tilde{b}_{\rm m}+\frac{1}{2}\right) &= 0\,.\end{aligned} \tag{4.12}$$

Furthermore, from the O(a) improvement of the basic 2-point functions we also obtain

$$\tilde{b}_2 = 1\,. \tag{4.13}$$

The fact that $\tilde{b}_\psi$ and $\tilde{b}_1$ are not determined independently is again due to the invariance of the continuum theory under axial rotations of the fields and a compensating change in the mass parameters. Hence our findings in the free theory are completely in line with the general expectation expressed in subsection 2.5. Choosing $\tilde{b}_{\rm m}$ as the free parameter and setting it to $-1/2$ leads to $b_\mu = \tilde{b}_{\rm A} = \tilde{b}_{\rm V} = 0$ and $\tilde{b}_1 = 1$, while e.g. for $\tilde{b}_{\rm m} = 0$ the tree level value $\tilde{b}_1 = 5/4$ is somewhat inconvenient.

5. The one-loop computation

We now want to expand the correlation functions to one-loop order. We work with vanishing boundary values C_k and C_k'. The gauge fixing procedure then is the same as in ref. [4] and will not be described here. In the following we only describe those aspects that are new and otherwise assume the reader to be familiar with refs. [4, 5].

5.1 Renormalized amplitudes

Once the flavour traces have been taken, the one-loop calculation at fixed lattice size is almost identical to the standard case [4, 5]. In order to take the continuum limit at fixed physical space-time volume, we then keep $m_{\rm R}$, $\mu_{\rm R}$, x_0 and T fixed in units of L. Here the renormalized mass parameters are defined in a mass-independent renormalization scheme which may remain unspecified for the moment.

To first order of perturbation theory the substitutions for the coupling constant and the quark mass then amount to

$$\begin{aligned} g_0^2 &= g_{\rm R}^2 + {\rm O}(g_{\rm R}^4)\,, \\ m_0 &= m_0^{(0)} + g_{\rm R}^2 m_0^{(1)} + {\rm O}(g_{\rm R}^4)\,, \\ \mu_{\rm q} &= \mu_{\rm q}^{(0)} + g_{\rm R}^2 \mu_{\rm q}^{(1)} + {\rm O}(g_{\rm R}^4)\,, \end{aligned} \tag{5.1}$$

where the precise form of the coefficients

$$\begin{aligned} m_0^{(0)} &= \frac{1}{a}\left[1-\sqrt{1-2am_{\rm R}-a^2\mu_{\rm R}^2}\right], \\ m_0^{(1)} &= m_{\rm c}^{(1)} - \left\{ Z_{\rm m}^{(1)} m_{\rm R} + b_{\rm m}^{(1)} a \left(m_0^{(0)}\right)^2 + a\mu_{\rm R}^2\left[\tilde{b}_{\rm m}^{(1)} + Z_\mu^{(1)} + b_\mu^{(1)} a m_0^{(0)}\right]\right\} \times \\ &\quad \times \left[1 - a m_0^{(0)}\right]^{-1}, \\ \mu_{\rm q}^{(0)} &= \mu_{\rm R}\,, \\ \mu_{\rm q}^{(1)} &= -\mu_{\rm q}^{(0)}\left\{Z_\mu^{(1)} + b_\mu^{(1)} a m_0^{(0)}\right\}, \end{aligned} \tag{5.2}$$

is a direct consequence of the definitions made in subsection 2.1, and already includes the tree-level results obtained in the preceding section with the particular choice $\tilde{b}_{\rm m}^{(0)} = -1/2$.

The renormalized correlation functions,

$$
\begin{aligned}
[f_{\rm V}^{12}(x_0)]_{\rm R} &= Z_{\rm V}(1+b_{\rm V}am_{\rm q})Z_\zeta^2(1+b_\zeta am_{\rm q})^2\left\{f_{\rm V}^{12}(x_0)+\tilde{b}_{\rm V}a\mu_{\rm q}f_{\rm A}^{11}(x_0)\right\},\\
[f_{\rm P}^{11}(x_0)]_{\rm R} &= Z_{\rm P}(1+b_{\rm P}am_{\rm q})Z_\zeta^2(1+b_\zeta am_{\rm q})^2 f_{\rm P}^{11}(x_0),\\
[f_{\rm A}^{11}(x_0)]_{\rm R} &= Z_{\rm A}(1+b_{\rm A}am_{\rm q})Z_\zeta^2(1+b_\zeta am_{\rm q})^2\times\\
&\quad\times\left\{f_{\rm A}^{11}(x_0)+c_{\rm A}a\tilde{\partial}_0 f_{\rm P}^{11}(x_0)-\tilde{b}_{\rm A}a\mu_{\rm q}f_{\rm V}^{12}(x_0)\right\},
\end{aligned}
\tag{5.3}
$$

have a well-defined perturbation expansion in the renormalized coupling $g_{\rm R}$, with coefficients that are computable functions of a/L. For instance the expansion of $[f_{\rm V}^{12}]_{\rm R}$ reads

$$
\begin{aligned}
[f_{\rm V}^{12}(x_0)]_{\rm R} = f_{\rm V}^{12}(x_0)^{(0)} + g_{\rm R}^2\Big\{ & f_{\rm V}^{12}(x_0)^{(1)} + m_0^{(1)}\frac{\partial}{\partial m_0}f_{\rm V}^{12}(x_0)^{(0)} +\\
&+\left(Z_{\rm V}^{(1)}+2Z_\zeta^{(1)}+am_{\rm R}\left[b_{\rm V}^{(1)}+2b_\zeta^{(1)}\right]\right)f_{\rm V}^{12}(x_0)^{(0)}+\\
&+\mu_{\rm q}^{(1)}\frac{\partial}{\partial\mu_{\rm q}}f_{\rm V}^{12}(x_0)^{(0)}+a\mu_{\rm R}\tilde{b}_{\rm V}^{(1)}f_{\rm A}^{11}(x_0)^{(0)}\Big\},
\end{aligned}
\tag{5.4}
$$

where terms of order a^2 and $g_{\rm R}^4$ have been neglected, and it is understood that the correlation functions are evaluated at $m_0 = m_0^{(0)}$ and $\mu_{\rm q} = \mu_{\rm q}^{(0)}$.

Following ref. [4] we now set $x_0 = T/2$ and scale all dimensionful quantities in units of L. With the parameters $z_m = m_{\rm R}L$, $z_\mu = \mu_{\rm R}L$ and $\tau = T/L$ we then consider the dimensionless functions,

$$
\begin{aligned}
h_{\rm A}\left(\theta,z_m,z_\mu,\tau,\frac{a}{L}\right) &= [f_{\rm A}^{11}(x_0)]_{\rm R}\big|_{x_0=T/2},\\
h_{\rm V}\left(\theta,z_m,z_\mu,\tau,\frac{a}{L}\right) &= [f_{\rm V}^{12}(x_0)]_{\rm R}\big|_{x_0=T/2},\\
h_{\rm P}\left(\theta,z_m,z_\mu,\tau,\frac{a}{L}\right) &= [f_{\rm P}^{11}(x_0)]_{\rm R}\big|_{x_0=T/2},\\
h_{\rm dA}\left(\theta,z_m,z_\mu,\tau,\frac{a}{L}\right) &= L\tilde{\partial}_0[f_{\rm A}^{11}(x_0)]_{\rm R}\Big|_{x_0=T/2},\\
h_{\rm dV}\left(\theta,z_m,z_\mu,\tau,\frac{a}{L}\right) &= L\tilde{\partial}_0[f_{\rm V}^{12}(x_0)]_{\rm R}\Big|_{x_0=T/2}.
\end{aligned}
\tag{5.5}
$$

One then infers,

$$
\begin{aligned}
h_{\rm A} = v_0 + g_{\rm R}^2\Big\{ & v_1+\tilde{c}_{\rm t}^{(1)}v_2+am_0^{(1)}v_3+c_{\rm A}^{(1)}v_4+a\mu_{\rm q}^{(1)}v_5+z_\mu\tilde{b}_1^{(1)}v_6-\frac{a}{L}z_\mu\tilde{b}_{\rm A}^{(1)}q_0+\\
&+\left(Z_{\rm A}^{(1)}+2Z_\zeta^{(1)}+\frac{a}{L}z_m\left[b_{\rm A}^{(1)}+2b_\zeta^{(1)}\right]\right)v_0\Big\},
\end{aligned}
\tag{5.6}
$$

$$
h_{\rm V} = q_0 + g_{\rm R}^2\Big\{q_1+\tilde{c}_{\rm t}^{(1)}q_2+am_0^{(1)}q_3+a\mu_{\rm q}^{(1)}q_5+z_\mu\tilde{b}_1^{(1)}q_6+\frac{a}{L}z_\mu\tilde{b}_{\rm V}^{(1)}v_0+
$$

$$+\left(Z_{\rm V}^{(1)}+2Z_\zeta^{(1)}+\frac{a}{L}z_m\left[b_{\rm V}^{(1)}+2b_\zeta^{(1)}\right]\right)q_0\Big\}\,, \tag{5.7}$$

$$h_{\rm P} = u_0+g_{\rm R}^2\Big\{u_1+\tilde{c}_{\rm t}^{(1)}u_2+am_0^{(1)}u_3+a\mu_{\rm q}^{(1)}u_5+z_\mu\tilde{b}_1^{(1)}u_6+ \\ +\left(Z_{\rm P}^{(1)}+2Z_\zeta^{(1)}+\frac{a}{L}z_m\left[b_{\rm P}^{(1)}+2b_\zeta^{(1)}\right]\right)u_0\Big\}\,, \tag{5.8}$$

$$h_{\rm dA} = w_0+g_{\rm R}^2\Big\{w_1+\tilde{c}_{\rm t}^{(1)}w_2+am_0^{(1)}w_3+c_{\rm A}^{(1)}w_4+a\mu_{\rm q}^{(1)}w_5+z_\mu\tilde{b}_1^{(1)}w_6-\frac{a}{L}z_\mu\tilde{b}_{\rm A}^{(1)}r_0+ \\ +\left(Z_{\rm A}^{(1)}+2Z_\zeta^{(1)}+\frac{a}{L}z_m\left[b_{\rm A}^{(1)}+2b_\zeta^{(1)}\right]\right)w_0\Big\}\,, \tag{5.9}$$

$$h_{\rm dV} = r_0+g_{\rm R}^2\Big\{r_1+\tilde{c}_{\rm t}^{(1)}r_2+am_0^{(1)}r_3+a\mu_{\rm q}^{(1)}r_5+z_\mu\tilde{b}_1^{(1)}r_6+\frac{a}{L}z_\mu\tilde{b}_{\rm V}^{(1)}w_0+ \\ +\left(Z_{\rm V}^{(1)}+2Z_\zeta^{(1)}+\frac{a}{L}z_m\left[b_{\rm V}^{(1)}+2b_\zeta^{(1)}\right]\right)r_0\Big\}\,. \tag{5.10}$$

Since we are neglecting terms of order a^2, the expansions,

$$m_0^{(1)} = m_{\rm c}^{(1)}-Z_{\rm m}^{(1)}\frac{z_m}{L}-\frac{az_m^2}{L^2}\left[Z_{\rm m}^{(1)}+b_{\rm m}^{(1)}\right]-\frac{az_\mu^2}{L^2}\left[Z_\mu^{(1)}+\tilde{b}_{\rm m}^{(1)}\right]\,, \\ \mu_{\rm q}^{(1)} = -\frac{z_\mu}{L}\left[Z_\mu^{(1)}+b_\mu^{(1)}\frac{az_m}{L}\right]\,, \tag{5.11}$$

may be inserted in eqs. (5.6)–(5.10). All the coefficients $v_i,\ldots,r_i$ are still functions of τ, θ, z_m and z_μ. Analytic expressions can be derived for those coefficients involving the tree level correlation functions or the $\mathrm{O}(a)$ counterterms. Their asymptotic expansions for $a/L\to 0$ are collected in appendix B. The coefficients $v_1,\ldots,r_1$ are only obtained numerically and definite choices for the parameters had to be made. We generated numerical data for $\theta=0$ and $\theta=0.5$ for both $T=L$ and $T=2L$ and various combinations of the mass parameters z_m and $z_\mu\neq 0$ with values between 0 and 1.5. With these parameter choices the Feynman diagrams were then evaluated numerically in 64 bit precision arithmetic for a sequence of lattice sizes ranging from $L/a=4$ to $L/a=32$ (and in some cases to $L/a=36$).

5.2 Analysis and results

The renormalization constants are determined by requiring the renormalized amplitudes to be finite in the continuum limit, and by the requirement that the tmQCD Ward identities be satisfied [2]. A linear divergence is cancelled in all amplitudes by inserting the usual one-loop coefficient $am_{\rm c}^{(1)}$, or equivalently a series which converges to this coefficient in the limit $a/L\to 0$ [4]. We choose the lattice minimal-subtraction scheme to renormalize the pseudo-scalar density and the quark boundary fields, and the one-loop coefficients are then given by [with $C_{\rm F}=(N^2-1)/2N$],

$$Z_{\rm P}^{(1)} = -\frac{6C_{\rm F}}{16\pi^2}\ln\left(\frac{L}{a}\right),\qquad 2Z_\zeta^{(1)}=-Z_{\rm P}^{(1)}\,. \tag{5.12}$$

The current renormalization constants, and the renormalization of the standard and twisted mass parameters are determined by the Ward identities. For the one-loop coefficients we expect [2, 14, 15],

$$\begin{aligned} Z_{\rm A}^{(1)} &= -0.087344(2)\, C_{\rm F}\,, \\ Z_{\rm V}^{(1)} &= -0.097072(2)\, C_{\rm F}\,, \\ Z_{\rm m}^{(1)} &= -Z_{\rm P}^{(1)} - 0.019458(1)\, C_{\rm F}\,, \\ Z_{\mu}^{(1)} &= -Z_{\rm P}^{(1)}\,. \end{aligned} \tag{5.13}$$

With our data we were able to compute the one-loop coefficients of the combinations $Z_{\rm m}Z_{\rm P}/Z_{\rm A}$ and $Z_\mu Z_{\rm P}/Z_{\rm V}$, as well as the logarithmically divergent parts of all one-loop coefficients. Complete consistency with the above expectations was found, and we shall adopt these results in the following.

The corresponding coefficients in other schemes differ from those above by a-independent terms. With the renormalization constants chosen in this way we find e.g. for the combination of separately diverging terms appearing in the curly bracket of (5.8)

$$\begin{aligned} u_1 + am_{\rm c}^{(1)}u_3 + \left(Z_{\rm P}^{(1)} + 2Z_{\zeta}^{(1)}\right)u_0 - Z_{\rm m}^{(1)} z_m u_3^{(-1)} - Z_{\mu}^{(1)} z_\mu u_5^{(-1)} = \\ = \mathcal{U}_0 + \mathcal{U}_1 \frac{a}{L} + {\rm O}\left(\frac{a^2}{L^2}\right), \end{aligned} \tag{5.14}$$

where $\mathcal{U}_i$ are functions of $\tau\,,\theta\,, z_m$ and z_μ, and $u_i^{(-1)}$ are coefficients of L/a in the expansion of u_i for $L/a \to \infty$. Evidently similar equations hold for the other functions v_1, q_1, w_1, r_1. It is important to note that we expect no terms involving $(a/L)\ln(L/a)$ on the right-hand side of (5.14) because we have imposed tree level improvement, and this was indeed seen in our data analysis. Moreover there are no terms $\sim Z_{\rm m}^{(1)}a/L$ or $\sim Z_\mu^{(1)}a/L$ on the left hand side above because of eq. (B.7); thus the coefficient $\mathcal{U}_1$ is (contrary to $\mathcal{U}_0$) independent of the renormalization scheme. Estimates for the coefficients $\mathcal{U}_1$, $\mathcal{V}_1, \ldots$ were obtained for the various data sequences using the methods described in [16].

Now the improvement coefficients are determined by demanding that the renormalized amplitudes approach the continuum limit with corrections of ${\rm O}(a^2/L^2)$. For the cancellation of the ${\rm O}(a)$ terms the following equations should be satisfied (for undefined notation see appendix B):

$$\begin{aligned} z_\mu\left[z_\mu \tilde{b}_{\rm m}^{(1)} v_3^{(-1)} + z_m b_\mu^{(1)} v_5^{(-1)} + \tilde{b}_{\rm A}^{(1)} q_0^{(0)} - \tilde{b}_1^{(1)} v_6^{(1)}\right] &= \mathcal{V}_1 + \bar{\mathcal{V}}_1\,, \\ z_\mu\left[z_\mu \tilde{b}_{\rm m}^{(1)} q_3^{(-1)} + z_m b_\mu^{(1)} q_5^{(-1)} - \tilde{b}_{\rm V}^{(1)} v_0^{(0)} - \tilde{b}_1^{(1)} q_6^{(1)}\right] &= \mathcal{Q}_1 + \bar{\mathcal{Q}}_1\,, \\ z_\mu\left[z_\mu \tilde{b}_{\rm m}^{(1)} u_3^{(-1)} + z_m b_\mu^{(1)} u_5^{(-1)} - \tilde{b}_1^{(1)} u_6^{(1)}\right] &= \mathcal{U}_1 + \bar{\mathcal{U}}_1\,, \\ z_\mu\left[z_\mu \tilde{b}_{\rm m}^{(1)} w_3^{(-1)} + z_m b_\mu^{(1)} w_5^{(-1)} + \tilde{b}_{\rm A}^{(1)} r_0^{(0)} - \tilde{b}_1^{(1)} w_6^{(1)}\right] &= \mathcal{W}_1 + \bar{\mathcal{W}}_1\,, \\ z_\mu\left[z_\mu \tilde{b}_{\rm m}^{(1)} r_3^{(-1)} + z_m b_\mu^{(1)} r_5^{(-1)} - \tilde{b}_{\rm V}^{(1)} w_0^{(0)} - \tilde{b}_1^{(1)} r_6^{(1)}\right] &= \mathcal{R}_1 + \bar{\mathcal{R}}_1\,. \end{aligned} \tag{5.15}$$

In these equations all terms involving improvement coefficients which are necessary also in the untwisted theory, have been collected in the terms $\bar{\mathcal{U}}_1, \ldots$ on the right-hand sides and they are specified in eqs. (B.13). The numerical values of these improvement coefficients, obtained in previous analyses [4, 5], are:

$$\begin{aligned}
\tilde{c}_{\rm t}^{(1)} &= -0.01346(1)\, C_{\rm F}\,, \\
c_{\rm A}^{(1)} &= -0.005680(2)\, C_{\rm F}\,, \\
b_{\zeta}^{(1)} &= -0.06738(4)\, C_{\rm F}\,, \\
b_{\rm m}^{(1)} &= -0.07217(2)\, C_{\rm F}\,, \\
b_{\rm A}^{(1)} &= 0.11414(4)\, C_{\rm F}\,, \\
b_{\rm V}^{(1)} &= 0.11492(4)\, C_{\rm F}\,, \\
b_{\rm P}^{(1)} &= 0.11484(4)\, C_{\rm F}\,.
\end{aligned} \tag{5.16}$$

Before we proceed with the numerical analysis of eqs. (5.15), it is essential to note that using the identities (B.11) they can be rewritten as

$$z_\mu \left[z_m b_\mu'^{(1)} v_5^{(-1)} + \tilde{b}_{\rm A}'^{(1)} q_0^{(0)} - \tilde{b}_1'^{(1)} v_6^{(1)} \right] = \mathcal{V}_1 + \bar{\mathcal{V}}_1\,, \tag{5.17}$$

$$z_\mu \left[z_m b_\mu'^{(1)} q_5^{(-1)} - \tilde{b}_{\rm V}'^{(1)} v_0^{(0)} - \tilde{b}_1'^{(1)} q_6^{(1)} \right] = \mathcal{Q}_1 + \bar{\mathcal{Q}}_1\,, \tag{5.18}$$

$$z_\mu \left[z_m b_\mu'^{(1)} u_5^{(-1)} - \tilde{b}_1'^{(1)} u_6^{(1)} \right] = \mathcal{U}_1 + \bar{\mathcal{U}}_1\,, \tag{5.19}$$

$$z_\mu \left[z_m b_\mu'^{(1)} w_5^{(-1)} + \tilde{b}_{\rm A}'^{(1)} r_0^{(0)} - \tilde{b}_1'^{(1)} w_6^{(1)} \right] = \mathcal{W}_1 + \bar{\mathcal{W}}_1\,, \tag{5.20}$$

$$z_\mu \left[z_m b_\mu'^{(1)} r_5^{(-1)} - \tilde{b}_{\rm V}'^{(1)} w_0^{(0)} - \tilde{b}_1'^{(1)} r_6^{(1)} \right] = \mathcal{R}_1 + \bar{\mathcal{R}}_1\,, \tag{5.21}$$

where the primed coefficients appearing here are defined through

$$\begin{aligned}
b_\mu'^{(1)} &= b_\mu^{(1)} + \tilde{b}_{\rm m}^{(1)}\,, \\
\tilde{b}_1'^{(1)} &= \tilde{b}_1^{(1)} - \frac{1}{2}\tilde{b}_{\rm m}^{(1)}\,, \\
\tilde{b}_{\rm A}'^{(1)} &= \tilde{b}_{\rm A}^{(1)} - \tilde{b}_{\rm m}^{(1)}\,, \\
\tilde{b}_{\rm V}'^{(1)} &= \tilde{b}_{\rm V}^{(1)} - \tilde{b}_{\rm m}^{(1)}\,.
\end{aligned} \tag{5.22}$$

In other words, from our equations we can only obtain information on four linearly independent combinations of the new improvement coefficients appearing in the twisted theory. This was in fact to be anticipated from our general discussion in subsection 2.5, where we argued that we are free to chose for example the coefficient $\tilde{b}_{\rm m}^{(1)}$ as we please.

Since our equations are over-determined and also having generated such a large selection of data sets, we had many ways to proceed to determine the coefficients $b_\mu'^{(1)}, \tilde{b}_1'^{(1)}, \tilde{b}_{\rm A}'^{(1)}$ and $\tilde{b}_{\rm V}'^{(1)}$, and a multitude of consistency checks on the results. We first note that if we consider the linear combination of amplitudes $h_{\mathrm{dA}} - 2z_m h_{\mathrm{P}}$ and $h_{\mathrm{dV}} + 2z_\mu h_{\mathrm{P}}$ associated with the PCAC and PCVC relations, respectively we obtain

$$
\begin{aligned}
-2z_\mu^2 u_0^{(0)} \tilde{b}_{\mathrm{A}}'^{(1)} &= \mathcal{W}_1 + \bar{\mathcal{W}}_1 - 2z_m \left(\mathcal{U}_1 + \bar{\mathcal{U}}_1\right), \\
-2z_\mu z_m u_0^{(0)} \left(b_\mu'^{(1)} + \tilde{b}_{\mathrm{V}}'^{(1)}\right) &= \mathcal{R}_1 + \bar{\mathcal{R}}_1 + 2z_\mu \left(\mathcal{U}_1 + \bar{\mathcal{U}}_1\right). \qquad (5.23)
\end{aligned}
$$

With knowledge of the right-hand sides, each equation determines a particular linear combination of improvement coefficients. In these equations the boundary coefficient $\tilde{b}_1^{(1)}$ does not appear as expected. On the other hand the coefficient $\tilde{b}_1'^{(1)}$ is all that appears on the left hand sides of eqs. (5.19) and (5.21) for the data sets with $z_m = 0$.

By solving simultaneously the three equations (5.17), (5.19) and (5.20) for one data set with $z_m \neq 0$, we could obtain the three coefficients[2] $b_\mu'^{(1)}, \tilde{b}_{\mathrm{A}}'^{(1)}$ and $\tilde{b}_1'^{(1)}$ (and of course analogously for the equations involving the vector current). We also extracted the two coefficients $b_\mu'^{(1)}, \tilde{b}_1'^{(1)}$ by solving just eq. (5.19) for two different data sets (of which at least one has $z_m \neq 0$).

Unfortunately due to rounding errors, the one-loop cutoff effects like $\mathcal{U}_1$ were rarely determined better than to within a few percent. The consequence of this was that many routes of analyses described above and when applied to various (combinations of) data sets, led to results for the improvement coefficients with very large errors. Nevertheless there remained sufficiently many analyses which delivered useful results with relatively small errors, and in these cases all results were consistent with each other and with our following "best estimates":

$$
\begin{aligned}
b_\mu'^{(1)} &= -0.103(3)\, C_{\mathrm{F}}, \\
\tilde{b}_1'^{(1)} &= 0.035(2)\, C_{\mathrm{F}}, \\
\tilde{b}_{\mathrm{A}}'^{(1)} &= 0.086(4)\, C_{\mathrm{F}}, \\
\tilde{b}_{\mathrm{V}}'^{(1)} &= 0.074(3)\, C_{\mathrm{F}}. \qquad (5.24)
\end{aligned}
$$

As one practical choice for applications in numerical simulations we advocate $\tilde{b}_{\mathrm{m}} = -1/2$ to all orders of perturbation theory, which would result in setting $\tilde{b}_{\mathrm{m}}^{(1)} = 0$ in the above equations.

6. Conclusions

In this paper we have introduced the set-up of O(a) improved twisted mass lattice QCD in its simplest form with two mass-degenerate quarks. In perturbation theory to one-loop order we have verified that O(a) improvement works out as expected. We have identified the new counterterms and computed their coefficients at the tree-level and to one-loop order. In practice perturbative estimates may be satisfactory, as tmQCD has been primarily designed to explore the chiral region of QCD, where

[2] Particularly good results were obtained e.g. with the data set $z_m = 0, z_\mu = 0.5, \theta = 0$, where we in fact had data up to $L/a = 36$.

the contribution of the new counterterms should be small anyway. This expectation is confirmed by a non-perturbative scaling test in a physically small volume, which employs the perturbative values of the new improvement coefficients reported here [19]. However, a non-perturbative determination of some of the new coefficients is certainly desirable and may be possible along the lines of ref. [8].

An interesting aspect of $\mathrm{O}(a)$ improved tmQCD is the absence of any new counterterm corresponding to a rescaling of the bare coupling g_0. This singles out the choice for the angle $\alpha = \pi/2$ for which the physical quark mass is entirely defined in terms of the twisted mass parameter. A quark mass dependent rescaling of g_0 is hence completely avoided, and one may hope that this eases the chiral extrapolation or interpolation of numerical simulation data. Furthermore, using the over-completeness of the counterterms (cf. subsection 2.5) to fix $\tilde{b}_{\mathrm{m}}$ exactly, no tuning is necessary to obtain $\alpha = \pi/2$ up to $\mathrm{O}(a^2)$ effects, provided the standard critical mass m_{c} and the standard improvement coefficients of the massless theory c_{sw} and c_{A} are known. We also note that, at $\alpha = \pi/2$, both sides of the exact PCVC relation are automatically renormalized and $\mathrm{O}(a)$ improved. This can be exploited for an $\mathrm{O}(a)$ improved determination of F_π [20], as the vector current at $\alpha = \pi/2$ is physically interpreted as the axial current [2].

In the future one may wish to extend the framework of $\mathrm{O}(a)$ improved tmQCD to include the heavier quarks in the way suggested in ref. [2]. The analysis of $\mathrm{O}(a)$ counterterms still remains to be done, but we do not expect any new conceptual problems here.

Finally, we have defined the Schrödinger functional for tmQCD, based on the appropriate generalisation of Lüscher's transfer matrix construction for tmQCD. We expect that the Schrödinger functional will be useful in the determination of hadronic matrix elements along the lines of refs. [17, 18], and work in this direction is currently in progress [20, 21].

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A. The transfer matrix for twisted mass lattice QCD

In this appendix we briefly indicate the generalization of the transfer matrix construction for twisted mass lattice QCD with $c_{\mathrm{sw}} = 0$. We use the original notation of ref. [6] with the conventions of ref. [10]. The transfer matrix as an operator in Fock space and as an integral kernel with respect to the gauge fields has the structure

$$T_0[U,U'] = \hat{T}_{\rm F}^{\dagger}(U) K_0[U,U'] \hat{T}_{\rm F}(U')\,, \tag{A.1}$$

with pure gauge kernel K_0 and the fermionic part

$$\hat{T}_{\rm F}(U) = \det(2\kappa B)^{1/4} \exp(\hat{\chi}^{\dagger} P_{-} C \hat{\chi}) \exp(-\hat{\chi}^{\dagger}\gamma_0 M \hat{\chi})\,. \tag{A.2}$$

Here, the operators $\hat{\chi}_i(\mathbf{x})$ are canonical (i is a shorthand for colour, spin and flavour indices) viz.

$$\{\hat{\chi}_i(\mathbf{x}), \hat{\chi}_j^{\dagger}(\mathbf{y})\} = \delta_{ij} a^{-3} \delta_{\mathbf{xy}}\,, \tag{A.3}$$

and B and C are matrix representations of the difference operators

$$B = 1 - 6\kappa - a^2\kappa \sum_{k=1}^{3} \nabla_k^* \nabla_k\,,$$

$$C = a\sum_{k=1}^{3} \gamma_k \frac{1}{2}(\nabla_k + \nabla_k^*) + ia\mu_{\rm q}\gamma_5\tau^3\,. \tag{A.4}$$

As in the standard case the positivity of the transfer matrix hinges on the positivity of the matrix B, which is guaranteed for $||\kappa|| < 1/6$. This is the standard bound which also ensures that the matrix M,

$$M = \frac{1}{2}\ln\left(\frac{1}{2}B\kappa^{-1}\right)\,, \tag{A.5}$$

is well-defined. No restriction applies to the twisted mass parameter, except that $\mu_{\rm q}$ must be real for the transfer matrix (A.1) to reproduce the twisted mass lattice QCD action.

B. Analytic expressions for expansion coefficients

In this appendix we provide explicit analytic expressions for the tree-level amplitudes and the counterterms appearing in eqs. (5.6)–(5.10) which are needed to compute the one-loop amplitudes up to terms of $\mathrm{O}(a^2)$. We have checked that the analytic expressions correctly reproduce the numerical values obtained by directly programming the correlation functions and counterterm insertions.

First we define

$$\begin{aligned}
\omega &= \sqrt{z_m^2 + 3\theta^2 + z_\mu^2}\,,\\
\mathrm{co} &= \cosh(\omega\tau)\,,\\
\mathrm{si} &= \sinh(\omega\tau)\,,\\
\rho &= \omega\,\mathrm{co} + z_m\,\mathrm{si}\,,\\
\nu &= \omega\,\mathrm{si} + z_m\,\mathrm{co}\,,
\end{aligned} \tag{B.1}$$

where $\tau = T/L$. Then we have $u_0 = u_0^{(0)} + \mathrm{O}(a^2/L^2)$ etc. with

$$
\begin{aligned}
u_0^{(0)} &= \frac{N\omega}{\rho}\,, \\
v_0^{(0)} &= -\frac{N(3\theta^2 + z_\mu^2 + z_m\nu)}{\rho^2}\,, \\
q_0^{(0)} &= \frac{N z_\mu(-z_m + \nu)}{\rho^2}\,, \\
w_0^{(0)} &= 2 z_m u_0^{(0)}\,, \\
r_0^{(0)} &= -2 z_\mu u_0^{(0)}\,.
\end{aligned} \tag{B.2}
$$

For the boundary terms we define

$$
\hat{r} = z_m + \frac{2(3\theta^2 + z_\mu^2)\,\mathrm{si}}{\rho}\,, \tag{B.3}
$$

and then $u_2 = a u_2^{(1)}/L + \mathrm{O}(a^2/L^2)$ etc. with

$$
\begin{aligned}
u_2^{(1)} &= 2\hat{r} u_0^{(0)}\,, \\
v_2^{(1)} &= 2\hat{r} v_0^{(0)} - \frac{4N\omega(3\theta^2 + z_\mu^2)(-z_m + \nu)}{\rho^3}\,, \\
q_2^{(1)} &= 2\hat{r} q_0^{(0)} - \frac{4N\omega z_\mu(3\theta^2 + z_\mu^2 + z_m\nu)}{\rho^3}\,, \\
w_2^{(1)} &= 2\hat{r} w_0^{(0)}\,, \\
r_2^{(1)} &= 2\hat{r} r_0^{(0)}\,.
\end{aligned} \tag{B.4}
$$

Similarly, $u_6 = a u_6^{(1)}/L + \mathrm{O}(a^2/L^2)$ etc. with

$$
\begin{aligned}
u_6^{(1)} &= -\frac{2 z_\mu\,\mathrm{si}}{\rho} u_0^{(0)}\,, \\
v_6^{(1)} &= -\frac{2 z_\mu\,\mathrm{si}}{\rho} v_0^{(0)} + \frac{2N\omega z_\mu(-z_m + \nu)}{\rho^3}\,, \\
q_6^{(1)} &= -\frac{2 z_\mu\,\mathrm{si}}{\rho} q_0^{(0)} + \frac{2N\omega\left(\omega\rho + z_\mu^2(1 - \mathrm{co})\right)}{\rho^3}\,, \\
w_6^{(1)} &= -\frac{2 z_\mu\,\mathrm{si}}{\rho} w_0^{(0)}\,, \\
r_6^{(1)} &= -\frac{2 z_\mu\,\mathrm{si}}{\rho} r_0^{(0)}\,.
\end{aligned} \tag{B.5}
$$

For the derivatives with respect to the mass parameters we have,

$$
u_i = \left(\frac{L}{a}\right) u_i^{(-1)} + u_i^{(0)} + \mathrm{O}\left(\frac{a}{L}\right), \qquad (i = 3, 5) \tag{B.6}
$$

with

$$u_3^{(0)} = -z_m u_3^{(-1)} \,, \qquad u_5^{(0)} = -z_\mu u_3^{(-1)} \,, \tag{B.7}$$

and analogous equations hold in all other cases. Defining

$$\begin{aligned} X &= \frac{\nu(1+z_m\tau)}{\omega} \,, \\ Y &= \frac{\rho(1+z_m\tau)}{\omega} \,, \\ \tilde{X} &= \frac{z_\mu(\nu\tau+\mathrm{co})}{\omega} \,, \\ \tilde{Y} &= \frac{z_\mu(\rho\tau+\mathrm{si})}{\omega} \,, \end{aligned} \tag{B.8}$$

one has

$$\begin{aligned} u_3^{(-1)} &= -\frac{Xu_0^{(0)}}{\rho} + \frac{Nz_m}{\omega\rho} \,, \\ v_3^{(-1)} &= -\frac{2Xv_0^{(0)}}{\rho} - \frac{N(\nu+z_mY)}{\rho^2} \,, \\ q_3^{(-1)} &= -\frac{2Xq_0^{(0)}}{\rho} - \frac{Nz_\mu(1-Y)}{\rho^2} \,, \\ w_3^{(-1)} &= 2(z_m u_3^{(-1)} + u_0^{(0)}) \,, \\ r_3^{(-1)} &= -2z_\mu u_3^{(-1)} \,, \end{aligned} \tag{B.9}$$

and

$$\begin{aligned} u_5^{(-1)} &= -\frac{\tilde{X}u_0^{(0)}}{\rho} + \frac{Nz_\mu}{\omega\rho} \,, \\ v_5^{(-1)} &= -\frac{2\tilde{X}v_0^{(0)}}{\rho} - \frac{N(2z_\mu+z_m\tilde{Y})}{\rho^2} \,, \\ q_5^{(-1)} &= -\frac{2\tilde{X}q_0^{(0)}}{\rho} + \frac{N(z_\mu\tilde{Y}-z_m+\nu)}{\rho^2} \,, \\ w_5^{(-1)} &= 2z_m u_5^{(-1)} \,, \\ r_5^{(-1)} &= -2z_\mu u_5^{(-1)} - 2u_0^{(0)} \,. \end{aligned} \tag{B.10}$$

Note the identities

$$\begin{aligned} 0 &= 2z_\mu u_3^{(-1)} - 2z_m u_5^{(-1)} - u_6^{(1)} \,, \\ 0 &= 2z_\mu v_3^{(-1)} - 2z_m v_5^{(-1)} - v_6^{(1)} + 2q_0^{(0)} \,, \\ 0 &= 2z_\mu q_3^{(-1)} - 2z_m q_5^{(-1)} - q_6^{(1)} - 2v_0^{(0)} \,, \\ 0 &= 2z_\mu w_3^{(-1)} - 2z_m w_5^{(-1)} - w_6^{(1)} + 2r_0^{(0)} \,, \\ 0 &= 2z_\mu r_3^{(-1)} - 2z_m r_5^{(-1)} - r_6^{(1)} - 2w_0^{(0)} \,. \end{aligned} \tag{B.11}$$

The remaining coefficients to be specified are $v_4 = av_4^{(1)}/L + \mathrm{O}(a^2/L^2)$ and $w_4 = aw_4^{(1)}/L + \mathrm{O}(a^2/L^2)$ with

$$\begin{aligned} v_4^{(1)} &= -\frac{2N\omega^2\nu}{\rho^2}\,, \\ w_4^{(1)} &= \frac{4N\omega^3}{\rho}\,. \end{aligned} \tag{B.12}$$

Finally we specify the terms $\bar{\mathcal{U}}_1, \ldots$ appearing on the right-hand side of eqs. (5.15):

$$\begin{aligned} \bar{\mathcal{V}}_1 &= \tilde{c}_{\mathrm{t}}^{(1)} v_2^{(1)} - z_m^2 b_{\mathrm{m}}^{(1)} v_3^{(-1)} + z_m[b_{\mathrm{A}}^{(1)} + 2b_\zeta^{(1)}]v_0^{(0)} + c_{\mathrm{A}}^{(1)} v_4\,, \\ \bar{\mathcal{Q}}_1 &= \tilde{c}_{\mathrm{t}}^{(1)} q_2^{(1)} - z_m^2 b_{\mathrm{m}}^{(1)} q_3^{(-1)} + z_m[b_{\mathrm{V}}^{(1)} + 2b_\zeta^{(1)}]q_0^{(0)}\,, \\ \bar{\mathcal{U}}_1 &= \tilde{c}_{\mathrm{t}}^{(1)} u_2^{(1)} - z_m^2 b_{\mathrm{m}}^{(1)} u_3^{(-1)} + z_m[b_{\mathrm{P}}^{(1)} + 2b_\zeta^{(1)}]u_0^{(0)}\,, \\ \bar{\mathcal{W}}_1 &= \tilde{c}_{\mathrm{t}}^{(1)} w_2^{(1)} - z_m^2 b_{\mathrm{m}}^{(1)} w_3^{(-1)} + z_m[b_{\mathrm{A}}^{(1)} + 2b_\zeta^{(1)}]w_0^{(0)} + c_{\mathrm{A}}^{(1)} w_4\,, \\ \bar{\mathcal{R}}_1 &= \tilde{c}_{\mathrm{t}}^{(1)} r_2^{(1)} - z_m^2 b_{\mathrm{m}}^{(1)} r_3^{(-1)} + z_m[b_{\mathrm{V}}^{(1)} + 2b_\zeta^{(1)}]r_0^{(0)}\,. \end{aligned} \tag{B.13}$$

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