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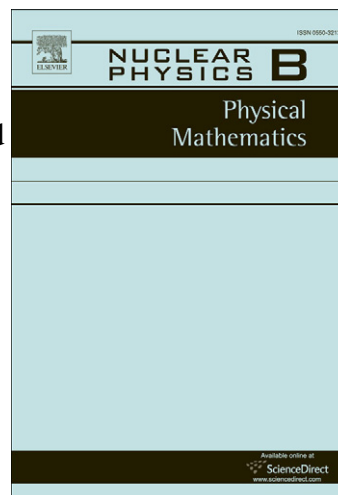
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The chirally rotated Schrödinger functional with Wilson fermions and automatic $O(a)$ improvement

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Abstract

A modified formulation of the Schrödinger functional (SF) is proposed. In the continuum it is related to the standard SF by a non-singlet chiral field rotation and therefore referred to as the chirally rotated SF (χ SF). On the lattice with Wilson fermions the relation is not exact, suggesting some interesting tests of universality. The main advantage of the χ SF consists in its compatibility with the mechanism of automatic $O(a)$ improvement. In this paper the basic set-up is introduced and discussed. Chirally rotated SF boundary conditions are implemented on the lattice using an orbifold construction. The lattice symmetries imply a list of counterterms, which determine how the action and the basic fermionic two-point functions are renormalised and $O(a)$ improved. As with the standard SF, a logarithmically divergent boundary counterterm leads to a multiplicative renormalisation of the quark boundary fields. In addition, a finite dimension 3 boundary counterterm must be tuned in order to preserve the chirally rotated boundary conditions in the interacting theory. Once this is achieved, $O(a)$ effects originating from the bulk action or from insertions of composite operators in the bulk can be avoided by the mechanism of automatic $O(a)$ improvement. The remaining $O(a)$ effects arise from the boundaries and can be cancelled by tuning a couple of $O(a)$ boundary counterterms. The general results are illustrated in the free theory where the Sheikholeslami-Wohlert term is shown to affect correlation functions only at $O(a^2)$, irrespective of its coefficient.

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1 Introduction

The Schrödinger functional (SF) [1–3] has become a general tool to address non-perturbative renormalization problems in lattice QCD [4]¹ and is now even used in candidate theories which might describe a strongly interacting electroweak sector [13–17]. Renormalization schemes based on the SF are gauge invariant, quark mass independent through renormalization in the chiral limit and suitable for evaluation by both Monte Carlo and perturbative methods. Moreover, as the finite space-time volume is used to set the renormalization scale, recursive finite size techniques can be applied to bridge large scale differences, thereby avoiding to resolve widely different scales on a single lattice. As systematic errors in large scale lattice simulations are becoming smaller, the need for a better controlled continuum limit will likely stir more interest in SF schemes, and it is therefore necessary to address its remaining shortcomings.

A first problem consists in the difficulty to implement the SF boundary conditions for fermion regularisations other than Wilson fermions. This has been largely solved, and formulations of the SF with staggered and Ginsparg-Wilson-type fermions have been given in [18–20] and [21–25], respectively.

The main problem with SF schemes is the presence of lattice artefacts which are linear in the lattice spacing a . Some of these $O(a)$ effects are caused by the mere presence of the Euclidean time boundaries, together with local Dirichlet conditions for the fields. Such $O(a)$ boundary effects will be present with any regularisation, since they do not arise from the breaking of a continuum symmetry. In practical applications, these effects are cancelled by adding a couple of boundary counterterms to the action, with coefficients determined perturbatively up to two-loop order [26, 27]. While this is often sufficient in practice, a non-perturbative determination of such boundary counterterms would be desirable and is indeed conceivable.

With Wilson quarks there is a second category of $O(a)$ effects which are cancelled by the usual $O(a)$ counterterms to the Wilson quark action and the composite fields which appear in the correlation functions. At first sight it may be surprising that these standard $O(a)$ counterterms are required at all, given that massless Wilson quarks in a finite volume enjoy the property of automatic $O(a)$ improvement [28]. However, the argument for automatic $O(a)$ improvement relies on a discrete chiral symmetry which is expected to be recovered in the continuum limit. The argument fails as the standard SF boundary conditions break chiral symmetry, so that observables cannot be classified as either even or odd under this symmetry [29,30].

In this paper a modified definition of the Schrödinger functional for Wilson-type quarks is introduced, which is suitable for QCD with an even number of quark

¹see [5] for early references and [6–12] for a selection of more recent applications and further references.

flavours, and which is compatible with automatic $O(a)$ improvement. In the continuum limit this modified SF is related to the standard SF by a chiral field rotation and is therefore referred to as the chirally rotated SF (χ SF). A first account of this work has been given a while ago in refs. [29,30]. The paper is organised as follows: in Section 2 the argument of automatic $O(a)$ improvement is reviewed and the reason why it fails in the presence of SF boundary conditions. Possible modifications of the SF boundary conditions which may restore this argument are discussed next. Concentrating on the solution provided by the chirally rotated SF, its lattice implementation through an orbifold construction is explained in Section 4. The lattice symmetries imply the counterterm structure relevant for renormalisation and $O(a)$ improvement (Section 5). In Section 6, the renormalisation constants and boundary $O(a)$ improvement coefficients are determined to tree-level of perturbation theory, and automatic bulk $O(a)$ improvement is demonstrated to this order. The paper ends with some concluding remarks and an outlook (Section 7). Finally, Appendix A demonstrates the absence of zero modes in the continuum Dirac operator and Appendix B collects some useful formulae for the free fermion propagator both on and off the lattice.

2 Automatic $O(a)$ improvement and SF boundary conditions

In order to understand how the SF boundary conditions interfere with $O(a)$ improvement, it is useful to recall the argument why massless Wilson fermions are expected to be automatically $O(a)$ improved in a finite volume without boundaries.

2.1 Symanzik's effective theory and automatic $O(a)$ improvement

The Wilson fermion action is given by

$$S_f = a^4 \sum_x \bar{\psi}(x) (D_W + m_0) \psi(x), \quad (2.1)$$

$$D_W = \sum_{\mu=0}^3 \frac{1}{2} \{ (\nabla_\mu + \nabla_\mu^*) \gamma_\mu - a \nabla_\mu^* \nabla_\mu \} + c_{\text{sw}} \frac{i}{4} a \sum_{\mu,\nu=0}^3 \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x). \quad (2.2)$$

Here, m_0 is a bare mass parameter, the covariant lattice derivatives in the Wilson-Dirac operator are defined as usual, and the last term is the Sheikholeslami-Wohlert term with $\hat{F}_{\mu\nu}$ denoting the clover leaf definition of the field strength tensor (see ref. [31] for conventions and unexplained notation). Standard Wilson quarks are obtained for $c_{\text{sw}} = 0$. We will focus on the massless limit, which is obtained by tuning the bare mass parameter to its critical value, $m_0 = m_{\text{cr}}$.

Cutoff effects can be studied using Symanzik's effective continuum theory [32, 31]. The effective action,

$$S_{\text{eff}} = S_0 + aS_1 + a^2S_2 + O(a^3), \quad (2.3)$$

starts out with the massless QCD continuum action,

$$S_0 = -\frac{1}{2g^2} \int d^4x \operatorname{tr} \{F_{\mu\nu}(x)F_{\mu\nu}(x)\} + \int d^4x \bar{\psi}(x) \not{D} \psi(x). \quad (2.4)$$

The terms which may appear in S_1 must be integrals over local composite fields of mass dimension 5. In the chiral limit there are only two such terms,

$$S_1 = ic_1 \int d^4x \bar{\psi}(x) \sigma_{\mu\nu} F_{\mu\nu}(x) \psi(x) + c_2 \int d^4x \bar{\psi}(x) D_\mu D_\mu \psi(x), \quad (2.5)$$

which can be reduced to a single term by restricting attention to on-shell quantities. The effective action renders the cutoff dependence explicit, up to logarithmic terms (cf. ref. [33]). The leading cutoff effects in a renormalised connected correlation function of a (multi-local) observable O are then described by the corresponding continuum correlation functions with insertions of either S_1 or the $O(a)$ counterterm δO for the observable O ,

$$\langle O \rangle_c = \langle O \rangle_c^{\text{cont}} - a \langle S_1 O \rangle_c^{\text{cont}} + a \langle \delta O \rangle_c^{\text{cont}} + O(a^2). \quad (2.6)$$

Here, $\langle \cdot \rangle_c^{\text{cont}}$ refers to Euclidean expectation values taken with respect to the continuum action S_0 , only taking into account connected diagrams. Obviously, the continuum action, S_0 , is chirally symmetric. In particular, the discrete γ_5 -transformation

$$\psi \rightarrow \gamma_5 \psi, \quad \bar{\psi} \rightarrow -\bar{\psi} \gamma_5, \quad (2.7)$$

leaves S_0 invariant, while it changes the sign of S_1 . Since the γ_5 -transformation squares to the identity, one may decompose any composite field into parts which are either even or odd under this transformation. Note that, despite the loss of chiral invariance on the lattice, such a decomposition can be made unambiguously for any lattice field. An important observation then is that the $O(a)$ counterterm, δO_{even} for any γ_5 -even field O_{even} must be γ_5 -odd and vice versa [28]. Provided that the functional measure is invariant under the change of variables to the γ_5 -transformed fields, one is then led to conclude that

$$\langle S_1 O_{\text{even}} \rangle_c^{\text{cont}} = -\langle S_1 O_{\text{even}} \rangle_c^{\text{cont}} = 0, \quad (2.8)$$

$$\langle \delta O_{\text{even}} \rangle_c^{\text{cont}} = -\langle \delta O_{\text{even}} \rangle_c^{\text{cont}} = 0, \quad (2.9)$$

i.e. Eq. (2.6) for γ_5 -even observables reads

$$\langle O_{\text{even}} \rangle_c = \langle O_{\text{even}} \rangle_c^{\text{cont}} + O(a^2). \quad (2.10)$$

This does not mean that $O(a)$ effects are absent, rather these are present in correlation functions of γ_5 -odd observables O_{odd} , for which the leading term in (2.6) vanishes, so that

$$\langle O_{\text{odd}} \rangle_c = -a \langle S_1 O_{\text{odd}} \rangle_c^{\text{cont}} + a \langle \delta O_{\text{odd}} \rangle_c^{\text{cont}} + O(a^3). \quad (2.11)$$

Note that the corrections here are of order a^3 , rather than a^2 . In fact, the mechanism of automatic $O(a)$ improvement more generally implies that lattice effects in γ_5 -even (γ_5 -odd) correlation functions only come with even (odd) powers of the lattice spacing a [28,34].

It should be emphasised that the inherent $O(a)$ ambiguity in the definition of the chiral limit with Wilson quarks does not alter this picture. To understand this, suppose that m_0 has been tuned critical e.g. by requiring the divergence of the axial current to vanish for some particular matrix element. By making a different choice, a non-zero quark mass $m' = a\Lambda^2$ is generated relative to the previous definition, with Λ denoting some mass scale. Its effect can be accounted for by an insertion of a fermionic mass term. Since this term is γ_5 -odd, its insertion into an even correlation function vanishes,

$$\int d^4x \langle O_{\text{even}} \bar{\psi}(x) \psi(x) \rangle_c^{\text{cont}} = 0. \quad (2.12)$$

In order to obtain a finite contribution to γ_5 -even observables at least a double insertion of this term is required, making it an a^2 -effect, as anticipated.

Note that the above arguments rely on the assumption that the functional measure is invariant under the change of variables to the γ_5 -transformed fields. To check this assumption it is useful to think of the effective Symanzik theory as being formulated on a very fine lattice with a spacing b very much smaller than a such that the theory is essentially continuum-like. Nevertheless, the functional integral in a finite volume is still finite-dimensional and mathematically well-defined. Furthermore, with Ginsparg-Wilson quarks, the fermionic part of the continuum like action

$$S_{0,f} = b^4 \sum_x \bar{\psi}(x) D_N \psi(x), \quad (2.13)$$

has an exact chiral symmetry [35]. Here, D_N is the Neuberger operator [36], which satisfies the Ginsparg-Wilson relation [37],

$$\gamma_5 D_N + D_N \gamma_5 = b D_N \gamma_5 D_N. \quad (2.14)$$

Combined with the γ_5 -conjugation property, $D_N^\dagger = \gamma_5 D_N \gamma_5$, this gives rise to the definition of $\hat{\gamma}_5$,

$$\hat{\gamma}_5 = \gamma_5 V, \quad V = 1 - b D_N, \quad (2.15)$$

which is hermitian and squares to the identity. However, in contrast to the ordinary γ_5 , it depends implicitly on the gauge field through the unitary matrix V . Replacing the γ_5 -transformation (2.7) with its version on the fine lattice,

$$\psi \rightarrow \hat{\gamma}_5 \psi, \quad \bar{\psi} \rightarrow -\bar{\psi} \gamma_5, \quad (2.16)$$

one readily verifies the invariance of the action (2.13), which follows from the Ginsparg-Wilson relation (2.14). Changing variables in the functional integral to the γ_5 -transformed fields, one finds that the Jacobian J is given by

$$J = \det(\gamma_5 \hat{\gamma}_5) = \det(V) = \det(\gamma_5 V \gamma_5) = \det(V^\dagger) = \pm 1. \quad (2.17)$$

For N_f quark flavours, each γ_5 -transformed flavour thus contributes a factor J , so that the total Jacobian becomes J^{N_f} . Hence, for even N_f , the γ_5 -transformation (2.16) is an exact symmetry of the path integral measure². In conclusion, one expects that lattice QCD with an even number of Wilson type quarks is indeed automatically $O(a)$ improved, at least in a finite volume with periodic boundary conditions.

However, the situation changes in the presence of SF boundary conditions, which, for the fermionic fields, read [2] ,

$$\begin{aligned} P_+ \psi(x)|_{x_0=0} &= 0, & P_- \psi(x)|_{x_0=T} &= 0, \\ \bar{\psi}(x) P_-|_{x_0=0} &= 0, & \bar{\psi}(x) P_+|_{x_0=T} &= 0, \end{aligned} \quad (2.18)$$

with $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$. The γ_5 -transformation is then no longer a symmetry of the effective continuum theory, as the γ_5 -transformed fields satisfy the SF boundary conditions with the complementary projectors, e.g.

$$\psi' = \gamma_5 \psi \quad \Rightarrow \quad P_- \psi'|_{x_0=0} = \gamma_5 P_+ \psi|_{x_0=0} = 0. \quad (2.19)$$

This may be taken as a property of the fermion measure, since the function space integrated over is not the same before and after the change of variables. Hence, the transformed correlation functions cannot be proportional to the original ones, and the basic argument needed for automatic $O(a)$ improvement cannot be made.

2.2 Rendering automatic $O(a)$ improvement compatible with the SF

The question then arises whether there are ways to save automatic $O(a)$ improvement in the presence of SF boundary conditions. One needs to either find an alternative to the γ_5 -transformation or modify the SF boundary conditions such that

²For a single quark flavour, a gauge field dependent sign in the Jacobian remains, thereby spoiling the argument for automatic $O(a)$ improvement. While some additional argument would be needed for $N_f = 1$, the situation is slightly better for odd flavour numbers $N_f > 1$, as the argument can then be applied to any pair of fermion flavours.

the transformation remains a symmetry of the massless continuum action, while the (homogeneous) SF boundary conditions are left invariant. There are various ways to achieve this:

- Let ψ be a flavour doublet, and augment the γ_5 -transformation by a flavour permutation, i.e.

$$\psi \rightarrow \tau^1 \gamma_5 \psi, \quad \bar{\psi} \rightarrow -\bar{\psi} \gamma_5 \tau^1, \quad (2.20)$$

where τ^1 is a Pauli matrix. This flavour permutation does not affect the bulk action and $O(a)$ improvement for $\gamma_5 \tau^1$ -even observables in the bulk can be shown as before. Then, giving the boundary conditions a flavour structure through the replacement

$$P_{\pm} = \frac{1}{2}(1 \pm \gamma_0) \longrightarrow \tilde{P}_{\pm} = \frac{1}{2}(1 \pm \gamma_0 \tau^3), \quad (2.21)$$

one easily sees that, due to

$$[\gamma_5 \tau^1, \tilde{P}_{\pm}] = 0, \quad (2.22)$$

the boundary conditions are preserved by the $\gamma_5 \tau^1$ -transformation.

- Another possibility consists in combining the $\gamma_5 \tau^1$ -transformation (2.20) with Dirichlet boundary conditions using the projectors

$$\tilde{Q}_{\pm} = \frac{1}{2}(1 \pm i\gamma_0 \gamma_5 \tau^3) \Rightarrow [\gamma_5 \tau^1, \tilde{Q}_{\pm}] = 0. \quad (2.23)$$

It is this option which will be investigated in much more detail below.

While it is relatively easy to find alternative SF boundary conditions and/or alternatives to the γ_5 -transformation, the difficult part is to show that this leads to a sensible alternative definition of the Schrödinger functional in the continuum limit. Besides renormalizability one would like to maintain the properties of the standard SF such as the absence of fermionic zero modes, which is crucial for practical applications. Another difficulty lies in the actual implementation of these boundary conditions on the lattice. All these questions will be addressed in the following for the proposed solution involving the projectors in Eq. (2.23).

3 Continuum considerations

The boundary conditions involving the projectors $\tilde{Q}_{\pm}$ can be thought of as a chirally rotated version of the standard SF boundary conditions. As the non-singlet chiral rotation is part of the continuum symmetries of massless QCD, the alternative formulation of the SF to be introduced here will in fact be closely related to the standard SF. It is useful to have a closer look at this relationship before passing to the lattice formulation.

3.1 Chirally rotated SF boundary conditions

Let ψ' and $\bar{\psi}'$ be isospin doublets of quark and anti-quark fields satisfying the homogeneous SF boundary conditions, Eq.(2.18). Performing a non-singlet chiral field rotation,

$$\psi' = R(\alpha)\psi, \quad \bar{\psi}' = \bar{\psi}R(\alpha), \quad R(\alpha) = \exp(i\alpha\gamma_5\tau^3/2), \quad (3.1)$$

the rotated fields satisfy the chirally rotated boundary conditions,

$$\begin{aligned} P_+(\alpha)\psi(x)|_{x_0=0} &= 0, & P_-(\alpha)\psi(x)|_{x_0=T} &= 0, \\ \bar{\psi}(x)\gamma_0 P_-(\alpha)|_{x_0=0} &= 0, & \bar{\psi}(x)\gamma_0 P_+(\alpha)|_{x_0=T} &= 0, \end{aligned} \quad (3.2)$$

with the projectors

$$P_{\pm}(\alpha) = \frac{1}{2} [1 \pm \gamma_0 \exp(i\alpha\gamma_5\tau^3)]. \quad (3.3)$$

For $\alpha = 0$ the standard projectors $P_{\pm} = P_{\pm}(0)$ are recovered, while for $\alpha = \pi/2$ one finds,

$$P_{\pm}(\pi/2) \equiv \tilde{Q}_{\pm} = \frac{1}{2} (1 \pm i\gamma_0\gamma_5\tau^3). \quad (3.4)$$

Since $\gamma_0\tilde{Q}_{\pm} = \tilde{Q}_{\mp}\gamma_0$, the boundary conditions (3.2) in this special case read

$$\begin{aligned} \tilde{Q}_+\psi(x)|_{x_0=0} &= 0, & \tilde{Q}_-\psi(x)|_{x_0=T} &= 0, \\ \bar{\psi}(x)\tilde{Q}_+|_{x_0=0} &= 0, & \bar{\psi}(x)\tilde{Q}_-|_{x_0=T} &= 0. \end{aligned} \quad (3.5)$$

We thus see that boundary conditions involving the projectors $\tilde{Q}_{\pm}$ appear naturally when chirally rotating quark and anti-quark fields which satisfy the standard SF boundary conditions.

3.2 Properties of the continuum Dirac operator

In the continuum the rotation angle α parameterizes a family of linear spaces of functions which satisfy homogeneous Dirichlet boundary conditions in Euclidean time. In the spatial directions we assume L -periodicity and we allow for a constant U(1) gauge background field $i\theta_{\mu}/L$. Formally this field may be included in the Dirac operator by promoting the SU(N) colour gauge field to a U(N) gauge field as follows:

$$A_{\mu}(x) = \sum_{a=0}^{N^2-1} A_{\mu}^a(x)T^a, \quad A_{\mu}^0(x)T^0 = i\frac{\theta_{\mu}}{L}\mathbf{1}. \quad (3.6)$$

Following [38,31], we set $\theta_1 = \theta_2 = \theta_3 = \theta$ and $\theta_0 = 0$. With respect to the natural inner product,

$$(\varphi, \chi) = \int_0^T dx_0 \int d^3\mathbf{x} \varphi(x)^{\dagger} \chi(x), \quad (3.7)$$

the Dirac operator for a quark doublet and generic angle α is γ_5 -hermitian up to a flavour exchange, i.e.

$$(\gamma_5 \tau^1 [\mathcal{D} + m + i\mu_q \gamma_5 \tau^3])^\dagger = \gamma_5 \tau^1 [\mathcal{D} + m + i\mu_q \gamma_5 \tau^3]. \quad (3.8)$$

For later reference both a standard and a twisted mass term have been included. Hence, a well-defined eigenvalue problem is obtained for any value³ of α . Denoting the eigenfunctions in the standard SF by v_n , the eigenvalue equation reads

$$\gamma_5 \tau^1 [\mathcal{D} + m + i\mu_q \gamma_5 \tau^3] v_n = \lambda_n v_n. \quad (3.9)$$

Performing the chiral rotation as in Eq.(3.1),

$$v_n = R(\alpha) w_n \quad (3.10)$$

and using

$$R(\alpha) [\mathcal{D} + m + i\mu_q \gamma_5 \tau^3] R(\alpha) = \mathcal{D} + \tilde{m} + i\tilde{\mu}_q \gamma_5 \tau^3, \quad (3.11)$$

one finds,

$$\gamma_5 \tau^1 [\mathcal{D} + \tilde{m} + i\tilde{\mu}_q \gamma_5 \tau^3] w_n = \lambda_n w_n. \quad (3.12)$$

Hence, the eigenfunctions are related by a chiral rotation, and the eigenvalues are exactly the same as in the standard SF, provided the mass parameters either vanish or are transformed covariantly, according to

$$\tilde{m} = m \cos \alpha - \mu_q \sin \alpha, \quad \tilde{\mu}_q = m \sin \alpha + \mu_q \cos \alpha. \quad (3.13)$$

Moreover, the absence of zero modes in the massless theory can be established following Lüscher [24], and some details have been deferred to Appendix A. Given the absence of zero modes, the free continuum quark propagator can then be calculated using standard techniques. Some results are collected in Appendix B.

3.3 Relating correlation functions at different values of α

The chiral rotation (3.1) is not anomalous, so that one may perform a corresponding change of variables in the functional integral. One obtains relations between correlation functions defined with the standard and the chirally rotated SF boundary conditions. This is similar to and generalises the relations between correlation functions in twisted mass and standard QCD [39,30]. In particular, one expects that these formal continuum relations will hold up to cutoff effects, for appropriately renormalised correlation functions on the lattice.

³As an aside note that for $\alpha = \pi/2$ the massless operator $i\mathcal{D}$ is hermitian for a single fermion with boundary conditions corresponding to either the up or the down flavour in Eq. (3.5).

It is instructive to include both a standard and a twisted mass term in the fermionic action at $\alpha = 0$,

$$S_f[m, \mu_q] = \int_0^T dx_0 \int_0^L d^3\mathbf{x} \bar{\psi}'(x)(\not{D} + m + i\mu_q\gamma_5\tau^3)\psi'(x), \quad (3.14)$$

even though the focus will later be on massless QCD. Performing the change of variables, Eq. (3.1), in the Euclidean functional integral one obtains the generic identities,

$$\langle O[\psi, \bar{\psi}] \rangle_{(m, \mu_q, P_{\pm})} = \langle O[R(\alpha)\psi, \bar{\psi}R(\alpha)] \rangle_{(\tilde{m}, \tilde{\mu}_q, P_{\pm}(\alpha))}, \quad (3.15)$$

where the integration variables are assumed to be ψ and $\bar{\psi}$ on both sides of the equation. In addition to the boundary conditions for ψ at $x_0 = 0, T$, the subscript to the correlation functions indicates the mass parameters in the action and the mass parameters are related as in Eq. (3.13). The relation (3.15) establishes a mapping of correlation functions defined at different values of α . An equivalent form of this mapping is given by

$$\langle O[\psi, \bar{\psi}] \rangle_{(\tilde{m}, \tilde{\mu}_q, \tilde{Q}_{\pm})} = \langle O[R(-\alpha)\psi, \bar{\psi}R(-\alpha)] \rangle_{(m, \mu_q, P_{\pm}(\frac{\pi}{2}-\alpha))}. \quad (3.16)$$

Setting the twisted mass term to zero in the chirally rotated SF, and choosing $\alpha = \pi/2$, this simplifies to

$$\langle O[\psi, \bar{\psi}] \rangle_{(m, 0, \tilde{Q}_{\pm})} = \langle O[R(-\pi/2)\psi, \bar{\psi}R(-\pi/2)] \rangle_{(0, -m, P_{\pm})}, \quad (3.17)$$

which shows that the standard mass parameter in the chirally rotated SF is equivalent to a (negative) twisted mass parameter in the standard SF.

The simplest fermionic correlation function is the quark propagator. Using the explicit expressions of Appendix B, one may easily verify the identity (3.1) in the free theory, viz.

$$\langle \psi(x)\bar{\psi}(y) \rangle_{(m, \mu_q, P_{\pm})}^{(g=0)} = R(\alpha) \langle \psi(x)\bar{\psi}(y) \rangle_{(\tilde{m}, \tilde{\mu}_q, P_{\pm}(\alpha))}^{(g=0)} R(\alpha). \quad (3.18)$$

Gauge invariant correlation functions corresponding to the ones defined in the standard SF [31,40] can be defined as well. For this we need the fermionic boundary fields, ζ, ζ' and $\bar{\zeta}, \bar{\zeta}'$, which are naturally included in the mapping (3.15) by identifying them with the non-Dirichlet components near the time boundaries. More precisely we set

$$\begin{aligned} \zeta(\mathbf{x}) &= P_-(\alpha)\psi(0, \mathbf{x}), & \zeta'(\mathbf{x}) &= P_+(\alpha)\psi(T, \mathbf{x}), \\ \bar{\zeta}(\mathbf{x}) &= \bar{\psi}(0, \mathbf{x})P_+(-\alpha), & \bar{\zeta}'(\mathbf{x}) &= \bar{\psi}(T, \mathbf{x})P_-(-\alpha), \end{aligned} \quad (3.19)$$

thus leaving the α -dependence implicit. This should not lead to any confusion, as the fermionic boundary fields mostly appear as insertions into correlation functions with the subscripts indicating the projectors used for the boundary conditions.

3.4 Symmetries and conventions

The standard SF boundary conditions break all chiral symmetries, as is best illustrated by the Ward identities [24]. With the global axial and vector non-singlet variations,

$$\begin{aligned}\delta_A^a \psi &= \gamma_5 \frac{\tau^a}{2} \psi, & \delta_V^a \psi &= \frac{\tau^a}{2} \psi, \\ \delta_A^a \bar{\psi} &= \bar{\psi} \gamma_5 \frac{\tau^a}{2}, & \delta_V^a \bar{\psi} &= -\bar{\psi} \frac{\tau^a}{2},\end{aligned}\quad (3.20)$$

the Ward identities take the form,

$$\langle \delta_X^a O \rangle_{(P_\pm)} = \langle \delta_X^a S O \rangle_{(P_\pm)}, \quad X = A, V, \quad (3.21)$$

where O denotes an arbitrary composite field, and the subscript to the expectation values indicates the boundary conditions for ψ at $x_0 = 0, T$. The variation of the action is given by

$$\delta_X S = - \int d^4x \partial_\mu X_\mu^a(x), \quad (3.22)$$

with the Noether currents

$$A_\mu^a(x) = \bar{\psi}(x) \gamma_\mu \gamma_5 \frac{\tau^a}{2} \psi(x), \quad V_\mu^a(x) = \bar{\psi}(x) \gamma_\mu \frac{\tau^a}{2} \psi(x). \quad (3.23)$$

The boundary conditions in the spatial directions being periodic, the integral over the total divergence yields only surface terms in the time direction. The r.h.s. of Eq. (3.21) becomes

$$\langle \delta_X^a S O \rangle_{(P_\pm)} = \int d^3\mathbf{x} \langle [X_0^a(0, \mathbf{x}) - X_0^a(T, \mathbf{x})] O \rangle_{(P_\pm)}. \quad (3.24)$$

Using the standard SF boundary conditions, Eqs. (2.18) and the identity $\gamma_0 P_\pm = \pm P_\pm$, one obtains

$$A_0^a(0, x) = \bar{\psi}(0, \mathbf{x}) P_+ \gamma_5 \frac{\tau^a}{2} P_- \psi(0, \mathbf{x}) = \bar{\zeta}(\mathbf{x}) \gamma_5 \frac{\tau^a}{2} \zeta(\mathbf{x}), \quad (3.25)$$

$$A_0^a(T, x) = \bar{\psi}(T, \mathbf{x}) P_- \gamma_5 \frac{\tau^a}{2} P_+ \psi(0, \mathbf{x}) = \bar{\zeta}'(\mathbf{x}) \gamma_5 \frac{\tau^a}{2} \zeta'(\mathbf{x}), \quad (3.26)$$

whereas $V_0^a(0, \mathbf{x})$ and $V_0^a(T, \mathbf{x})$ vanish. One thus arrives at the Ward identities,

$$\langle \delta_A^a O \rangle_{(P_\pm)} = \frac{1}{2} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \gamma_5 \tau^a \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \gamma_5 \tau^a \zeta'(\mathbf{z})] O \rangle_{(P_\pm)}, \quad (3.27)$$

$$\langle \delta_V^a O \rangle_{(P_\pm)} = 0, \quad (3.28)$$

which show that the standard $SU(2)$ vector symmetry is conserved, while chiral symmetry is broken by terms which are localized at the time boundaries, with coefficients of $O(1)$.

Proceeding analogously we may derive the Ward identities in the presence of chirally rotated SF boundary conditions,

$$\langle \delta_A^a O \rangle_{(P_{\pm}(\alpha))} = \frac{1}{2} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \gamma_0 \gamma_5 \tau^a \zeta(\mathbf{z}) - \bar{\zeta}'(\mathbf{z}) \gamma_0 \gamma_5 \tau^a \zeta'(\mathbf{z})] O \rangle_{(P_{\pm}(\alpha))} \quad (3.29)$$

$$\langle \delta_V^a O \rangle_{(P_{\pm}(\alpha))} = \frac{1}{2} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \gamma_0 \tau^a \zeta(\mathbf{z}) - \bar{\zeta}'(\mathbf{z}) \gamma_0 \tau^a \zeta'(\mathbf{z})] O \rangle_{(P_{\pm}(\alpha))}. \quad (3.30)$$

Using the projector structure implicit in the fermionic boundary fields, Eq. (3.19), the r.h.s. of the vector Ward identity (3.30) with index $a = 3$ is seen to vanish. Moreover, there are two further linear combinations of Eqs. (3.29,3.30) for which the r.h.s. vanishes, so that three generators correspond to conserved symmetries. This is not surprising, as the chiral rotation merely transforms the vector symmetry of the standard SF to an unusual form, a situation which is familiar from twisted mass QCD [39,30]. To illustrate this further, consider the case of most interest, $\alpha = \pi/2$, where the Ward identities take the form

$$\langle \delta_A^a O \rangle_{(\tilde{Q}_{\pm})} = \frac{i}{2} \delta^{3a} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \zeta'(\mathbf{z})] O \rangle_{(\tilde{Q}_{\pm})}, \quad (3.31)$$

$$\langle \delta_V^a O \rangle_{(\tilde{Q}_{\pm})} = \frac{i}{2} \varepsilon^{3ab} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \gamma_5 \tau^b \zeta(\mathbf{z}) - \bar{\zeta}'(\mathbf{z}) \gamma_5 \tau^b \zeta'(\mathbf{z})] O \rangle_{(\tilde{Q}_{\pm})}. \quad (3.32)$$

Apparently a mixture of vector and axial symmetries are broken by boundary terms. However, in massless QCD this is really a convention dependent statement. A preferred or “physical” basis is only available in the presence of a mass term: those symmetry transformations which leave the mass term invariant are identified as vector symmetries whereas the remaining chiral flavour transformations are classified as axial symmetries. In massless QCD with SF type boundary conditions we will choose a similar convention, and define the “physical” basis as the one with standard SF boundary conditions. This implies that the broken symmetries are in all cases the axial symmetries, whereas the vector or isospin symmetries are conserved. The situation is then completely analogous to twisted mass QCD, in particular, the “dictionary” translating composite fields between both bases can be taken over from twisted mass QCD.

4 χ SF boundary conditions on the lattice

Implementing boundary conditions on the lattice is not straightforward, since boundary conditions cannot really be imposed. Rather, they arise dynamically from the

structure of the lattice action near the boundaries. An attractive, though not universally applicable technique to obtain a lattice theory with the desired boundary conditions is based on an orbifold construction. In the context of lattice QCD orbifold techniques have previously been applied by Taniguchi [21] in order to implement SF boundary conditions for Ginsparg-Wilson quarks. The rôle of the orbifold construction is to define the action of the lattice operator near the time boundaries, such that the desired boundary conditions are obtained for the free theory. In a second step one needs to analyse the symmetries and list the allowed boundary counterterms which will be generated by the interactions. From the list of possible counterterms one may conclude whether the desired boundary conditions will be obeyed in the renormalised theory, or whether this requires the fine tuning of some counterterm coefficients (cf. Sect. 5).

4.1 Orbifold construction

The starting point is a single Wilson quark flavour χ with lattice action

$$S_f[\chi, \bar{\chi}, U] = a^4 \sum_{-T < x_0 \leq T} \sum_{\mathbf{x}} \bar{\chi}(x) (D_W + m_0) \chi(x). \quad (4.1)$$

The fermionic fields are taken to be $2T$ -anti-periodic in the Euclidean time direction,

$$\chi(x_0 + 2T, \mathbf{x}) = -\chi(x), \quad \bar{\chi}(x_0 + 2T, \mathbf{x}) = -\bar{\chi}(x). \quad (4.2)$$

The orbifold reflection $\mathcal{T}$ about the Euclidean time $x_0 = 0$ is defined by,

$$\mathcal{T} : \chi(x) \rightarrow (\mathcal{T}\chi)(x) = i\gamma_0\gamma_5\chi(-x_0, \mathbf{x}), \quad \bar{\chi}(x) \rightarrow (\bar{\chi}\mathcal{T})(x) = \bar{\chi}(-x_0, \mathbf{x})i\gamma_0\gamma_5. \quad (4.3)$$

Following ref. [21] the gauge field is treated as an external field. It is first extended to the doubled time interval $[-T, T]$, through

$$U_k(-x_0, \mathbf{x}) = U_k(x_0, \mathbf{x}), \quad U_0(-x_0 - a, \mathbf{x})^\dagger = U_0(x), \quad (4.4)$$

and then $2T$ -periodically continued to all Euclidean times. Since $\mathcal{T}$ is an involution, one may define associated projectors and project on $\mathcal{T}$ -even and -odd fields as follows:

$$\chi_\pm = \frac{1}{2}(1 \pm \mathcal{T})\chi, \quad \bar{\chi}_\pm = \bar{\chi}\frac{1}{2}(1 \pm \mathcal{T}). \quad (4.5)$$

Even and odd fields then satisfy homogeneous Dirichlet conditions at $x_0 = 0$,

$$(1 \mp i\gamma_0\gamma_5)\chi_\pm(0, \mathbf{x}) = 0, \quad \bar{\chi}_\pm(0, \mathbf{x})(1 \mp i\gamma_0\gamma_5) = 0. \quad (4.6)$$

Furthermore, due to the $2T$ -anti-periodicity in time, Dirichlet conditions with the complementary projectors are obtained at $x_0 = T$,

$$(1 \pm i\gamma_0\gamma_5)\chi_\pm(T, \mathbf{x}) = 0, \quad \bar{\chi}_\pm(T, \mathbf{x})(1 \pm i\gamma_0\gamma_5) = 0. \quad (4.7)$$

$\mathcal{T}$ -even and odd anti-quark fields are defined analogously. For the orbifold projection to be consistent with the lattice theory, it is necessary that the reflection $\mathcal{T}$ commutes (or anti-commutes) with the Wilson-Dirac operator. The lattice action can then be decomposed according to

$$S_f[\chi, \bar{\chi}, U] = S_f[\chi_+ + \chi_-, \bar{\chi}_+ + \bar{\chi}_-, U] = S_f[\chi_+, \bar{\chi}_+, U] + S_f[\chi_-, \bar{\chi}_-, U]. \quad (4.8)$$

To check whether this is indeed the case for the reflection (4.3), the crucial relations to note are

$$\mathcal{T}\nabla_0^* = -\nabla_0\mathcal{T}, \quad \mathcal{T}\nabla_0 = -\nabla_0^*\mathcal{T}, \quad (4.9)$$

for the forward and backward covariant time derivatives. On the other hand, all spatial derivatives simply commute with $\mathcal{T}$. Taking into account the γ -matrix structure in the Wilson-Dirac operator this then leads to $[\mathcal{T}, D_W] = 0$, as required.

As a consequence, one may consistently restrict attention to either the $\mathcal{T}$ -even or the $\mathcal{T}$ -odd fields. For instance, using only the $\mathcal{T}$ -odd fields, the fermionic functional integral is taken to be

$$\int D[\chi_-, \bar{\chi}_-] \exp(-S_f[\chi_-, \bar{\chi}_-, U]). \quad (4.10)$$

Both $\mathcal{T}$ -even and $\mathcal{T}$ -odd fields are determined for negative times $x_0 \in [-T, 0]$, once specified for $x_0 \in [0, T]$. Hence, the field values at the negative times are no independent degrees of freedom, and the integration measure over the odd fields in Eq. (4.10) can be written as a measure over the fields at Euclidean times $x_0 \in [0, T]$,

$$D[\chi_-, \bar{\chi}_-] = \prod_{\mathbf{x}} d\varphi(\mathbf{x}) d\bar{\varphi}(\mathbf{x}) \prod_{0 < x_0 < T} d\chi_-(x) d\bar{\chi}_-(x), \quad (4.11)$$

where the non-Dirichlet components have been combined in the spinors $\varphi(\mathbf{x})$ and $\bar{\varphi}(\mathbf{x})$, viz.

$$\varphi(\mathbf{x}) = Q_- \chi_-(0, \mathbf{x}) + Q_+ \chi_-(T, \mathbf{x}), \quad (4.12)$$

$$\bar{\varphi}(\mathbf{x}) = \bar{\chi}_-(0, \mathbf{x}) Q_- + \bar{\chi}_-(T, \mathbf{x}) Q_+, \quad (4.13)$$

with $Q_{\pm} = \frac{1}{2}(1 \pm i\gamma_0\gamma_5)$. Also the action can be reduced to the interval $[0, T]$: taking into account Eq. (4.4), the action for the fields at negative times $x_0 \in [-T, 0]$ turns out to be the same as for the fields at positive times. Eventually, the only trace left by the orbifold reflection is the structure of the Wilson-Dirac operator near the time boundaries.

The case of a flavour doublet with boundary conditions given in terms of the projectors $\tilde{Q}_{\pm}$, is naturally obtained by interpreting the even and odd fields as the components of a flavour doublet. More precisely, one sets

$$\psi = \sqrt{2} \begin{pmatrix} \chi_- \\ \chi_+ \end{pmatrix}, \quad \bar{\psi} = \sqrt{2} (\bar{\chi}_-, \bar{\chi}_+). \quad (4.14)$$

With this convention the fields ψ and $\bar{\psi}$ satisfy the boundary conditions (3.5). The prefactor has been included in order to obtain the correct normalisation of the kinetic term, once the action is reduced to the interval $[0, T]$. In the case at hand the dynamical degrees of freedom are the fields $\psi(x)$ and $\bar{\psi}(x)$ for $0 < x_0 < T$ as well as the non-Dirichlet components at the boundaries, i.e. $\tilde{Q}_-\psi(0, \mathbf{x})$, $\tilde{Q}_+\psi(T, \mathbf{x})$ and $\bar{\psi}(0, \mathbf{x})\tilde{Q}_-$, $\bar{\psi}(T, \mathbf{x})\tilde{Q}_+$. The Dirac operator is implicitly defined when the action is reduced to the time interval $[0, T]$:

$$\begin{aligned} S_f[\chi, \bar{\chi}, U] &= S_f[\chi_+, \bar{\chi}_+, U] + S_f[\chi_-, \bar{\chi}_-, U] \\ &= \frac{1}{2}a^4 \sum_{-T < x_0 \leq T} \sum_{\mathbf{x}} \bar{\psi}(x)(D_W + m_0)\psi(x) \\ &= a^4 \sum_{0 \leq x_0 \leq T} \sum_{\mathbf{x}} \bar{\psi}(x)(D_W + m_0)\psi(x). \end{aligned} \quad (4.15)$$

More explicitly, writing D_W as a time difference operator,

$$aD_W\psi(x) = -U_0(x)P_-\psi(x + a\hat{0}) + K\psi(x) - U_0(x - a\hat{0})^\dagger P_+\psi(x - a\hat{0}), \quad (4.16)$$

with the time diagonal kernel being given by

$$\begin{aligned} K\psi(x) &= \left(1 + \frac{1}{2} \sum_{k=1}^3 \{a(\nabla_k + \nabla_k^*)\gamma_k - a^2 \nabla_k^* \nabla_k\}\right) \psi(x) \\ &\quad + c_{\text{sw}} \frac{i}{4} a \sum_{\mu, \nu=0}^3 \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x) \psi(x), \end{aligned} \quad (4.17)$$

one finds

$$aD_W\psi(x) = \begin{cases} \frac{1}{2}\tilde{Q}_-K\tilde{Q}_-\psi(x) - \tilde{Q}_-P_-\psi(x + a\hat{0}) & \text{if } x_0 = 0, \\ -P_+\tilde{Q}_-\psi(x - a\hat{0}) + K\psi(x) - P_-\psi(x + a\hat{0}) & \text{if } x_0 = a, \\ aD_W\psi(x) & \text{if } a < x_0 < T - a, \\ -P_+\psi(x - a\hat{0}) + K\psi(x) - P_-\tilde{Q}_+\psi(x + a\hat{0}) & \text{if } x_0 = T - a, \\ -\tilde{Q}_+P_+\psi(x - a\hat{0}) + \frac{1}{2}\tilde{Q}_+K\tilde{Q}_+\psi(x) & \text{if } x_0 = T, \end{cases} \quad (4.18)$$

where the temporal links have been set to unit matrices for better readability. Note that this structure follows from the boundary conditions for both ψ and $\bar{\psi}$, and the explicit factor 1/2 at the boundaries arises from the standard normalisation of the kinetic term. The orbifold construction also determines the Sheikholeslami-Wohlert term at the time boundaries. However, in practical applications it may be easier to set the coefficient of the Sheikholeslami-Wohlert term at the time boundaries to zero. This amounts to a change of a dimension 5 operator at the boundaries, i.e. a change in the action by a term of $O(a^2)$.

4.2 Orbifold reflection with an $O(a)$ offset

On a hypercubic lattice it is natural to distinguish between site and link reflections. The orbifold construction just described corresponds to using a site reflection about the time $x_0 = 0$. Orbifold constructions based on link reflections correspond to an offset by $a/2$ of the reflection point, i.e $x_0 = \pm a/2$. Both options may be interesting in practice and are discussed in turn, beginning with link reflection about $x_0 = -a/2$. It is convenient to set $T' = T + a$. Then the starting point is the same as in Eq. (4.1), with the replacement $T \rightarrow T'$, and the fermion fields are now taken to be anti-periodic with period $2T'$. The orbifold reflection is defined by

$$\mathcal{T}_+ : \chi(x) \rightarrow i\gamma_0\gamma_5\chi(-a - x_0, \mathbf{x}), \quad \bar{\chi}(x) \rightarrow \bar{\chi}(-a - x_0, \mathbf{x})i\gamma_0\gamma_5. \quad (4.19)$$

and the external gauge field is extended to the interval $[-T', T']$,

$$U_k(-a - x_0, \mathbf{x}) = U_k(x_0, \mathbf{x}), \quad U_0(-2a - x_0, \mathbf{x})^\dagger = U_0(x), \quad (4.20)$$

and then $2T'$ -periodically continued. This implies that the spatial gauge fields at the time boundaries are duplicated and the time-like links connecting the doubled boundary layers are set to unit matrices.

Again the orbifold reflection $\mathcal{T}_+$ commutes with the Wilson-Dirac operator, and $\mathcal{T}_+$ -even and -odd quark fields can be defined as previously,

$$\chi_\pm = \frac{1}{2}(1 \pm \mathcal{T}_+)\chi, \quad \bar{\chi}_\pm = \bar{\chi}\frac{1}{2}(1 \pm \mathcal{T}_+). \quad (4.21)$$

However, it is obvious that these fields will not exactly satisfy the desired continuum boundary conditions. For instance, for the odd fields one finds,

$$\chi_-(0, \mathbf{x}) = i\gamma_0\gamma_5\chi(-a, \mathbf{x}), \quad \chi_-(T, \mathbf{x}) = -i\gamma_0\gamma_5\chi(T + a, \mathbf{x}), \quad (4.22)$$

i.e. boundary conditions would be obtained at $x_0 = -a/2$ or $x_0 = T + a/2$, where there are no lattice points available. One may however say that the boundary conditions are satisfied up to $O(a)$ effects. In fact, combining the even and odd fields in quark doublets ψ and $\bar{\psi}$ as in Eq. (4.14), one may write, in terms of the ordinary lattice forward and backward derivatives,

$$\begin{aligned} \tilde{Q}_+(1 - \frac{1}{2}a\partial_0^*)\psi(x)|_{x_0=0} &= 0, & \tilde{Q}_-(1 + \frac{1}{2}a\partial_0)\psi(x)|_{x_0=T} &= 0, \\ \bar{\psi}(x)\tilde{Q}_+(1 - \frac{1}{2}a\overleftarrow{\partial}_0^*)|_{x_0=0} &= 0, & \bar{\psi}(x)\tilde{Q}_-(1 + \frac{1}{2}a\overleftarrow{\partial}_0)|_{x_0=T} &= 0. \end{aligned} \quad (4.23)$$

Note that there is no problem with gauge invariance here, as the time-like links between the doubled boundary layer are set to unit matrices.

Once again the action and the dynamical variables can be reduced explicitly to the time interval $[0, T]$, and the final result can be written as

$$S_f = a^4 \sum_{x_0=0}^T \sum_{\mathbf{x}} \bar{\psi}(x) (\mathcal{D}_W + m_0) \psi(x), \quad (4.24)$$

where the Wilson-Dirac operator is specified by

$$a\mathcal{D}_W\psi(x) = \begin{cases} -U_0(x)P_-\psi(x + a\hat{\mathbf{0}}) + (K + i\gamma_5\tau^3P_-)\psi(x) & \text{if } x_0 = 0, \\ aD_W\psi(x) & \text{if } 0 < x_0 < T, \\ (K + i\gamma_5\tau^3P_+)\psi(x) - U_0(x - a\hat{\mathbf{0}})^\dagger P_+\psi(x - a\hat{\mathbf{0}}) & \text{for } x_0 = T. \end{cases} \quad (4.25)$$

The dynamical field variables (i.e. the integration variables in the functional integral) are now given by the fields $\psi(x)$ and $\bar{\psi}(x)$ for times $0 \leq x_0 \leq T$. Note also that the form of the Dirac operator $\mathcal{D}_W$ can be obtained directly by acting with the infinite volume operator D_W on functions $\psi(x)$ for $0 \leq x_0 \leq T$, supplemented with the “syntactic extension”,

$$\psi(-a, \mathbf{x}) = -i\gamma_0\gamma_5\tau^3\psi(0, \mathbf{x}), \quad \psi(T + a, \mathbf{x}) = i\gamma_0\gamma_5\tau^3\psi(T, \mathbf{x}), \quad (4.26)$$

and taken to vanish at all other times. Note that a similar statement can not be made for the orbifold construction based on the site-reflection $\mathcal{T}$, as the expression of the Dirac operator in Eq. (4.18) also refers to the boundary conditions for $\bar{\psi}$.

4.3 Orbifold construction with link reflection about $x_0 = a/2$

We start again from Eq. (4.1), but with the replacement $T \rightarrow T' = T - a$. The fermion fields are taken to be $2T'$ -anti-periodic and the orbifold reflection is defined by

$$\mathcal{T}_- : \chi(x) \rightarrow i\gamma_0\gamma_5\chi(a - x_0, \mathbf{x}), \quad \bar{\chi}(x) \rightarrow \bar{\chi}(a - x_0, \mathbf{x})i\gamma_0\gamma_5. \quad (4.27)$$

In this case, however, it is not possible to treat the SF gauge field consistently as an external field, as this would e.g. require to set

$$U_k(a, \mathbf{x}) = U_k(0, \mathbf{x}), \quad (4.28)$$

i.e. the gauge field near the boundary would be equal to the gauge field at the boundary. However, this is not really important as the orbifold construction is not end in itself. It merely serves to teach us the structure of the Wilson-Dirac operator near the boundaries for the non-interacting theory. Hence the introduction of gauge fields can be postponed until the end, and whether or not the interacting theory

satisfies the boundary conditions will depend on the symmetries and the allowed counterterms.

Proceeding in this way we obtain the action,

$$S_f = a^4 \sum_{x_0=a}^{T-a} \sum_{\mathbf{x}} \bar{\psi}(x) (\mathcal{D}_W + m_0) \psi(x), \quad (4.29)$$

where the Wilson-Dirac operator is specified by

$$a\mathcal{D}_W\psi(x) = \begin{cases} -U_0(x)P_-\psi(x+a\hat{0}) + (K + i\gamma_5\tau^3P_-)\psi(x) & \text{if } x_0 = a, \\ a\mathcal{D}_W\psi(x) & \text{if } a < x_0 < T-a, \\ (K + i\gamma_5\tau^3P_+)\psi(x) - U_0(x-a\hat{0})^\dagger P_+\psi(x-a\hat{0}) & \text{for } x_0 = T-a. \end{cases} \quad (4.30)$$

Note that the dynamical field variables in this case are $\psi(x)$ and $\bar{\psi}(x)$ at times $0 < x_0 < T$, which is analogous to the standard SF for Wilson quarks.

4.4 The free quark propagator

In order to check whether the boundary conditions are indeed satisfied in the free theory one may compute the free quark propagator in a time-momentum representation, and compare to its expected continuum limit. There are various ways to proceed and some explicit results can be found in Appendix B. In fact the orbifold construction itself allows to calculate the propagator, taking the propagator on a hypertorus as starting point. The 3 different orbifold procedures can be combined by introducing the parameter $\tau = \pm 1, 0$: we set $T' = T + \tau a$ and identify the site reflection $\mathcal{T}$ with $\mathcal{T}_0$. Performing the inverse Fourier transform in time of the propagator in four-momentum space, one obtains

$$S_{\mathbf{p}}^{2T'}(x_0 - y_0) = \frac{1}{2T'} \sum_{p_0} e^{ip_0(x_0 - y_0)} \tilde{D}_W^{-1}(p), \quad (4.31)$$

where

$$\tilde{D}_W(p) = i\tilde{\not{p}} + m_0 + \frac{1}{2}a\hat{p}^2, \quad (4.32)$$

denotes the symbol of the Wilson-Dirac operator with the inverse

$$\tilde{D}_W^{-1}(p) = \frac{-i\tilde{\not{p}} + (m_0 + \frac{1}{2}a\hat{p}^2)}{\tilde{p}^2 + (m_0 + \frac{1}{2}a\hat{p}^2)^2}. \quad (4.33)$$

Here, lattice momenta have been denoted by

$$\tilde{p}_\mu = \frac{1}{a} \sin ap_\mu, \quad \hat{p}_\mu = \frac{2}{a} \sin \frac{ap_\mu}{2}. \quad (4.34)$$

Note that there are $2T'/a$ allowed values for p_0 , parameterised by an integer k ,

$$p_0(k) = \frac{(2k+1)\pi}{2T'}, \quad k = -T'/a, -T'/a + 1, \dots, T'/a, \quad (4.35)$$

so that the sum over p_0 can be interpreted as a sum over k ,

$$\sum_{p_0} \equiv \sum_{p_0(k)} \equiv \sum_{k=-T'/a}^{T'/a-1}. \quad (4.36)$$

All one needs to do to obtain the propagator in the orbifolded setting is to project on the appropriate $\mathcal{T}_\tau$ -even and -odd field components, and take the field normalisation, Eq. (4.14), into account. Combining the orbifold projection for both flavours by setting

$$\tilde{\mathcal{T}}_\tau = \text{diag}(\mathcal{T}_\tau, -\mathcal{T}_\tau), \quad (4.37)$$

one obtains

$$S_{\mathbf{p}}^\tau(x_0, y_0) = \frac{1}{2}(1 - \tilde{\mathcal{T}}_\tau) S_{\mathbf{p}}^{2T'}(x_0 - y_0)(1 - \tilde{\mathcal{T}}_\tau) \quad (4.38)$$

$$= S_{\mathbf{p}}^{2T'}(x_0 - y_0) - S_{\mathbf{p}}^{2T'}(x_0 + y_0 + \tau a) i\gamma_0 \gamma_5 \tau^3. \quad (4.39)$$

where the orbifold projection from the left (right) acts on $S_{\mathbf{p}}^{2T'}(x_0 - y_0)$ taken as a function of x_0 (y_0). Note that in going from Eq. (4.38) to Eq. (4.39) the behaviour under time reversal has been used,

$$S_{\mathbf{p}}^{2T'}(t) = i\gamma_0 \gamma_5 S_{\mathbf{p}}^{2T'}(-t) i\gamma_0 \gamma_5. \quad (4.40)$$

It is now straightforward to check that the defining equations of the fermion propagator are satisfied, i.e.

$$\mathcal{D}_W^\tau a^3 \sum_{\mathbf{x}} e^{i\mathbf{p}(\mathbf{x}-\mathbf{y})} S_{\mathbf{p}}^\tau(x_0, y_0) = a^{-4} \delta_{x,y}, \quad (4.41)$$

provided the arguments are restricted to $0 \leq x_0, y_0 \leq T$ for $\tau = 0, +1$ and to $0 < x_0, y_0 < T$ for $\tau = -1$. Furthermore, the homogeneous boundary conditions are indeed satisfied, for instance,

$$\tilde{Q}_+ S_{\mathbf{p}}^\tau(0, y_0) = \tilde{Q}_+ \left[S_{\mathbf{p}}^{2T'}(-y_0) - S_{\mathbf{p}}^{2T'}(-y_0 - \tau a) \right], \quad (4.42)$$

vanishes for $\tau = 0$ and is of $\mathcal{O}(a)$ for $\tau = \pm 1$. Note that, formally, the boundary conditions are satisfied at $x_0 = -\tau a/2$, which may be used as a check, even though there is no lattice point at $x_0 = \pm a/2$.

A more explicit expression for the quark propagator can be obtained using the procedure of [40]. The resulting expressions are given in Appendix B and coincide

numerically with the above orbifolded expression⁴, provided one restricts the time arguments to $0 \leq x_0, y_0 \leq T'$ for $\tau = 0, +1$ and to $0 < x_0, y_0 \leq T'$ for $\tau = -1$.

Finally, the orbifold procedure makes it clear that the free spectrum of $\gamma_5 \tau^1 \mathcal{D}_W^\tau$ is the same as obtained on a torus with $2T'$ -anti-periodic boundary conditions. More precisely, the eigenvalues are of the form

$$\lambda = \pm \sqrt{\tilde{p}^2 + (m_0 + \frac{1}{2}a\hat{p}^2)^2}. \quad (4.43)$$

In particular, the smallest (in modulus) eigenvalue is obtained for $\mathbf{p} = \mathbf{0}$ and is (for $m_0 = 0$ and $\theta = 0$) given by

$$|\lambda_{\min}| = \frac{2}{a} \left| \sin \left(\frac{a\pi}{4T'} \right) \right| \stackrel{a \rightarrow 0}{\sim} \frac{\pi}{2T'}, \quad (4.44)$$

which converges to the known continuum result [2].

4.5 Orbifold construction, summary

The orbifold construction yields the structure of the Wilson-Dirac operator near the time boundaries, such that the chirally rotated boundary conditions are realised in the free theory, possibly up to $O(a)$ effects. Using the link reflections $\mathcal{T}_\pm$, the action of the Wilson-Dirac operator on the interval can be specified by a syntactic extension of the function space it acts upon. This is not the case for the site reflection $\mathcal{T}$, where in addition one needs to refer to the boundary condition for the anti-quark fields.

In all three cases the relation,

$$(\gamma_5 \tau^1 \mathcal{D}_W)^\dagger = \gamma_5 \tau^1 \mathcal{D}_W, \quad (4.45)$$

implies that the determinant of the Wilson Dirac operator is real. Moreover, a well defined eigenvalue problem is obtained for $\gamma_5 \tau^1 \mathcal{D}_W$. In the free theory, the eigenvalues are determined by the possible values of the time momentum component for anti-periodic boundary conditions on the doubled time interval. In particular, the lowest eigenvalue is determined by $\pi/(2T')$, where $T' = T + \tau a$ and $\tau = \pm 1, 0$ for the three versions of the orbifold discussed above.

Concerning mass terms, we have seen that the standard mass term can be added without any problem. Adding a twisted mass term $i\mu_q \gamma_5 \tau^3$ is, on the other hand, only possible by including a time profile following ref. [21]. Introducing the mass term in another flavour direction, e.g. $i\mu_q \gamma_5 \tau^2$ is however possible without such a time profile, and corresponds to a twisted mass term in the standard SF basis, too.

⁴For $\tau = 0$, this is correct except for $x_0 = y_0 = 0, T$. However, this contact term in the propagator is never referred to provided the boundary quark and anti-quark fields are defined at $x_0 = a, T - a$ (cf. Sect. 5).

In order to incorporate such a mass term in the orbifold construction it is best to start directly with flavour doublet fields and define the orbifold reflection directly for this case. The twisted mass term is then seen to commute with the spin-flavour matrix $i\gamma_0\gamma_5\tau^3$ in the orbifold reflection $\tilde{T}_\tau$, and therefore with $\tilde{T}_\tau$ itself.

5 Symmetries, renormalisation and $O(a)$ improvement

Given the fermionic lattice action with the correct boundary conditions at tree level, the next step consists in identifying the exact lattice symmetries and the allowed boundary counterterms. One then needs to choose a counterterm basis and discuss their lattice implementation and their effect on the basic fermionic 2-point functions.

5.1 Counterterms of dimension 3 and 4

The Ward identities, Eqs. (3.31,3.32) suggest that the symmetry breaking induced by the chirally rotated SF boundary conditions is quite similar to the breaking by a twisted mass term, except that the breaking terms are localised at the boundaries and come with dimensionless coefficients. Therefore it should not be too surprising that the symmetries of the lattice action in the chirally rotated Schrödinger functional are the same as in twisted mass lattice QCD [39], except for those space-time symmetries which mix time and spatial directions. In particular, there is charge conjugation, spatial lattice rotations, space and time reflections combined with a flavour exchange and global U(1) vector like rotations with generator $\tau^3/2$.

Given the symmetries, a list of fermionic operators of dimension 3 and 4 can be worked out. Their integrals over space, taken at $x_0 = 0$ and $x_0 = T$ define the possible counterterms to the lattice action that are needed to renormalise and $O(a)$ improve the boundary effects in the Schrödinger functional. We do not need to discuss the bulk counterterms here, as these are the same as in infinite volume [31].

Symmetrising with respect to charge conjugation we find the following operators allowed by the symmetries: there are 3 operators of mass dimension 3,

$$\mathcal{O}_1 = \bar{\psi}\gamma_0\tilde{Q}_+\psi - \bar{\psi}\gamma_0\tilde{Q}_-\psi = \bar{\psi}i\gamma_5\tau^3\psi, \quad (5.1)$$

$$\mathcal{O}_2 = \bar{\psi}\tilde{Q}_+\psi, \quad (5.2)$$

$$\mathcal{O}_3 = \bar{\psi}\tilde{Q}_-\psi, \quad (5.3)$$

and further 8 operators of mass dimension 4:

$$\mathcal{O}_4 = \bar{\psi} \tilde{Q}_+ \gamma_k D_k \psi - \bar{\psi} \overleftarrow{D}_k \gamma_k \tilde{Q}_+ \psi, \quad (5.4)$$

$$\mathcal{O}_5 = \bar{\psi} \tilde{Q}_- \gamma_k D_k \psi - \bar{\psi} \overleftarrow{D}_k \gamma_k \tilde{Q}_- \psi, \quad (5.5)$$

$$\mathcal{O}_6 = \bar{\psi} \tilde{Q}_+ \gamma_0 D_0 \psi - \bar{\psi} \overleftarrow{D}_0 \gamma_0 \tilde{Q}_+ \psi, \quad (5.6)$$

$$\mathcal{O}_7 = \bar{\psi} \tilde{Q}_- \gamma_0 D_0 \psi - \bar{\psi} \overleftarrow{D}_0 \gamma_0 \tilde{Q}_- \psi, \quad (5.7)$$

$$\mathcal{O}_8 = \bar{\psi} \tilde{Q}_+ D_0 \psi + \bar{\psi} \overleftarrow{D}_0 \tilde{Q}_+ \psi, \quad (5.8)$$

$$\mathcal{O}_9 = \bar{\psi} \tilde{Q}_- D_0 \psi + \bar{\psi} \overleftarrow{D}_0 \tilde{Q}_- \psi, \quad (5.9)$$

$$\mathcal{O}_{10} = \bar{\psi} \tilde{Q}_+ \gamma_0 \gamma_k D_k \psi + \bar{\psi} \overleftarrow{D}_k \gamma_k \gamma_0 \tilde{Q}_+ \psi, \quad (5.10)$$

$$\mathcal{O}_{11} = \bar{\psi} \tilde{Q}_- \gamma_0 \gamma_k D_k \psi + \bar{\psi} \overleftarrow{D}_k \gamma_k \gamma_0 \tilde{Q}_- \psi. \quad (5.11)$$

The dimension 4 operators are related by the equations of motion

$$\not{D}\psi = 0, \quad \bar{\psi} \overleftarrow{\not{D}} = 0, \quad (5.12)$$

which imply four relations

$$\mathcal{O}_4 + \mathcal{O}_6 = 0, \quad (5.13)$$

$$\mathcal{O}_5 + \mathcal{O}_7 = 0, \quad (5.14)$$

$$\mathcal{O}_8 + \mathcal{O}_{10} = 0, \quad (5.15)$$

$$\mathcal{O}_9 + \mathcal{O}_{11} = 0. \quad (5.16)$$

Furthermore, the combination,

$$\mathcal{O}_{10} - \mathcal{O}_{11} = \partial_k (\bar{\psi} \gamma_k i \gamma_5 \tau^3 \psi), \quad (5.17)$$

yields a total spatial derivative and therefore does not contribute to the action. In summary, we have 5 relations among the 8 counterterms of mass dimension 4. No such simplification is possible for the dimension 3 operators. Hence one needs to consider 3 $\mathcal{O}(1)$ and 3 $\mathcal{O}(a)$ counterterms, which must be added to the SF lattice action with appropriately chosen coefficients.

5.2 Formal continuum theory with inhomogeneous boundary conditions

In order to understand how the boundary counterterms affect SF correlation functions one would ideally start from the lattice theory with *inhomogeneous* boundary conditions, following the steps taken for the standard SF [40]. Given the counterterms to the action, the renormalised and $\mathcal{O}(a)$ improved 2-point functions are obtained by differentiating with respect to the fermionic boundary values and bulk source fields, which are subsequently set to zero. Arbitrary SF correlation functions

can be built from these basic 2-point functions, and their renormalization and $O(a)$ improvement properties then follow, too. The main problem one faces is that the formulation of the lattice theory with inhomogeneous boundary conditions is not directly available. Indeed, our construction of the lattice theory based on the orbifold procedure yields homogeneous boundary conditions. While this is all that will be needed eventually, some alternative method is required to understand the rôle of the boundary counterterms. The approach taken here is based on the fact that the allowed counterterms of dimension 3 and 4 completely fix the structure of the unknown lattice theory to $O(a)$. This turns out to be sufficient to extract the desired information which may then be used to parametrize the renormalized lattice theory.

As a first step let us go through the formal continuum theory with inhomogeneous boundary conditions, specified by

$$\begin{aligned}\tilde{Q}_+\psi(x)|_{x_0=0} &= \rho(\mathbf{x}), & \tilde{Q}_-\psi(x)|_{x_0=T} &= \rho'(\mathbf{x}), \\ \bar{\psi}(x)\tilde{Q}_+|_{x_0=0} &= \bar{\rho}(\mathbf{x}), & \bar{\psi}(x)\tilde{Q}_-|_{x_0=T} &= \bar{\rho}'(\mathbf{x}).\end{aligned}\quad (5.18)$$

As in the case of the standard SF [2], the action is not just given by the bulk action but also requires local boundary terms. We thus make the ansatz

$$\begin{aligned}S_f^{\text{cont}}[\psi, \bar{\psi}, A] &= \int d^4x \bar{\psi}(x) \frac{1}{2} \overleftrightarrow{D} \psi(x) + \int d^3\mathbf{x} [\bar{\psi}(x) R_0(\mathbf{x}) \psi(x)]_{x_0=0} \\ &\quad + \int d^3\mathbf{x} [\bar{\psi}(x) R_T(\mathbf{x}) \psi(x)]_{x_0=T},\end{aligned}\quad (5.19)$$

with $R_0(\mathbf{x})$ and $R_T(\mathbf{x})$ to be determined. Here, A_μ denotes the external gauge field, and the symmetrisation of the derivative implies that bulk and boundary parts of the action density must be separately invariant under charge conjugation. In order to determine the boundary terms we now follow the steps in ref. [2], and demand that the action must have smooth stationary points, i.e. classical solutions ψ_{cl} and $\bar{\psi}_{\text{cl}}$ which satisfy both the boundary conditions, Eqs. (5.18), and the equations of motion,

$$D\psi_{\text{cl}} = 0, \quad \bar{\psi}_{\text{cl}} \overleftarrow{D} = 0. \quad (5.20)$$

This is ensured if R_0 and R_T are of the form

$$R_0(\mathbf{x}) = -\frac{i}{2} \gamma_5 \tau^3 + \tilde{Q}_+ \Gamma_0(\mathbf{x}) \tilde{Q}_+, \quad R_T(\mathbf{x}) = -\frac{i}{2} \gamma_5 \tau^3 + \tilde{Q}_- \Gamma_T(\mathbf{x}) \tilde{Q}_-, \quad (5.21)$$

with arbitrary Γ_0 and Γ_T , subject only to symmetry requirements. Imposing the continuum symmetries of the standard SF, in particular parity and flavour symmetries, one finds that these terms must vanish, so that,

$$R_0(\mathbf{x}) = R_T(\mathbf{x}) = -\frac{i}{2} \gamma_5 \tau^3. \quad (5.22)$$

Not surprisingly, the resulting action coincides with the chirally rotated continuum action of the standard SF [2]. Using this action, we now consider the functional integral over the fermion fields,

$$\mathcal{Z}_F[\rho, \bar{\rho}; \rho', \bar{\rho}'; \eta, \bar{\eta}] = \int D[\psi, \bar{\psi}] \exp \left\{ -S_f^{\text{cont}}[\psi, \bar{\psi}, A] + (\bar{\eta}, \psi) + (\bar{\psi}, \eta) \right\}, \quad (5.23)$$

which implicitly depends on the fermionic boundary values in Eq. (5.18). We have also included source fields η and $\bar{\eta}$ in the bulk using the notation

$$(\bar{\eta}, \psi) = \int d^4x \bar{\eta}(x) \psi(x). \quad (5.24)$$

The functional integration is best carried out after shifting variables,

$$\psi = \psi_{\text{cl}} + v, \quad \bar{\psi} = \bar{\psi}_{\text{cl}} + \bar{v}, \quad (5.25)$$

where the fluctuation fields v and $\bar{v}$ satisfy homogeneous boundary conditions, and the classical solutions of the field equations are explicitly given by

$$\psi_{\text{cl}}(x) = \int d^3\mathbf{y} \left[S(x; 0, \mathbf{y}) \gamma_0 \tilde{Q}_+ \rho(\mathbf{y}) - S(x; T, \mathbf{y}) \gamma_0 \tilde{Q}_- \rho'(\mathbf{y}) \right], \quad (5.26)$$

$$\bar{\psi}_{\text{cl}}(x) = \int d^3\mathbf{y} \left[\bar{\rho}'(\mathbf{y}) \gamma_0 \tilde{Q}_+ S(T, \mathbf{y}; x) - \bar{\rho}(\mathbf{y}) \gamma_0 \tilde{Q}_- S(0, \mathbf{y}; x) \right]. \quad (5.27)$$

Here, $S(x, y)$ denotes the continuum quark propagator in the external gauge field A_μ . Integration over the v and $\bar{v}$ yields

$$\ln \mathcal{Z}_F = \ln \mathcal{Z}_{F,0} - S_f^{\text{cont}}[\psi_{\text{cl}}, \bar{\psi}_{\text{cl}}, A] + (\bar{\eta}, S\eta) + (\bar{\eta}, \psi_{\text{cl}}) + (\bar{\psi}_{\text{cl}}, \eta), \quad (5.28)$$

with

$$\mathcal{Z}_{F,0} = \mathcal{Z}_F[0, 0; 0, 0; 0, 0], \quad (S\eta)(x) = \int d^4y S(x, y) \eta(y). \quad (5.29)$$

The dependence upon the source fields becomes completely explicit when inserting the classical solutions (5.26) and (5.27) into equation (5.28). In particular the continuum action of the classical fields takes the form

$$\begin{aligned} S_f^{\text{cont}}[\psi_{\text{cl}}, \bar{\psi}_{\text{cl}}, A] = & \int d^3\mathbf{x} d^3\mathbf{y} \left[\bar{\rho}(\mathbf{x}) \gamma_0 \tilde{Q}_- S(0, \mathbf{x}; 0, \mathbf{y}) \tilde{Q}_- \gamma_0 \rho(\mathbf{y}) \right. \\ & - \bar{\rho}(\mathbf{x}) \gamma_0 \tilde{Q}_- S(0, \mathbf{x}; T, \mathbf{y}) \tilde{Q}_+ \gamma_0 \rho'(\mathbf{y}) \\ & - \bar{\rho}'(\mathbf{x}) \gamma_0 \tilde{Q}_+ S(T, \mathbf{x}; 0, \mathbf{y}) \tilde{Q}_- \gamma_0 \rho(\mathbf{y}) \\ & \left. + \bar{\rho}'(\mathbf{x}) \gamma_0 \tilde{Q}_+ S(T, \mathbf{x}; T, \mathbf{y}) \tilde{Q}_+ \gamma_0 \rho'(\mathbf{y}) \right]. \quad (5.30) \end{aligned}$$

It is convenient to follow ref. [40] and define fermionic expectation values through⁵

$$[O]_F = \left\{ \frac{1}{\mathcal{Z}_F} O \mathcal{Z}_F \right\}_{\bar{\rho}=\dots=\eta=0}. \quad (5.31)$$

Here the observables O may contain derivatives with respect to the source fields. Since the effective action is bilinear in the source fields, the fermionic expectation value of any observable can be given in terms of the basic fermionic 2-point functions, defined as all possible second derivatives of $\ln \mathcal{Z}_F$ with respect to the source fields. In order to be compatible with Eqs. (3.19), for $\alpha = \pi/2$, one identifies

$$\begin{aligned} \zeta(\mathbf{x}) &\leftrightarrow -\frac{\delta}{\delta[\bar{\rho}(\mathbf{x})\gamma_0]}, & \bar{\zeta}(\mathbf{x}) &\leftrightarrow -\frac{\delta}{\delta[\gamma_0\rho(\mathbf{x})]}, \\ \zeta'(\mathbf{x}) &\leftrightarrow \frac{\delta}{\delta[\bar{\rho}'(\mathbf{x})\gamma_0]}, & \bar{\zeta}'(\mathbf{x}) &\leftrightarrow \frac{\delta}{\delta[\gamma_0\rho'(\mathbf{x})]}. \end{aligned} \quad (5.32)$$

Using this notation, and, similarly,

$$\psi(x) \leftrightarrow \frac{\delta}{\delta\bar{\eta}(x)}, \quad \bar{\psi}(x) \leftrightarrow -\frac{\delta}{\delta\eta(x)}, \quad (5.33)$$

all the basic fermionic 2-point functions are given by

$$[\psi(x)\bar{\psi}(y)]_F = S(x, y), \quad (5.34)$$

$$[\psi(x)\bar{\zeta}(\mathbf{y})]_F = S(x; 0, \mathbf{y})\tilde{Q}_-, \quad (5.35)$$

$$[\psi(x)\bar{\zeta}'(\mathbf{y})]_F = S(x; T, \mathbf{y})\tilde{Q}_+, \quad (5.36)$$

$$[\zeta(\mathbf{x})\bar{\psi}(y)]_F = \tilde{Q}_- S(0, \mathbf{x}; y), \quad (5.37)$$

$$[\zeta'(\mathbf{x})\bar{\psi}(y)]_F = \tilde{Q}_+ S(T, \mathbf{x}; y), \quad (5.38)$$

$$[\zeta(\mathbf{x})\bar{\zeta}(\mathbf{y})]_F = \tilde{Q}_- S(0, \mathbf{x}; 0, \mathbf{y})\tilde{Q}_-, \quad (5.39)$$

$$[\zeta(\mathbf{x})\bar{\zeta}'(\mathbf{y})]_F = \tilde{Q}_- S(0, \mathbf{x}; T, \mathbf{y})\tilde{Q}_+, \quad (5.40)$$

$$[\zeta'(\mathbf{x})\bar{\zeta}(\mathbf{y})]_F = \tilde{Q}_+ S(T, \mathbf{x}; 0, \mathbf{y})\tilde{Q}_-, \quad (5.41)$$

$$[\zeta'(\mathbf{x})\bar{\zeta}'(\mathbf{y})]_F = \tilde{Q}_+ S(T, \mathbf{x}; T, \mathbf{y})\tilde{Q}_+. \quad (5.42)$$

Thus, in the formal continuum theory, the insertion into Eqs. (5.35–5.42) of the non-Dirichlet field components at the time boundaries (3.19), is indeed equivalent to their inclusion as functional derivatives, Eqs. (5.32, 5.33).

⁵The definition is such that the usual Euclidean expectation value is obtained by a subsequent integration over the gauge field, i.e. $\langle O \rangle = \langle [O]_F \rangle_G$, where the effective gauge field measure in $\langle \cdot \rangle_G$ includes both the pure gauge action and the fermionic determinant.

5.3 Including the counterterm action

The correctly renormalised and $O(a)$ improved lattice theory is expected to converge to the formal continuum theory up to terms of $O(a^2)$. By adding the counterterms with some as yet undetermined coefficients one essentially defines Symanzik's effective action for a generic lattice theory the formulation of which is not directly available. Obviously, the inclusion of dimension 3 boundary counterterms with arbitrary coefficients may alter the very continuum theory including the boundary conditions. This point will be addressed in Sect. 6, but we will ignore it here, as we are only looking for a structural result: by keeping arbitrary coefficients we may monitor their effect on the Dirac operator and the basic fermionic 2-point functions. This will then enable us to parameterize the counterterms in the lattice formulation.

For definiteness, we use the equations of motion to obtain a counterterm basis for the massless theory, where all operators with temporal derivatives are eliminated. The resulting set of operators,

$$\mathcal{O}_{1-5}, \mathcal{O}_{10}, \quad (5.43)$$

will be used at both time boundaries. The boundary counterterm action is given by

$$S_{f,b}^{\text{c.t.}} = \sum_{i=1}^3 c_i S_{f,b}^{(i)} + \sum_{i=4}^5 c_i a S_{f,b}^{(i)} + c_{10} a S_{f,b}^{(10)}, \quad (5.44)$$

where the individual terms are specified by

$$S_{f,b}^{(1)} = \int d^3 \mathbf{x} (\mathcal{O}_1|_{x_0=0} + \mathcal{O}_1|_{x_0=T}), \quad (5.45)$$

$$S_{f,b}^{(2)} = \int d^3 \mathbf{x} (\mathcal{O}_2|_{x_0=0} + \mathcal{O}_3|_{x_0=T}), \quad (5.46)$$

$$S_{f,b}^{(3)} = \int d^3 \mathbf{x} (\mathcal{O}_3|_{x_0=0} + \mathcal{O}_2|_{x_0=T}), \quad (5.47)$$

$$S_{f,b}^{(4)} = \int d^3 \mathbf{x} (\mathcal{O}_4|_{x_0=0} + \mathcal{O}_5|_{x_0=T}), \quad (5.48)$$

$$S_{f,b}^{(5)} = \int d^3 \mathbf{x} (\mathcal{O}_5|_{x_0=0} + \mathcal{O}_4|_{x_0=T}), \quad (5.49)$$

$$S_{f,b}^{(10)} = \int d^3 \mathbf{x} (\mathcal{O}_{10}|_{x_0=0} - \mathcal{O}_{10}|_{x_0=T}), \quad (5.50)$$

taking into account the behaviour under time reflections. Including the counterterm action, the total fermionic action becomes

$$S_f^{\text{total}} = S_f^{\text{cont}} + S_{f,b}^{\text{c.t.}} + a S_1. \quad (5.51)$$

The last term contains the volume $O(a)$ counterterms [cf. Eq. 2.5)]. Note that the elimination of counterterms containing time derivatives implies that $O(a)$ effects

such as in Eqs. (4.23) are absent. Hence, disregarding $O(a^2)$ effects, the boundary conditions can still be imposed at $x_0 = 0$ and $x_0 = T$. In a first attempt we will thus try to maintain the boundary conditions (5.18) to $O(a)$. The first question to answer is whether there are still smooth classical solutions with the $O(a)$ enhanced action. Varying the action one immediately notices that there are three categories of counterterms. First, there are those which only refer to field components at the boundaries which are subject to the Dirichlet conditions, such as $\tilde{Q}_+\psi$ and $\bar{\psi}\tilde{Q}_+$ at $x_0 = 0$. This is the case for the counterterms $\propto c_2, c_4$. Then there are those which mix Dirichlet and non-Dirichlet components ($\propto c_1, c_{10}$) and finally the ones only referring to non-Dirichlet components ($\propto c_3, c_5$). Since the non-Dirichlet components are integration variables in the functional integral, the last category of counterterms can be absorbed in a re-definition of the Dirac operator. The same holds true for the bulk $O(a)$ improvement terms in S_1 . This leads to a redefined Dirac operator which we shall denote by $\mathcal{D}^{(r)}$. Defining classical solutions,

$$\mathcal{D}^{(r)}\psi_{\text{cl}} = 0, \quad \bar{\psi}_{\text{cl}}\overleftarrow{\mathcal{D}}^{(r)} = 0, \quad (5.52)$$

subject to the boundary conditions (5.18), the question is whether the presence of the counterterms $\propto c_1, c_2, c_4$ and c_{10} , allows for the classical solutions to be smooth. We need to check what kind of structures R_0 and R_T correspond to the counterterms $\propto c_1, c_2, c_4$ and c_{10} , and whether these take the form given in Eq. (5.21). This is indeed the case for the counterterms $\propto c_2, c_4$, which induce non-vanishing Γ_0 and Γ_T terms. However, the counterterms $\propto c_1, c_{10}$ cannot be cast in this form. Some thought reveals that one may take the counterterms $\propto c_1, c_{10}$ into consideration by a modification of the boundary conditions rather than by including them in the action. We set

$$\begin{aligned} \tilde{Q}_+\psi(x)|_{x_0=0} &= \rho_r(\mathbf{x}), & \tilde{Q}_-\psi(x)|_{x_0=T} &= \rho'_r(\mathbf{x}), \\ \bar{\psi}(x)\tilde{Q}_+|_{x_0=0} &= \bar{\rho}_r(\mathbf{x}), & \bar{\psi}(x)\tilde{Q}_-|_{x_0=T} &= \bar{\rho}'_r(\mathbf{x}), \end{aligned} \quad (5.53)$$

where we have re-defined the boundary values as follows,

$$\rho_r(\mathbf{x}) = \sqrt{1-2c_1} (1 - \bar{c}_{10}a\gamma_k D_k) \rho(\mathbf{x}), \quad (5.54)$$

$$\bar{\rho}_r(\mathbf{x}) = \bar{\rho}(\mathbf{x}) (1 + \bar{c}_{10}a\gamma_k \overleftarrow{D}_k) \sqrt{1-2c_1}, \quad \bar{c}_{10} = c_{10}/(1-2c_1), \quad (5.55)$$

and analogously for the primed fields. When considered as a function of $\rho, \bar{\rho}, \rho'$ and $\bar{\rho}'$ the reduced action

$$S_f^{(r)} = S_f^{\text{cont}} + \sum_{i=2}^3 c_i S_{f,b}^{(i)} + \sum_{i=4}^5 c_i a S_{f,b}^{(i)} + a S_1. \quad (5.56)$$

coincides up to terms of $O(a^2)$ with the total action, Eq. (5.51), taken with the original boundary conditions. We re-define the Dirac operator as before, so that the fermionic action takes the form

$$\begin{aligned} S_f^{(r)}[\psi, \bar{\psi}, A] &= \int d^4x \bar{\psi}(x) \frac{1}{2} \overleftrightarrow{D}^{(r)} \psi(x) - \frac{1}{2} \int d^3\mathbf{x} [\bar{\psi}(x) i\gamma_5 \tau^3 \psi(x)]_{x_0=0} \\ &\quad - \frac{1}{2} \int d^3\mathbf{x} [\bar{\psi}(x) i\gamma_5 \tau^3 \psi(x)]_{x_0=T} \\ &\quad + c_2 S_{f,b}^{(2)}[\psi, \bar{\psi}, A] + c_4 a S_{f,b}^{(4)}[\psi, \bar{\psi}, A]. \end{aligned} \quad (5.57)$$

The classical solutions $\psi_{\text{cl},r}$ and $\bar{\psi}_{\text{cl},r}$ are defined by

$$D^{(r)} \psi_{\text{cl},r} = 0, \quad \bar{\psi}_{\text{cl},r} \overleftrightarrow{D}^{(r)} = 0, \quad (5.58)$$

subject to the modified boundary conditions Eq. (5.53). Explicit expressions are similar to Eqs. (5.26,5.27), where the differences are accounted for by replacing the boundary values $\rho \rightarrow \rho_r$ etc., and the propagator $S(x, y) \rightarrow S_r(x, y)$, defined as the Green's function for $D^{(r)}$. Separating classical and fluctuation fields the fermionic action splits in two parts,

$$S_f^{(r)}[\psi_{\text{cl},r} + v, \bar{\psi}_{\text{cl},r} + \bar{v}, A] = S_f^{(r)}[v, \bar{v}, A] + S_f^{(r)}[\psi_{\text{cl},r}, \bar{\psi}_{\text{cl},r}, A]. \quad (5.59)$$

The second term on the r.h.s. contains the whole dependence on the boundary source fields, and can be written in the form,

$$\begin{aligned} S_f^{(r)}[\psi_{\text{cl},r}, \bar{\psi}_{\text{cl},r}, A] &= c_2 \int d^3\mathbf{x} [\bar{\rho}_r(\mathbf{x}) \tilde{Q}_+ \rho_r(\mathbf{x}) + \bar{\rho}'_r(\mathbf{x}) \tilde{Q}_- \rho'_r(\mathbf{x})] \\ &\quad + 2c_4 a \int d^3\mathbf{x} [\bar{\rho}_r(\mathbf{x}) \tilde{Q}_+ D_k \rho_r(\mathbf{x}) + \bar{\rho}'_r(\mathbf{x}) \tilde{Q}_- \gamma_k D_k \rho'_r(\mathbf{x})] \\ &\quad + \int d^3\mathbf{x} d^3\mathbf{y} [\bar{\rho}_r(\mathbf{x}) \gamma_0 \tilde{Q}_- S_r(0, \mathbf{x}; 0, \mathbf{y}) \tilde{Q}_- \gamma_0 \rho_r(\mathbf{y}) \\ &\quad - \bar{\rho}_r(\mathbf{x}) \gamma_0 \tilde{Q}_- S_r(0, \mathbf{x}; T, \mathbf{y}) \tilde{Q}_+ \gamma_0 \rho'_r(\mathbf{y}) \\ &\quad - \bar{\rho}'_r(\mathbf{x}) \gamma_0 \tilde{Q}_+ S_r(T, \mathbf{x}; 0, \mathbf{y}) \tilde{Q}_- \gamma_0 \rho_r(\mathbf{y}) \\ &\quad + \bar{\rho}'_r(\mathbf{x}) \gamma_0 \tilde{Q}_+ S_r(T, \mathbf{x}; T, \mathbf{y}) \tilde{Q}_+ \gamma_0 \rho'_r(\mathbf{y})]. \end{aligned} \quad (5.60)$$

Introducing again the bulk source fields, we arrive at the expression of the fermionic generating functional,

$$\begin{aligned} \ln \mathcal{Z}_F^{(r)} &= \ln \mathcal{Z}_{F,0}^{(r)} - S_f^{(r)}[\psi_{\text{cl},r}, \bar{\psi}_{\text{cl},r}, A] + (\bar{\eta}, S_r \eta) \\ &\quad + (\bar{\eta}, \psi_{\text{cl},r}) + (\bar{\psi}_{\text{cl},r}, \eta), \end{aligned} \quad (5.61)$$

where the dependence on the source fields is completely explicit. Before taking derivatives with respect to the source fields one may partially integrate the terms

proportional to $\bar{c}_{10}$ so that all the spatial derivatives act on the fermion propagator. It is then straightforward to compute all fermionic 2-point functions, e.g.

$$[\zeta(\mathbf{x})\bar{\psi}(y)]_F = \sqrt{1-2c_1}(1-\bar{c}_{10}a\gamma_k D_k)\tilde{Q}_-S_r(0,\mathbf{x};y), \quad (5.62)$$

$$[\psi(x)\bar{\zeta}(\mathbf{y})]_F = \sqrt{1-2c_1}S_r(x;0,\mathbf{y})\tilde{Q}_-(1+\bar{c}_{10}a\gamma_k \overleftarrow{D}_k). \quad (5.63)$$

By comparing with Eqs. (5.34–5.42), we thus obtain a clear picture of how the counterterms affect the basic 2-point functions and the Dirac operator. Based on this information one may now parametrize both the $O(a)$ improved Wilson-Dirac operator and the basic 2-point functions on the lattice.

5.4 Lattice parameterisation

We here focus primarily on the version of the χ SF obtained with the orbifold reflection $\mathcal{T}_\tau$ with $\tau = +1$ (cf. Sect. 4). Hence, the fermionic fields at Euclidean times $x_0 = 0$ and $x_0 = T$ are integration variables in the functional integral and the counterterms in the chosen basis can be defined at $x_0 = 0$ and $x_0 = T$. Starting with the Wilson-Dirac operator, the necessary counterterms are included by replacing $\mathcal{D}_W$ of Eq. (4.25) with $\mathcal{D}_W + \delta\mathcal{D}_W$, where we define

$$\delta\mathcal{D}_W\psi(x) = (\delta_{x_0,0} + \delta_{x_0,T}) \left[(z_f - 1) + (d_s - 1)a\mathbf{D}_s \right] \psi(x), \quad (5.64)$$

$$\mathbf{D}_s = \frac{1}{2}(\nabla_k + \nabla_k^*)\gamma_k. \quad (5.65)$$

On the lattice the fields are always subject to (a lattice version of) homogeneous boundary conditions (cf. subsection 4.2), so that ψ and $\bar{\psi}$ correspond to the fluctuation fields $\bar{v}$ and v in the continuum theory. This implies relations such as

$$\bar{\psi}(x)\psi(x)\Big|_{x_0=0} = \bar{\psi}(x)\tilde{Q}_-\psi(x)\Big|_{x_0=0} + O(a) \quad (5.66)$$

which have been used to simplify the parametrization⁶ (5.64). Note that $O(a)$ corrections to such continuum relations either re-define the coefficients of the existing $O(a)$ counterterms or modify $O(a^2)$ terms in the action, which are considered irrelevant in the present context.

There is also considerable freedom in parametrizing the basic 2-point functions. We will here follow the convention used in the standard SF and obtain fermionic boundary fields from the fermion fields at times $x_0 = a$ and $x_0 = T - a$, parallel

⁶When defining $\delta\mathcal{D}_W$ for $\tau = 0$ one needs to keep the projectors $\tilde{Q}_\pm$, in order to project out the Dirichlet component of the fields at $x_0 = 0$ and $x_0 = T$ which are not integrated over in the functional integral (cf. Sect. 4). In the case $\tau = -1$, one may use the same parameterisation as in Eq. (5.64) except that the Kronecker δ 's should be localised at $x_0 = a$ and $x_0 = T - a$.

transported back to the boundaries at $x_0 = 0$ and $x_0 = T$. In view of this, we introduce a shorthand notation for the parallel transported boundary-to-boundary propagators,

$$\bar{S}(0, \mathbf{x}; 0, \mathbf{y}) = U_0(0, \mathbf{x}) S(a, \mathbf{x}; a, \mathbf{y}) U_0(0, \mathbf{y})^\dagger, \quad (5.67)$$

$$\bar{S}(0, \mathbf{x}; T, \mathbf{y}) = U_0(0, \mathbf{x}) S(a, \mathbf{x}; T - a, \mathbf{y}) U_0(T - a, \mathbf{y}) \quad (5.68)$$

$$\bar{S}(T, \mathbf{x}; 0, \mathbf{y}) = U_0(T - a, \mathbf{x})^\dagger S(T - a, \mathbf{x}; a, \mathbf{y}) U_0(0, \mathbf{y})^\dagger, \quad (5.69)$$

$$\bar{S}(T, \mathbf{x}; T, \mathbf{y}) = U_0(T - a, \mathbf{x})^\dagger S(T - a, \mathbf{x}; T - a, \mathbf{y}) U_0(T - a, \mathbf{y}). \quad (5.70)$$

where the quark propagator is defined by

$$(\mathcal{D}_W + \delta\mathcal{D}_W + m_0) S(x, y) = a^{-4} \delta_{x,y}, \quad (5.71)$$

and we set $m_0 = m_{\text{cr}}$. The unrenormalised, $\mathcal{O}(a)$ improved fermionic 2-point functions in the massless lattice theory are then parametrized as follows:

$$[\psi(x) \bar{\psi}(y)]_F = S(x, y), \quad (5.72)$$

$$[\psi(x) \bar{\zeta}(\mathbf{y})]_F = S(x; a, \mathbf{y}) U_0(0, \mathbf{y})^\dagger (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s) \tilde{Q}_-, \quad (5.73)$$

$$[\psi(x) \bar{\zeta}'(\mathbf{y})]_F = S(x; T - a, \mathbf{y}) U_0(T - a, \mathbf{y}) (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s) \tilde{Q}_+, \quad (5.74)$$

$$[\zeta(\mathbf{x}) \bar{\psi}(y)]_F = \tilde{Q}_- (1 + \bar{d}_s a \mathbf{D}_s) U_0(0, \mathbf{x}) S(a, \mathbf{x}; y), \quad (5.75)$$

$$[\zeta'(\mathbf{x}) \bar{\psi}(y)]_F = \tilde{Q}_+ (1 + \bar{d}_s a \mathbf{D}_s) U_0(T - a, \mathbf{x})^\dagger S(T - a, \mathbf{x}; y), \quad (5.76)$$

$$\begin{aligned} [\zeta(\mathbf{x}) \bar{\zeta}(\mathbf{y})]_F &= \tilde{Q}_- (1 + \bar{d}_s a \mathbf{D}_s) \left[\bar{S}(0, \mathbf{x}; 0, \mathbf{y}) \right. \\ &\quad \left. - (\tilde{z}_f + \bar{d}_s a \mathbf{D}_s) \delta(\mathbf{x} - \mathbf{y}) \right] (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s) \tilde{Q}_-, \end{aligned} \quad (5.77)$$

$$[\zeta(\mathbf{x}) \bar{\zeta}'(\mathbf{y})]_F = \tilde{Q}_- (1 + \bar{d}_s a \mathbf{D}_s) \bar{S}(0, \mathbf{x}; T, \mathbf{y}) (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s) \tilde{Q}_+, \quad (5.78)$$

$$[\zeta'(\mathbf{x}) \bar{\zeta}(\mathbf{y})]_F = \tilde{Q}_+ (1 + \bar{d}_s a \mathbf{D}_s) \bar{S}(T, \mathbf{x}; 0, \mathbf{y}) (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s) \tilde{Q}_-, \quad (5.79)$$

$$\begin{aligned} [\zeta'(\mathbf{x}) \bar{\zeta}'(\mathbf{y})]_F &= \tilde{Q}_+ (1 + \bar{d}_s a \mathbf{D}_s) \left[\bar{S}(T, \mathbf{x}; T, \mathbf{y}) \right. \\ &\quad \left. - (\tilde{z}_f + \bar{d}_s a \mathbf{D}_s) \delta(\mathbf{x} - \mathbf{y}) \right] (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s) \tilde{Q}_+, \end{aligned} \quad (5.80)$$

where $\overleftarrow{\mathbf{D}}_s = \frac{1}{2} (\overleftarrow{\nabla}_k + \overleftarrow{\nabla}_k^*) \gamma_k$ is the counterpart to $\mathbf{D}_s$ in Eq. (5.65). This defines the building blocks for any fermionic correlation function and therefore completes the set-up for the massless theory. It also implicitly defines the fermionic boundary fields as integrands in the functional integral. For instance, one has

$$\zeta(\mathbf{x}) = (1 + \bar{d}_s a \mathbf{D}_s) U_0(0, \mathbf{x}) \tilde{Q}_- \psi(a, \mathbf{x}), \quad (5.81)$$

$$\bar{\zeta}(\mathbf{x}) = \bar{\psi}(a, \mathbf{x}) \tilde{Q}_- U_0(x)^\dagger (1 - \bar{d}_s a \overleftarrow{\mathbf{D}}_s), \quad (5.82)$$

except that these equations do not take into account the contact terms proportional to $\tilde{z}_f$ and $\bar{d}_s$, which need to be subtracted whenever the possible Wick contractions

yield the 2-point functions $[\zeta(\mathbf{x})\bar{\zeta}(\mathbf{y})]_F$ or $[\zeta'(\mathbf{x})\bar{\zeta}'(\mathbf{y})]_F$ at coinciding spatial points $\mathbf{x} = \mathbf{y}$.

The 2 renormalisation constants z_f and $\tilde{z}_f$ and the 3 $O(a)$ improvement coefficients d_s , $\tilde{d}_s$ and $\bar{d}_s$ implement lattice variants of the 5 counterterms $\mathcal{O}_i$ with $i = 2, 3, 4, 5, 10$. The only missing counterterm is $\mathcal{O}_1$, which can be taken care of by a multiplicative renormalization of the fermionic boundary fields,

$$\zeta_R = Z_\zeta \zeta, \quad \bar{\zeta}_R = Z_\zeta \bar{\zeta}, \quad \zeta'_R = Z_\zeta \zeta', \quad \bar{\zeta}'_R = Z_\zeta \bar{\zeta}', \quad (5.83)$$

in complete analogy to the standard SF [3,31]. While the $O(a)$ improvement coefficients d_s and $\tilde{d}_s$ have their standard SF counterparts in $\tilde{c}_t$ and $\tilde{c}_s$, the renormalization constants z_f and $\tilde{z}_f$ and the coefficient $\bar{d}_s$ are new and arise as a consequence of breaking the parity and flavour symmetries. However, the situation is not as bad as it seems, since correlation functions involving $\tilde{z}_f$ and $\bar{d}_s$ can be avoided in practice. Moreover, the counterterm proportional to $\bar{d}_s$ is $\gamma_5\tau^1$ -odd and only contributes $O(a^2)$ effects to $\gamma_5\tau^1$ -even correlation functions, thus rendering it irrelevant for most applications. In practice, this leaves us with the tuning of the renormalisation constant z_f as the main new feature as compared to the standard SF.

5.5 Away from the chiral limit

The possible counterterm structures in the presence of mass parameters can be obtained by applying the equations of motion for massive fermions to the counterterm basis obtained for the massless theory. Possible counterterms are then given by those combinations which are invariant under charge conjugation. Considering the mass terms

$$m\bar{\psi}\psi + \mu_q\bar{\psi}i\gamma_5\tau^3\psi, \quad (5.84)$$

one finds that the boundary counterterms of dimension 4 have the form,

$$\{m, \mu_q\} \times \{\mathcal{O}_1, \mathcal{O}_2, \mathcal{O}_3\}, \quad (5.85)$$

and are thus proportional to the existing counterterms of dimension 3. They can be absorbed in a mass dependent rescaling of the corresponding renormalisation constants Z_ζ , z_f and $\tilde{z}_f$. It should be emphasised that a non-zero standard mass term entails the loss of automatic $O(a)$ improvement. In order to maintain $O(a)$ improvement away from the chiral limit one thus needs to introduce all the usual $O(a)$ bulk counterterms, just like in the standard SF. This is to be contrasted with a twisted mass parameter, which preserves the $\gamma_5\tau^1$ -symmetry and is therefore compatible with automatic $O(a)$ improvement.

An interesting alternative mass term is obtained by introducing a twisted mass term in a different flavour direction⁷,

$$\mu'_q \bar{\psi} i \gamma_5 \tau^2 \psi. \quad (5.86)$$

Such a mass term is invariant under the chiral rotation (3.1) relating the standard and the chirally rotated SF, and is thus equivalent to a twisted mass parameter in the standard SF. Interestingly, in this case one needs a single counterterm, which can be chosen to be

$$\mu'_q \left(\bar{\psi} \tilde{Q}_+ i \gamma_0 \gamma_5 \tau^2 \psi - \bar{\psi} \tilde{Q}_- i \gamma_0 \gamma_5 \tau^2 \psi \right). \quad (5.87)$$

Note that this term is $\gamma_5 \tau^1$ -odd, so that it can be ignored, provided that $m = 0$ and attention is restricted to $\gamma_5 \tau^1$ -even observables. Thus, no additional $O(a)$ mass counterterm is needed whilst automatic $O(a)$ improvement is maintained. The obvious drawback consists in the fact that the action ceases to be flavour diagonal.

6 Renormalization and $O(a)$ improvement

The basic 2-point functions in the free theory can be used to determine the renormalization constants z_f and $\tilde{z}_f$ and the $O(a)$ improvement coefficients d_s , $\tilde{d}_s$ and $\bar{d}_s$ at the tree level of perturbation theory. Some insight is provided for the rôle played by the renormalisation constant z_f . Automatic $O(a)$ improvement is then demonstrated with the free quark propagator in an Abelian background field.

6.1 Interpretation of z_f and $\tilde{z}_f$

The renormalization constants z_f and $\tilde{z}_f$ are related to the counterterms $\mathcal{O}_2$ and $\mathcal{O}_3$ which are $\gamma_5 \tau^1$ -odd. When chirally rotated back to the standard SF basis these 2 operators become proportional to $\bar{\psi}' P_{\pm} i \gamma_5 \tau^3 \psi'$, which indicates a breaking of parity and flavour symmetry. Indeed, in terms of the standard SF fields the $\gamma_5 \tau^1$ -transformation becomes a discrete $SU(2)$ flavour transformation,

$$\psi' \rightarrow -\tau^2 \psi' \quad \bar{\psi}' \rightarrow -\bar{\psi}' \tau^2. \quad (6.1)$$

Since parity and flavour symmetries are good continuum symmetries one expects that both renormalization constants are finite, i.e. scale independent functions of the bare coupling, with an expansion of the form

$$z(g_0) = z^{(0)} + g_0^2 z^{(1)} + O(g_0^4). \quad (6.2)$$

⁷The author thanks Jenifer Gonzalez Lopez for reminding him of this option.

It is straightforward to determine their lowest order values, by comparing the basic 2-point functions with a vanishing gauge background field to their expected continuum limit (cf. Appendix B). The free quark propagator on the lattice is obtained analytically for $z_f = 1$. The fact that this yields the expected continuum quark propagator up to cutoff effects immediately implies

$$z_f^{(0)} = 1, \quad (6.3)$$

as the correct tree-level value. Furthermore, the absence of contact terms in the continuum counterparts (5.39) and (5.42) of the boundary-to-boundary 2-point functions (5.77,5.80) implies

$$\tilde{z}_f^{(0)} = \frac{1}{2}. \quad (6.4)$$

Note that these 2 finite renormalization constants restore the very $\gamma_5\tau^1$ -symmetry which enables automatic $O(a)$ improvement. A possible strategy to determine z_f and $\tilde{z}_f$ therefore consists in the requirement that 2 suitable $\gamma_5\tau^1$ -odd observables vanish exactly. Note that this strategy has implicitly been applied to obtain the results in Eqs. (6.3,6.4) since the $\gamma_5\tau^1$ -odd parts of the continuum 2-point functions all vanish identically. It should also be emphasized that z_f affects any observable via the Wilson-Dirac operator, whereas $\tilde{z}_f$ only appears in the additive counterterm to the 2-point functions, Eqs. (5.77,5.80). Hence the determination of $\tilde{z}_f$ can be avoided if the observables of interest do not involve these 2-point functions. This can often be arranged by choosing appropriate quark flavour assignments [44].

Another perspective on z_f is obtained by considering an infinitesimal perturbation δ around the lowest order value, Eq. (6.3). This would e.g. be the situation in perturbation theory with g_0^2 as the infinitesimal parameter. The first order correction is equivalent to a single counterterm insertion in the correlation function of interest. Considering the quark propagator in the time-momentum representation and neglecting $O(a)$ artefacts, one obtains the expansion

$$\begin{aligned} S_{\mathbf{p}}^T(x_0, y_0)|_{z_f=1+\delta} &= S_{\mathbf{p}}^{(\pi/2)}(x_0, y_0) - \delta \left[S_{\mathbf{p}}^{(\pi/2)}(x_0, 0) S_{\mathbf{p}}^{(\pi/2)}(0, y_0) \right. \\ &\quad \left. + S_{\mathbf{p}}^{(\pi/2)}(x_0, T) S_{\mathbf{p}}^{(\pi/2)}(T, y_0) \right] + O(a, \delta^2), \end{aligned} \quad (6.5)$$

where the value of the angle α in the continuum propagator has been indicated by a superscript. Interestingly, the first order correction can be expressed as a derivative of the continuum propagator with respect to the angle α ,

$$S_{\mathbf{p}}^{(\pi/2)}(x_0, 0) S_{\mathbf{p}}^{(\pi/2)}(0, y_0) + S_{\mathbf{p}}^{(\pi/2)}(x_0, T) S_{\mathbf{p}}^{(\pi/2)}(T, y_0) = -2 \frac{\partial}{\partial \alpha} S_{\mathbf{p}}^{(\alpha)}(x_0, y_0) \Big|_{\alpha=\pi/2}. \quad (6.6)$$

This gives rise to a complementary point of view regarding the rôle of z_f : starting from a free theory with boundary conditions involving the projectors $P_{\pm}(\alpha = \pi/2) = \tilde{Q}_{\pm}$, the interactions tend to rotate the angle α away from $\pi/2$. Since there is no lattice symmetry which protects the angle $\alpha = \pi/2$, one needs to tune z_f to maintain the angle at $\pi/2$ all the way to the continuum limit. This interpretation is further corroborated by a numerical experiment: one may tune z_f such that the free lattice propagator $S_{\mathbf{p}}^{\tau}(x_0, y_0)$ approaches the continuum propagator defined at arbitrary values of α , as long as both time arguments are in the range $0 < x_0, y_0 < T$.

In conclusion, the finite renormalization constants z_f and $\tilde{z}_f$ restore the $\gamma_5\tau^1$ -symmetry, which is interpreted as a flavour symmetry in the standard SF basis. With the chosen set-up for the fermionic boundary fields the tuning of z_f is equivalent to a renormalisation of the angle α such that the boundary conditions remain the ones with projectors $\tilde{Q}_{\pm}$. In practice z_f and $\tilde{z}_f$ can be fixed by tuning suitable $\gamma_5\tau^1$ -odd observables to zero. In analogy with the $O(a)$ uncertainty in the definition of the chiral limit (cf. Sect. 2), one expects different determinations of z_f or $\tilde{z}_f$ to differ by terms of $O(a)$. However, as in the case of the mass term, any $O(a)$ differences are expected to cause only $O(a^2)$ effects in $\gamma_5\tau^1$ -even observables.

6.2 $O(a)$ improvement coefficients at tree-level

To obtain $O(a)$ improvement at the tree level one needs to adapt the counterterm coefficients such that the continuum limit of the basic 2-point functions is approached with $O(a^2)$ corrections. All coefficients can be expanded in powers of g_0^2 in analogy to the finite renormalization constants, Eq. (6.2). The first step should be the determination of d_s since this counterterm enters the Wilson-Dirac operator and thus affects the fermion propagator in the bulk. Note that the exact expressions for the fermion propagator in Appendix B have been calculated without the counterterm $\delta\mathcal{D}_W$ (5.64), and therefore correspond to the choice $d_s = 1$. Calculating the $O(a)$ effects in the propagator for this case yields, in terms of the coefficient functions of Eqs. (B.31, B.32),

$$G_{\pm}^{\tau}(\mathbf{p}; x_0, y_0) = G_{\pm}(\mathbf{p}; x_0, y_0) + \frac{\tau a}{2 \cosh^2 \omega T} \left\{ \cosh \omega(x_0 - y_0) \mp \sinh \omega T \sinh \omega(x_0 + y_0 - T) \right\} + O(a^2), \quad (6.7)$$

$$H_{\pm}^{\tau}(\mathbf{p}; x_0, y_0) = H_{\pm}(\mathbf{p}; x_0, y_0) + \frac{\tau a \omega}{2 \cosh^2 \omega T} \left\{ \sinh \omega(x_0 - y_0) \mp \sinh \omega T \cosh \omega(x_0 + y_0 - T) \right\} + O(a^2). \quad (6.8)$$

We thus see that for $\tau = 0$ the $O(a)$ effects vanish so that $d_s^{(0)} = 1$ is the correct choice in this case. However, for $\tau = \pm 1$, there are uncanceled $O(a)$ effects, implying that $d_s^{(0)} = 1$ is incorrect in this case. In order to retain $d_s^{(0)}$ as a free parameter in

the lattice propagator to $O(a)$, one may proceed by calculating a single insertion of this counterterm into the propagator, viz.

$$\begin{aligned} S_{\mathbf{p}}^{\tau}(x_0, y_0) \Big|_{d_s=d_s^{(0)}} &= S_{\mathbf{p}}^{\tau}(x_0, y_0) \Big|_{d_s=1} \\ &\quad - a \left(d_s^{(0)} - 1 \right) \left[S_{\mathbf{p}}^{(\pi/2)}(x_0, 0) i p_k^+ \gamma_k S_{\mathbf{p}}^{(\pi/2)}(0, y_0) \right. \\ &\quad \left. + S_{\mathbf{p}}^{(\pi/2)}(x_0, T) i p_k^+ \gamma_k S_{\mathbf{p}}^{(\pi/2)}(T, y_0) \right] + O(a^2). \end{aligned} \quad (6.9)$$

Hence the $O(a)$ effects in the first term of the r.h.s., explicitly given by Eqs. (6.7,6.8) should be cancelled by the second term, which may be calculated directly in the continuum. After some algebra one finds that in all cases

$$d_s^{(0)} = 1 - \frac{\tau}{2}, \quad (6.10)$$

appears to be the correct choice⁸. This result has been confirmed by numerical inversion of the improved Wilson-Dirac operator in time-momentum space for a range of lattice resolutions, L/a .

Having determined the $O(a)$ improved bulk propagator, it is straightforward to insert it into the basic 2-point functions. Again we limit ourselves to $\tau = 0$ and $\tau = +1$. It turns out that $\tilde{d}_s^{(0)} = 0$ in both cases. Finally, requiring the contact terms in Eqs. (5.77,5.80) to be absent at $O(a)$ yields

$$\tilde{d}_s^{(0)} = 1. \quad (6.11)$$

6.3 A tree-level test of automatic $O(a)$ improvement

In the free theory the simplest non-trivial correlation function is the fermion propagator in a fixed external gauge field. We are thus led to consider “observables” of the type

$$I_{\Gamma_A}^{\pm} = -a^3 \sum_{\mathbf{x}} e^{-i\mathbf{p}(\mathbf{x}-\mathbf{y})} [\bar{\psi}(y) \Gamma_A \tilde{Q}_{\pm} \psi(x)]_F, \quad (6.12)$$

where Γ_A denotes any of the 16 linearly independent Hermitian 4×4 -matrices, $\gamma_{\mu}, 1, \gamma_5, i\gamma_{\mu}\gamma_5, \sigma_{\mu\nu}$ (for $\mu, \nu = 0, 1, 2, 3$ and $\mu < \nu$). Note that such bilocal quark-bilinear fields have a definite $\gamma_5\tau^1$ -parity, which is even (odd) if Γ_A anti-commutes (commutes) with γ_5 . Integrating over the fermions leads to

$$I_{\Gamma_A}^{\pm} = \text{tr} \left\{ \Gamma_A \tilde{Q}_{\pm} S_{\mathbf{p}}^{\tau=1}(x_0, y_0) \right\}, \quad (6.13)$$

where the trace is over flavour, spin and colour indices, as these are contracted in Eq. (6.12). In the continuum limit, a chiral rotation relates these observables to

⁸Note that for this equation to hold with $\tau = -1$ it is assumed that the counterterm $\delta\mathcal{D}_W$ (5.64) has been added to the Wilson-Dirac operator at Euclidean times $x_0 = a, T - a$.

standard SF correlators (cf. Sect. 3). With vanishing mass parameters and in the continuum limit one thus expects

$$I_{\Gamma_A, \text{cont}}^{\pm} = \text{tr} \left\{ \Gamma_A P_{\pm} S_{\mathbf{p}}^{(\alpha=0)}(x_0, y_0) \right\}, \quad \text{if } \{\gamma_5, \Gamma_A\} = 0, \quad (6.14)$$

whereas $\gamma_5 \tau^1$ -odd observables vanish identically, due to flavour and parity symmetry (at a more technical level, in the standard SF basis, such observables are proportional to $\text{tr}(\tau^3) = 0$). It is instructive to consider the same observables in the standard SF at finite lattice spacing, which will be denoted by $I_{\Gamma_A}^{\pm}$.

To take the continuum limit we keep all dimensionful parameters $(x_0, y_0, T, \dots)$, fixed in units of L . Furthermore, we assume that boundary $\mathcal{O}(a)$ improvement is correctly implemented. i.e. that the $\mathcal{O}(a)$ improvement coefficients, d_s or, in the case of the standard SF, $\tilde{c}_t$, are set to their known tree-level values $d_s^{(0)} = 1 - \tau/2$ (6.10) and $\tilde{c}_t^{(0)} = 1$ [31]. For Γ_A 's which anti-commute with γ_5 one then expects

$$I_{\Gamma_A}^{\pm} \Big|_{\{\Gamma_A, \gamma_5\}=0} = I_{\Gamma_A, \text{cont}}^{\pm} + \text{const} \times (c_{\text{sw}} - 1) \frac{a}{L} + \mathcal{O}(a^2), \quad (6.15)$$

$$I_{\Gamma_A}^{\pm} \Big|_{\{\Gamma_A, \gamma_5\}=0} = I_{\Gamma_A, \text{cont}}^{\pm} + \mathcal{O}(a^2). \quad (6.16)$$

While the standard SF observables in Eq. (6.15) require $c_{\text{sw}} = 1$ to be $\mathcal{O}(a)$ improved, χ SF observables in Eq. (6.16) should reach the same continuum limit with a rate of $\mathcal{O}(a^2)$, regardless of the value of c_{sw} . On the other hand, for $\gamma_5 \tau^1$ -odd observables one expects,

$$I_{\Gamma_A}^{\pm} \Big|_{[\Gamma_A, \gamma_5]=0} = 0, \quad (6.17)$$

$$I_{\Gamma_A}^{\pm} \Big|_{[\Gamma_A, \gamma_5]=0} = \text{const} \times (c_{\text{sw}} - 1) \frac{a}{L} + \mathcal{O}(a^2). \quad (6.18)$$

Like in the continuum, the exact flavour symmetry in the standard SF implies that $\gamma_5 \tau^1$ -odd observables are exactly zero [Eq. (6.17)]. While some of the χ SF observables vanish exactly, too, most are afflicted by $\mathcal{O}(a)$ effects which can be reduced to $\mathcal{O}(a^2)$ by Symanzik improvement with $c_{\text{sw}} = 1$, as indicated in Eq. (6.18).

In order to see the effect of the Sheikholeslami-Wohlert term at tree-level one needs the presence of a background gauge field. We will use the same constant Abelian $\text{SU}(2)$ background gauge field which has been used for the definition of the SF coupling in the $\text{SU}(2)$ Yang-Mills theory [41]. The fermion propagator in the continuum is known analytically in this case; however its lattice counterparts have so far only been calculated in the standard SF (cf. ref. [40]). We therefore resort to a numerical approach. We choose the set-up with $\tau = +1$, set $T = L$ and $\mathbf{p} = \mathbf{0}$, but keep a non-zero value $\theta = 1.0$. Specifying the Euclidean times $x_0 = T/2$ and $y_0 = T/4$ we choose the $+$ -components with $\Gamma_A = \gamma_0$ and $\Gamma_A = 1$ as

examples of $\gamma_5\tau^1$ -even and -odd quantities, respectively. Using the analytic result for the continuum propagator of Appendix B, their continuum limit can be calculated analytically, with the result,

$$I_{\gamma_0, \text{cont}}^+ = 4 \sum_{i=1}^2 \frac{\cosh [\omega_i(T/2) - \omega_i(T)] \cosh \omega_i(T/4)}{\cosh \omega_i(T)}, \quad (6.19)$$

whereas $I_{1, \text{cont}}^+ = 0$. The sum over colour components corresponds to the colour trace in the special case of the SU(2) Abelian background field. Computing these observables for $c_{\text{sw}} = 0$ and $c_{\text{sw}} = 1$, and lattice sizes from $L/a = 8$ up to $L/a = 72$, universality is indeed confirmed. In Figure 1 the relative deviations from the common continuum limit, rescaled by L/a , are plotted versus a/L . This extrapolates to a finite value in the case of $O(a)$ corrections, whereas a vanishing continuum limit indicates $O(a^2)$ or higher lattice artefacts. Finally, Fig. 2 shows the $\gamma_5\tau^1$ -odd observable I_1^+ , multiplied by L/a . Hence, a finite value in the continuum limit indicates $O(a)$ effects. This is the generic situation unless $c_{\text{sw}} = 1$ for which the observable becomes a pure lattice artefact of $O(a^2)$. In the free theory we have thus explicitly verified that automatic $O(a)$ improvement works as expected.

7 Concluding remarks and outlook

We have shown how the mechanism of automatic $O(a)$ improvement can be reconciled with SF boundary conditions. This means that any bulk $O(a)$ effects vanish in correlation functions which are even under the $\gamma_5\tau^1$ -symmetry. Any remaining $O(a)$ effects must arise from boundary effects and their elimination requires the tuning of a couple of boundary counterterms (proportional to d_s and c_t), similar to the standard SF. In order to achieve this one needs to tune the coefficient z_f of a dimension 3 boundary counterterm such that the physical parity symmetry is restored. One may say that the tuning problem for z_f is the price to be paid for avoiding the non-perturbative determination of c_{sw} and of any $O(a)$ improvement coefficients for composite fields in the correlation functions (such as c_A or c_V for the flavour currents [4]). The chirally rotated SF provides a well-defined framework which can be seen as an alternative regularisation of the standard SF, with the advantage of reduced cutoff effects. This will benefit the calculation of step-scaling functions for which the continuum extrapolation will be made easier, and it will reduce the potential problem of introducing $O(a)$ effects into hadronic matrix elements through SF scheme renormalization factors.

Since the formulation of the chirally rotated SF was given for a flavour doublet, a natural question to ask is whether it can be generalised to arbitrary flavour number N_f .

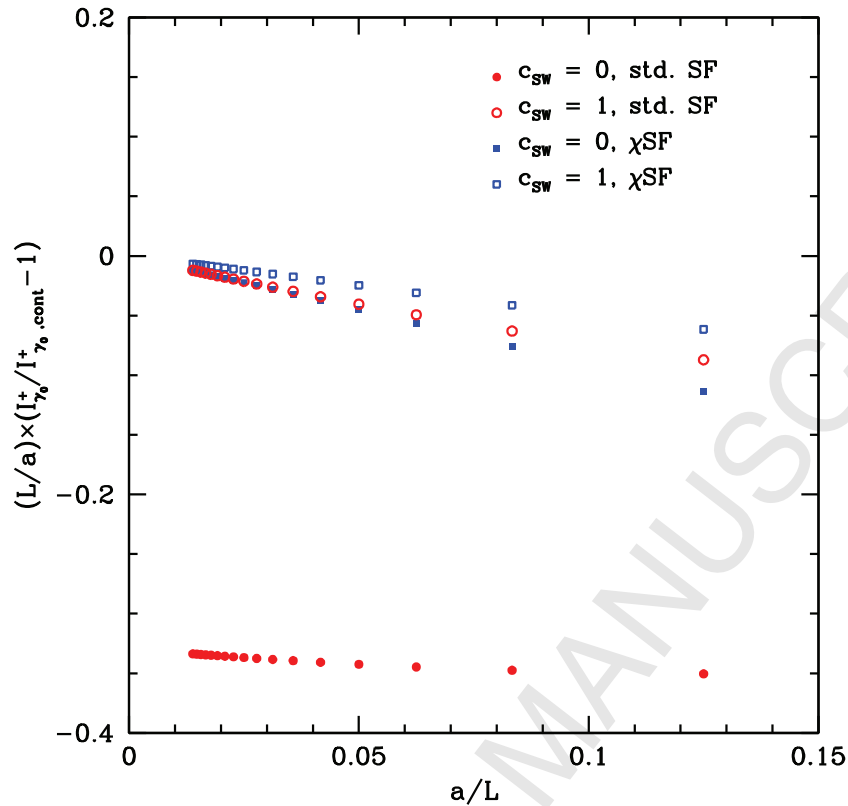


Figure 1: The relative deviation from the continuum limit, rescaled by L/a , is plotted vs. a/L for the $\gamma_5\tau^1$ -even observable $I_{\gamma_0}^+$ (cf. text for further details).

7.1 General N_f

Most of the discussion in this paper concerned the case of a quark flavour doublet, where a non-singlet axial rotation relates the correlation functions with those defined in the standard SF. In particular, invoking universality, one expects that the renormalisation works out in the same way as in the standard SF, up to scale-independent (finite) counterterms, which are the consequence of breaking the continuum flavour and parity symmetry by the regularisation. This is further supported by the formulation with Ginsparg-Wilson quarks, where the same symmetries are restored à la Ginsparg-Wilson [25].

While the inclusion of further doublets and thus the formulation for even flavour numbers is straightforward, the situation is a bit more complicated for odd N_f . First

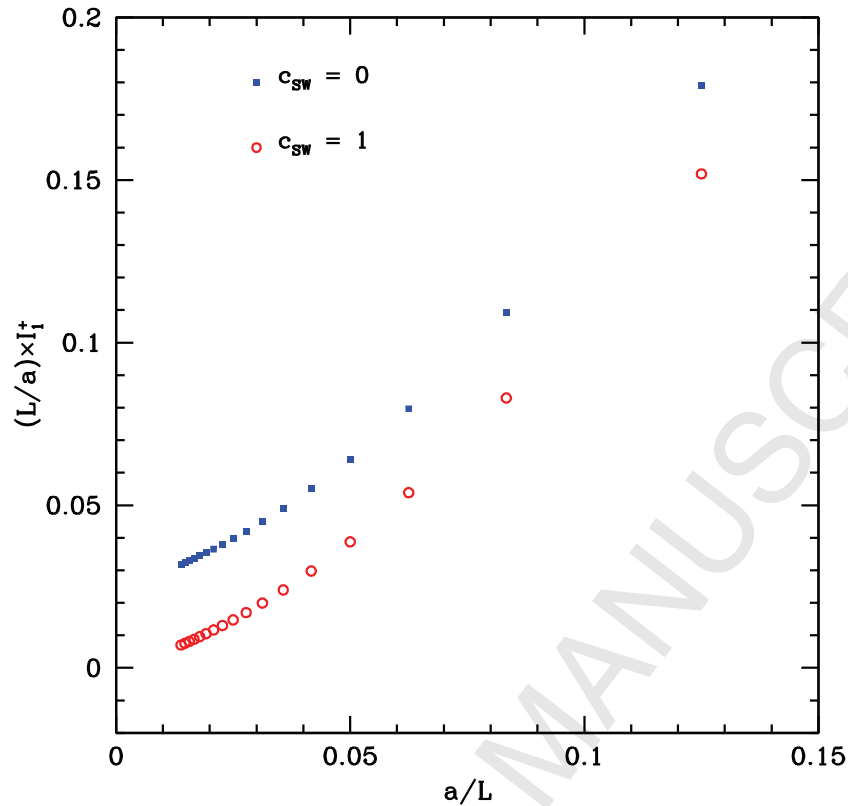


Figure 2: The $O(a)$ effect in the $\gamma_5 \tau^1$ -odd observable I_1^+ with $c_{sw} = 0$ is rendered visible by rescaling the observable with L/a . The effect of $O(a)$ improvement with $c_{sw} = 1$ reduces the lattice artefacts to $O(a^2)$.

of all, the discussion of the symmetries, and hence the counterterm structure, relied on a flavour exchange between up- and down-type flavours combined with space-time reflections. To apply this analysis to the single flavour case one may use a spurion field in the Wilson-Dirac operator, which switches sign under a space or time reflection, and thus takes over the rôle of the flavour exchange symmetry. The counterterm structure found in this way would then be the same as in the doublet case, appropriately reduced to either the up- or down-type flavour. This may in fact be generalised to any number N_f of flavours, with all flavours being of the up-flavour type, for example. As the relation to the standard SF is lost in this case, one would then tend to describe the symmetries as an exact $SU(N_f)$ flavour symmetry, with all

axial symmetries being broken by a singlet twisted mass term with $O(1)$ coefficient, localised at the boundaries. In addition to the axial symmetries also parity and time reflection symmetries are broken explicitly by the boundary conditions. Note, however, that the interpretation that z_f restores a continuum symmetry is lost in this case, and it is unclear to the author whether z_f remains scale-independent in this situation. A further, more practical question is whether such a set-up would be suitable for numerical simulations.

7.2 Numerical simulations including the fermion determinant

Currently, most numerical simulations are based on some variant of the Hybrid Monte Carlo algorithm [42], and the fermionic determinant is thus required to be real and positive. For the Wilson-Dirac operator in the two-flavour case with χ SF boundary conditions this property can easily be established. The hermiticity of $\gamma_5 \tau^1 \mathcal{D}_W$, implies for its flavour components,

$$\mathcal{D}_W = \text{diag} \left(\mathcal{D}_W^{(1)}, \mathcal{D}_W^{(2)} \right), \quad \gamma_5 \mathcal{D}_W^{(1)} \gamma_5 = \left(\mathcal{D}_W^{(2)} \right)^\dagger, \quad (7.1)$$

and therefore,

$$\begin{aligned} \det(\mathcal{D}_W + m_0) &= \det \left(\mathcal{D}_W^{(1)} + m_0 \right) \det \left(\mathcal{D}_W^{(2)} + m_0 \right) \\ &= \det \left[\left(\mathcal{D}_W^{(1)} + m_0 \right)^\dagger \left(\mathcal{D}_W^{(1)} + m_0 \right) \right] \geq 0. \end{aligned} \quad (7.2)$$

which has exactly the structure required for the standard algorithms. Twisted mass terms can be added, too. Allowing for two kinds of twisted mass terms,

$$i\mu_q \gamma_5 \tau^3 + i\mu'_q \gamma_5 \tau^2, \quad (7.3)$$

one realizes that the Wilson-Dirac operator is still $\gamma_5 \tau^1$ -hermitian so that its determinant must be real. Reducing the determinant in flavour space the r.h.s. of Eq. (7.2) generalises as follows,

$$\det \left[\left(\mathcal{D}_W^{(1)} + m_0 \right)^\dagger \left(\mathcal{D}_W^{(1)} + m_0 \right) + i\mu_q \gamma_5 \left(\mathcal{D}_W^{(1)} - \mathcal{D}_W^{(2)} \right) + \mu_q^2 + (\mu'_q)^2 \right]. \quad (7.4)$$

Note that μ_q multiplies a hermitian operator localised at the boundaries, which is diagonal in space-time and gauge field independent, at least for the set-up with $\tau = \pm 1$ (cf. Sect. 4).

The situation is less clear with odd numbers of flavours. In the free theory the determinant for a single flavour turns out to be real, even in the presence of a spatially constant Abelian background field. However, a numerical check on a small lattice with a random gauge configuration reveals that the determinant is in general complex⁹. Hence, some additional idea is needed in order to enable simulations of

⁹I thank B. Leder for performing this numerical check using MATLAB.

odd flavour numbers with χ SF-type boundary conditions. A simple alternative in this case would be a mixed formulation, where an even number of quarks is represented by chirally rotated quark doublets, whereas a single quark is implemented with standard SF boundary conditions. In the continuum limit this formulation will be equivalent to the standard SF with an odd number of flavours. Moreover, automatic $O(a)$ improvement would partially apply: while the Sheikholeslami-Wohlert term in the action would be required, correlation functions involving only chirally rotated quark flavours would be automatically $O(a)$ improved up to boundary effects. The price to pay is an additional $O(a)$ improvement coefficient at the boundaries since now both d_s and $\tilde{c}_t$ would be required.

7.3 Outlook

The chirally rotated SF offers a number of applications. Automatic $O(a)$ improvement will be particularly welcome when applying SF schemes e.g. to four-quark operators for which a non-perturbative determination of the $O(a)$ counterterms seems impractical. Furthermore, in the standard SF, the $O(a)$ improvement by the Sheikholeslami-Wohlert term often cancels large cutoff effects. In order to apply SF schemes to operators used in twisted mass QCD without the Sheikholeslami-Wohlert term (as currently used by the European twisted mass collaboration [43]), the chirally rotated SF is a natural choice, and may indeed be the only practical one. Further applications include multi-flavour QCD-like theories or lattice gauge theories with different gauge groups and fermion representations, where the determination of the Sheikholeslami-Wohlert coefficient c_{sw} can be avoided. Moreover, one may expect a reduced sensitivity to the precise definition of the critical quark mass. Finally, the chirally rotated SF provides new methods to determine finite renormalisation constants such as the axial current normalisation constant Z_A , and some of the usual $O(a)$ improvement coefficients [44]. Since standard Symanzik $O(a)$ improvement of Wilson fermions remains relevant for many collaborations, any improvement over the traditional methods based on Ward identities may indeed be welcome.

However, before these applications can be envisaged, one would like to perform a thorough non-perturbative test of the chirally rotated SF. In particular one needs to acquire some experience regarding the tuning of z_f and m_{cr} [45,44]. One would like to verify that the boundary conditions are correctly implemented in the interacting theory and that automatic $O(a)$ improvement works out as anticipated. Furthermore, universality could be checked by comparing with correlation functions defined in the standard SF. A non-perturbative study addressing all these questions is currently being performed in quenched lattice QCD [44]. Further checks will be carried out in perturbation theory [46]. In particular, one would like to obtain per-

turbative estimates for d_s and c_t , as these improvement coefficients are difficult to determine otherwise.

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A Absence of zero modes

The absence of zero modes for the massless continuum Dirac operator in a smooth external gauge field $A_\mu(x)$, can be established as in the case of the SF with standard boundary conditions [24]. We first deal with the case of a single quark flavour with $Q_\pm$ boundary conditions, and then consider the case of a quark doublet at generic values of the angle α .

A.1 Single flavour with $Q_\pm$ boundary conditions

Consider the massless Dirac operator $\mathcal{D} = \gamma_\mu(D_\mu + A_\mu)$ for a single flavour, acting in the Hilbert space of square integrable functions $\varphi(x)$ on a hyper cylinder, subject to the boundary conditions

$$Q_+\varphi(0, \mathbf{x}) = 0 = Q_-\varphi(T, \mathbf{x}), \quad Q_\pm = \frac{1}{2}(1 \pm i\gamma_0\gamma_5). \quad (\text{A.1})$$

With respect to the natural scalar product,

$$(\varphi, \chi) = \int_0^T dx_0 \int d^3\mathbf{x} \varphi(x)^\dagger \chi(x), \quad (\text{A.2})$$

the operator $i\mathcal{D}$ is hermitian. A well-defined eigenvalue problem is thus obtained,

$$i\mathcal{D}w_n = \lambda_n w_n, \quad (\text{A.3})$$

with real eigenvalues λ_n and smooth eigenfunctions w_n , which span the Hilbert space. In the following it is assumed that the eigenfunctions have been chosen such as to form an orthonormal basis of the Hilbert space, i.e.

$$(w_n, w_m) = \delta_{nm}, \quad \sum_n w_n(x)w_n(y)^\dagger = \delta^{(4)}(x - y). \quad (\text{A.4})$$

Next, consider the classical solution of the Dirac equation with inhomogeneous boundary conditions,

$$\not{D} \psi_{\text{cl}}(x) = 0, \quad Q_+ \psi_{\text{cl}}(0, \mathbf{x}) = \rho(\mathbf{x}), \quad Q_- \psi_{\text{cl}}(T, \mathbf{x}) = \rho'(\mathbf{x}). \quad (\text{A.5})$$

In order to obtain an explicit expression for the classical solution, one needs the propagator in the orthogonal subspace of the zero modes,

$$S^\perp(x, y) = -i \sum_{n: \lambda_n \neq 0} \frac{w_n(x) w_n(y)^\dagger}{\lambda_n}. \quad (\text{A.6})$$

Assume that there are a finite number of N_0 zero modes, $w_{n_i}(x)$, $i = 1, \dots, N_0$. The propagator in the orthogonal subspace then satisfies the equation

$$\not{D} S^\perp(x, y) = \delta^{(4)}(x - y) - \sum_{i=1}^{N_0} w_{n_i}(x) w_{n_i}(y)^\dagger. \quad (\text{A.7})$$

Furthermore, since any finite superposition of zero modes must be smooth, the discontinuity for $S^\perp(x, y)$ is given by

$$S^\perp_{>}(x_0, \mathbf{x}, x_0, \mathbf{y}) - S^\perp_{<}(x_0, \mathbf{x}, x_0, \mathbf{y}) = \gamma_0 \delta^{(3)}(\mathbf{x} - \mathbf{y}), \quad (\text{A.8})$$

where the subscripts refer to the ordering of the time arguments in the propagator. Using these properties, the classical solution can be written as follows,

$$\psi_{\text{cl}}(x) = \int d^3 \mathbf{y} \left[S^\perp(x, 0, \mathbf{y}) \gamma_0 Q_+ \rho(\mathbf{y}) - S^\perp(x, T, \mathbf{y}) \gamma_0 Q_- \rho'(\mathbf{y}) \right], \quad (\text{A.9})$$

showing that it is linearly related to the boundary values. Finally, note that any of the zero modes, $w_{n_i}(x)$, is a classical solution of the Dirac equation, and can be written in the form (A.9). Since its boundary values vanish, the zero modes must vanish, too, i.e. $w_{n_i} = 0$, $i = 1, \dots, N_0$.

The case of opposite boundary projectors is completely analogous. Hence, the absence of zero modes is guaranteed with any number of quark flavours, and for any mixture of up and down type flavours.

A.2 Flavour doublet at generic values of α

Essentially the same argument works for a flavour doublet at any value of α , except that the mathematical structure is a bit more complicated. The boundary conditions for ψ and $\bar{\psi}$ at fixed, but arbitrary α give rise to the definition of two different Hilbert spaces,

$$\mathcal{H}_\pm = \{\phi : P_\pm(\pm\alpha)\phi|_{x_0=0} = 0 = P_\mp(\pm\alpha)\phi|_{x_0=T}\}, \quad (\text{A.10})$$

and both $\mathcal{D}$ and $\gamma_5\tau^1$ can be seen as mappings between these two spaces. Hence, $\gamma_5\tau^1\mathcal{D}$ is a hermitian operator in either space, with a complete set of smooth eigenfunctions and real eigenvalues. Denoting its orthonormal eigenfunctions in $\mathcal{H}_+$ by φ_n ,

$$\gamma_5\tau^1\mathcal{D}\varphi_n = \lambda_n\varphi_n, \quad (\text{A.11})$$

it follows that the functions $\tilde{\varphi}_n = \gamma_5\tau^1\varphi_n$ form an orthonormal basis in $\mathcal{H}_-$, and

$$\mathcal{D}\gamma_5\tau^1\tilde{\varphi}_n = \mathcal{D}\varphi_n = \lambda_n\gamma_5\tau^1\varphi_n = \lambda_n\tilde{\varphi}_n. \quad (\text{A.12})$$

Completeness in either Hilbert space then implies

$$\delta^4(x-y) = \sum_n \varphi_n(x)\varphi_n(y)^\dagger = \sum_n \tilde{\varphi}_n(x)\tilde{\varphi}_n(y)^\dagger. \quad (\text{A.13})$$

To relate the classical solution of the Dirac equation, $\mathcal{D}\psi_{\text{cl}}(x) = 0$, to its boundary values,

$$P_+(\alpha)\psi_{\text{cl}}(0, \mathbf{x}) = \rho(\mathbf{x}), \quad P_-(\alpha)\psi_{\text{cl}}(T, \mathbf{x}) = \rho'(\mathbf{x}), \quad (\text{A.14})$$

one needs again the inverse of $\mathcal{D}$ on the non-zero modes,

$$S^\perp(x, y) = \sum_{n:\lambda_n \neq 0} \frac{\varphi_n(x)\tilde{\varphi}_n(y)^\dagger}{\lambda_n}. \quad (\text{A.15})$$

Assuming N_0 zero modes, this propagator satisfies

$$\mathcal{D}S^\perp(x, y) = \delta^4(x-y) - \sum_{i=1}^{N_0} \tilde{\varphi}_{n_i}(x)\tilde{\varphi}_{n_i}(y)^\dagger. \quad (\text{A.16})$$

The discontinuity is again described by Eq. (A.8), and the classical solution takes the form

$$\psi_{\text{cl}}(x) = \int d^3\mathbf{y} \left[S^\perp(x, 0, \mathbf{y})\gamma_0 P_+(\alpha)\rho(\mathbf{y}) - S^\perp(x, T, \mathbf{y})\gamma_0 P_-(\alpha)\rho'(\mathbf{y}) \right]. \quad (\text{A.17})$$

Again, any of the zero modes solves the Dirac equation and satisfies homogeneous boundary conditions, and must therefore vanish identically. Note that this argument also holds at $\alpha = 0$. In particular, the flavour permutation τ^1 is not required in this case, so that the proof applies virtually unchanged to the case of a single quark flavour with standard SF boundary conditions.

B The free quark propagator

We collect a few formulae for the free propagator both in the continuum and on the lattice. For the sake of notational simplicity the propagator is generically denoted by S and any additional parameter dependence or indeed whether it is the lattice or continuum propagator will be either clear from the context or otherwise indicated.

B.1 Continuum quark propagator for generic values of α

The free quark propagator in the continuum theory can be easily obtained using standard methods. Allowing for standard and twisted mass terms, the quark propagator satisfies,

$$(\not{D} + m + i\mu_q \gamma_5 \tau^3) S(x, y) = \delta^{(4)}(x - y), \quad (\text{B.1})$$

and the boundary conditions,

$$\begin{aligned} P_+(\alpha) S(x, y)|_{x_0=0} &= 0, & P_-(\alpha) S(x, y)|_{x_0=T} &= 0, \\ S(x, y) P_-(-\alpha)|_{y_0=0} &= 0, & S(x, y) P_+(-\alpha)|_{y_0=T} &= 0. \end{aligned} \quad (\text{B.2})$$

The boundary conditions in the second argument follow e.g. from the fact that the Dirac operator is $\gamma_5 \tau^1$ -hermitian (cf. Appendix A). For the same reason the complementary components satisfy (modified) Neumann conditions, i.e.

$$\begin{aligned} (D_0 - M_\alpha) P_-(\alpha) S(x, y)|_{x_0=0} &= 0, & (D_0 + M_\alpha) P_+(\alpha) S(x, y)|_{x_0=T} &= 0, \\ S(x, y) P_+(-\alpha) (\overleftarrow{D}_0 - M_\alpha)|_{y_0=0} &= 0, & S(x, y) P_-(-\alpha) (\overleftarrow{D}_0 + M_\alpha)|_{y_0=T} &= 0, \end{aligned} \quad (\text{B.3})$$

with

$$M_\alpha = m \cos \alpha + \mu_q \sin \alpha. \quad (\text{B.4})$$

These equations hold for arbitrary smooth gauge field $A_\mu(x)$. Setting the gauge field to zero, we use L -periodic spatial boundary conditions and include the phase θ as an Abelian background field in the spatial derivative:

$$\not{D} = \partial_0 \gamma_0 + \left(\partial_k + i \frac{\theta}{L} \right) \gamma_k. \quad (\text{B.5})$$

Spatial translation invariance suggests to pass to the time momentum representation,

$$S(x, y) = L^{-3} \sum_{\mathbf{p}} e^{i\mathbf{p}(\mathbf{x}-\mathbf{y})} S_{\mathbf{p}}(x_0, y_0), \quad (\text{B.6})$$

where the (infinite) sum is over all allowed momenta of the form $\mathbf{p} = 2\pi\mathbf{n}/L$, with $\mathbf{n}$ being a triple of integers. In time-momentum representation one then has

$$(\partial_0 - A) S_{\mathbf{p}}(x_0, y_0) = \gamma_0 \delta(x_0 - y_0), \quad (\text{B.7})$$

with

$$A = (ip_k^+ \gamma_k - m + i\mu_q \gamma_5 \tau^3) \gamma_0 = A^\dagger, \quad p_k^+ = p_k + \theta/L. \quad (\text{B.8})$$

There are many ways to represent the free propagator. A very compact form is

$$S_{\mathbf{p}}(x_0, y_0) = e^{x_0 A} \left\{ \frac{-1}{n(T)} P_-(\alpha) e^{TA} + \theta(x_0 - y_0) \right\} e^{-y_0 A} \gamma_0, \quad (\text{B.9})$$

where $\theta(t)$ denotes the Heaviside step function, and

$$n(T) = \cosh(\omega T) + \frac{M_\alpha}{\omega} \sinh(\omega T), \quad \omega = \sqrt{(\mathbf{p}^+)^2 + m^2 + \mu_q^2}. \quad (\text{B.10})$$

Using $A^2 = \omega^2$ one may easily evaluate the exponentials and obtain a more explicit representation,

$$\begin{aligned} S_{\mathbf{p}}(x_0, y_0) &= \gamma_0 P_-(-\alpha) H_+ + \gamma_0 P_+(-\alpha) H_- \\ &\quad - (A - M_\alpha) \gamma_0 P_-(-\alpha) G_+ - (A + M_\alpha) \gamma_0 P_+(-\alpha) G_-, \end{aligned} \quad (\text{B.11})$$

with coefficient functions $G_\pm$ and $H_\pm$ defined by

$$\begin{aligned} G_+(\mathbf{p}; x_0, y_0) &= \frac{1}{2\omega R_\alpha} \left\{ (M_\alpha - \omega) \left(e^{\omega(|x_0 - y_0| - T)} - e^{\omega(x_0 + y_0 - T)} \right) \right. \\ &\quad \left. + (M_\alpha + \omega) \left(e^{-\omega(|x_0 - y_0| - T)} - e^{-\omega(x_0 + y_0 - T)} \right) \right\}, \end{aligned} \quad (\text{B.12})$$

$$G_-(\mathbf{p}; x_0, y_0) = G_+(\mathbf{p}; T - x_0, T - y_0), \quad (\text{B.13})$$

$$H_\pm(\mathbf{p}; x_0, y_0) = (-\partial_0 \mp M_\alpha) G_\pm(\mathbf{p}; x_0, y_0), \quad (\text{B.14})$$

and

$$R_\alpha = (M_\alpha + \omega) e^{\omega T} - (M_\alpha - \omega) e^{-\omega T}. \quad (\text{B.15})$$

Note that the coefficient functions are indexed such as to conform with the projectors for $\alpha = \pi/2$, where $P_\pm(-\pi/2) = \tilde{Q}_\mp$. They enjoy the following properties:

$$G_\pm(\mathbf{p}; x_0, y_0) = G_\pm(\mathbf{p}; y_0, x_0), \quad H_\pm(\mathbf{p}; x_0, y_0) = -H_\mp(\mathbf{p}; y_0, x_0). \quad (\text{B.16})$$

The Dirichlet boundary conditions imply

$$G_+(\mathbf{p}; 0, y_0) = 0 = G_-(\mathbf{p}; T, y_0), \quad (\text{B.17})$$

and

$$H_-(\mathbf{p}; 0, y_0) = 0 = H_+(\mathbf{p}; y_0, 0), \quad H_+(\mathbf{p}; T, y_0) = 0 = H_-(\mathbf{p}; y_0, T). \quad (\text{B.18})$$

Of particular interest is the massless case, for which the formulae simplify,

$$\begin{aligned} G_\pm(\mathbf{p}; x_0, y_0) &= \frac{1}{2\omega \cosh \omega T} \left\{ -\sinh \omega(|x_0 - y_0| - T) \right. \\ &\quad \left. \pm \sinh \omega(x_0 + y_0 - T) \right\}, \end{aligned} \quad (\text{B.19})$$

$$\begin{aligned} H_\pm(\mathbf{p}; x_0, y_0) &= \frac{1}{2 \cosh \omega T} \left\{ \varepsilon(x_0 - y_0) \cosh \omega(|x_0 - y_0| - T) \right. \\ &\quad \left. \mp \cosh \omega(x_0 + y_0 - T) \right\}, \end{aligned} \quad (\text{B.20})$$

where $\varepsilon(t)$ denotes the sign function.

B.2 The massless continuum quark propagator in an Abelian and spatially constant background field

In this subsection, an explicit expression is given for the massless continuum quark propagator in an Abelian $SU(N)$ background field B_μ . The latter is taken to be spatially constant, i.e. $B_\mu = B_\mu(x_0)$, and in the $B_0 = 0$ gauge. Spatial translation invariance then allows to pass to the time-momentum representation, where the propagator satisfies,

$$(\partial_0 \gamma_0 + [ip_k^+ + B_k(x_0)] \gamma_k) S_{\mathbf{p}}(x_0, y_0) = \delta(x_0 - y_0). \quad (\text{B.21})$$

We are interested in the background fields used for the running coupling [1,41,47] or the determination of the Sheikholeslami-Wohlert coefficient [48]. These are of the form

$$B_k(x_0) = C_k + \frac{x_0}{T} (C'_k - C_k), \quad (\text{B.22})$$

where the boundary gauge fields are taken to be

$$C_k = i\phi/L, \quad C'_k = i\phi'/L, \quad (\text{B.23})$$

with diagonal $N \times N$ -matrices ϕ and ϕ' in colour space. Since these are chosen to be independent of the spatial index k , it is convenient to restrict attention to the special case where also the momentum components are k -independent, i.e. $p_k^+ = p^+$ for $k = 1, 2, 3$. Then, defining

$$\Sigma = \frac{i}{\sqrt{3}} (\gamma_1 + \gamma_2 + \gamma_3) \gamma_0, \quad (\text{B.24})$$

$$\omega(t) = t\sqrt{3} \left(p^+ + \frac{\phi}{L} + \frac{t}{2LT} [\phi' - \phi] \right), \quad (\text{B.25})$$

the result for the quark propagator can be written in the form

$$S_{\mathbf{p}}(x_0, y_0) = e^{\omega(x_0)\Sigma} \left\{ -\frac{1}{\cosh \omega(T)} P_-(\alpha) e^{\omega(T)\Sigma} + \theta(x_0 - y_0) \right\} e^{-\omega(y_0)\Sigma} \gamma_0. \quad (\text{B.26})$$

where $\theta(t)$ denotes the Heaviside step function. Using $\Sigma^2 = 1$, one may easily obtain the equivalent expression

$$\begin{aligned} S_{\mathbf{p}}(x_0, y_0) &= \gamma_0 P_-(-\alpha) H_+ + \gamma_0 P_+(-\alpha) H_- \\ &\quad - \omega'(T) \Sigma \gamma_0 \{ P_-(-\alpha) G_+ + P_+(-\alpha) G_- \}. \end{aligned} \quad (\text{B.27})$$

Here, $\omega'(t) \equiv d\omega(t)/dt$, and the coefficient functions are defined by

$$\begin{aligned} G_{\pm}(\mathbf{p}; x_0, y_0) &= \frac{1}{2\omega'(T) \cosh \omega(T)} \left\{ \pm \sinh [\omega(x_0) + \omega(y_0) - \omega(T)] \right. \\ &\quad \left. - \sinh [\varepsilon(x_0 - y_0) \{\omega(x_0) - \omega(y_0)\} - \omega(T)] \right\}, \quad (\text{B.28}) \\ H_{\pm}(\mathbf{p}; x_0, y_0) &= \frac{1}{2 \cosh \omega(T)} \left\{ \mp \cosh [\omega(x_0) + \omega(y_0) - \omega(T)] \right. \\ &\quad \left. + \varepsilon(x_0 - y_0) \cosh [\varepsilon(x_0 - y_0) \{\omega(x_0) - \omega(y_0)\} - \omega(T)] \right\}. \quad (\text{B.29}) \end{aligned}$$

Here all functions are diagonal in colour space, with colour components being obtained by specifying the colour components ϕ_i and ϕ'_i and thus ω_i , with $i = 1, \dots, N$. Setting $\phi_i = \phi'_i = 0$ amounts to the replacement of $\omega_i(t) \rightarrow \omega(\mathbf{p}^+)t$ and these expressions then reduce to the ones given in Eqs. (B.19) and (B.20), for the special case with $p_1^+ = p_2^+ = p_3^+ = p^+$.

B.3 The free quark propagator on the lattice

A straightforward way to calculate the free quark propagator on the lattice proceeds via the classical solution of the lattice Dirac equation, following [40], where the inhomogeneous boundary conditions are imposed either at Euclidean times $x_0 = 0, T$, or appropriately off set by $\pm a/2$. After spatial Fourier transform, the result can be written in the form

$$\begin{aligned} S_{\mathbf{p}}^T(x_0, y_0) &= \frac{1}{2A(\mathbf{p}^+)} \delta_{x_0, y_0} + \gamma_0 \tilde{Q}_+ H_+^T + \gamma_0 \tilde{Q}_- H_-^T \\ &\quad + (-i\tilde{p}_k^+ \gamma_k + M(\mathbf{p}^+)) [\tilde{Q}_+ G_+^T + \tilde{Q}_- G_-^T], \quad (\text{B.30}) \end{aligned}$$

where the coefficient functions are given by

$$\begin{aligned} G_{\pm}^T(\mathbf{p}; x_0, y_0) &= \frac{1}{2\tilde{\omega}A(\mathbf{p}^+) \cosh \omega T'} \left\{ -\sinh \omega(|x_0 - y_0| - T') \right. \\ &\quad \left. \pm \sinh \omega(x_0 + y_0 - T) \right\}, \quad (\text{B.31}) \end{aligned}$$

$$\begin{aligned} H_{\pm}^T(\mathbf{p}; x_0, y_0) &= \frac{1}{2A(\mathbf{p}^+) \cosh \omega T'} \left\{ \tilde{\varepsilon}(x_0 - y_0) \cosh \omega(|x_0 - y_0| - T') \right. \\ &\quad \left. \mp \cosh \omega(x_0 + y_0 - T) \right\}. \quad (\text{B.32}) \end{aligned}$$

Here, $T' = T + \tau a$ denotes the effective time extent for the fermionic degrees of freedom, for the orbifold construction with $\tau = 0$ and $\tau = \pm 1$ (cf. Sect. 4). With

$$A(\mathbf{p}) = 1 + am_0 + \frac{1}{2}a^2 \hat{\mathbf{p}}^2, \quad (\text{B.33})$$

the one-particle energy ω is defined by

$$\sinh\left(\frac{a}{2}\omega(\mathbf{p})\right) = \left\{ \frac{a^2\tilde{\mathbf{p}}^2 + \{A(\mathbf{p}) - 1\}^2}{4A(\mathbf{p})} \right\}^{\frac{1}{2}}. \quad (\text{B.34})$$

The notation is further specified by

$$\tilde{\omega} = \frac{1}{a} \sinh(a\omega), \quad (\text{B.35})$$

$$aM(\mathbf{p}) = A(\mathbf{p}) - \cosh[a\omega(\mathbf{p})], \quad (\text{B.36})$$

and the above lattice version of the sign function, $\tilde{\varepsilon}(t)$, is given by

$$\tilde{\varepsilon}(t) = \begin{cases} 1 & \text{if } t > 0, \\ 0 & \text{if } t = 0, \\ -1 & \text{if } t < 0. \end{cases} \quad (\text{B.37})$$

These expressions for the free quark propagator have been checked numerically by inverting the corresponding Dirac operators at fixed momentum, and semi-analytically by comparing with Eq. (4.39). For $\tau = 0$ a difference with Eq. (4.39) is found for the contact terms at the boundaries, i.e. for $x_0 = y_0 = 0$ and $x_0 = y_0 = T$. While the difference can be easily worked out, the result is not needed here. In fact, these contact terms are never referred to provided the fermionic boundary fields are defined as in Sect. 5.

References

- [1] M. Lüscher, R. Narayanan, P. Weisz and U. Wolff, Nucl. Phys. B **384** (1992) 168 [arXiv:hep-lat/9207009].
- [2] S. Sint, Nucl. Phys. B **421** (1994) 135 [arXiv:hep-lat/9312079].
- [3] S. Sint, Nucl. Phys. B **451** (1995) 416 [arXiv:hep-lat/9504005].
- [4] K. Jansen *et al.*, Phys. Lett. B **372** (1996) 275 [arXiv:hep-lat/9512009].
- [5] S. Sint, Nucl. Phys. Proc. Suppl. **94** (2001) 79 [arXiv:hep-lat/0011081].
- [6] M. Della Morte, R. Hoffmann, F. Knechtli, J. Rolf, R. Sommer, I. Wetzorke and U. Wolff [ALPHA Collaboration], Nucl. Phys. B **729** (2005) 117 [arXiv:hep-lat/0507035].
- [7] S. Aoki *et al.* [PACS-CS collaboration and PACS-CS collaboration and PACS-CS collaborat], arXiv:1006.1164 [hep-lat].

- [8] M. Della Morte, R. Frezzotti, J. Heitger, J. Rolf, R. Sommer and U. Wolff [ALPHA Collaboration], Nucl. Phys. B **713** (2005) 378 [arXiv:hep-lat/0411025].
- [9] S. Aoki *et al.* [PACS-CS Collaboration], JHEP **0910** (2009) 053 [arXiv:0906.3906 [hep-lat]].
- [10] F. Tekin, R. Sommer and U. Wolff, arXiv:1006.0672 [hep-lat].
- [11] M. Guagnelli, J. Heitger, C. Pena, S. Sint and A. Vladikas [ALPHA Collaboration], JHEP **0603**, 088 (2006) [arXiv:hep-lat/0505002].
- [12] R. Sommer, proceedings of the workshop “Perspectives in Lattice QCD”, Nara, Japan 31 October - 11 November 2005, Yoshinobu Kuramashi (ed.), World Scientific (2008) [arXiv:hep-lat/0611020].
- [13] T. Appelquist, G. T. Fleming and E. T. Neil, Phys. Rev. D **79** (2009) 076010 [arXiv:0901.3766 [hep-ph]].
- [14] A. J. Hietanen, K. Rummukainen and K. Tuominen, Phys. Rev. D **80** (2009) 094504 [arXiv:0904.0864 [hep-lat]].
- [15] F. Bursa, L. Del Debbio, L. Keegan, C. Pica and T. Pickup, Phys. Rev. D **81** (2010) 014505 [arXiv:0910.4535 [hep-ph]].
- [16] T. DeGrand, Y. Shamir and B. Svetitsky, arXiv:1006.0707 [hep-lat].
- [17] N. Yamada, M. Hayakawa, K. I. Ishikawa, Y. Osaki, S. Takeda and S. Uno, arXiv:1003.3288 [hep-lat].
- [18] U. M. Heller, Nucl. Phys. B **504** (1997) 435 [arXiv:hep-lat/9705012].
- [19] P. Perez-Rubio and S. Sint, PoS **LAT2007** (2007) 249 [arXiv:0710.0583 [hep-lat]].
- [20] P. Perez-Rubio and S. Sint, PoS **LATTICE2008** (2008) 221 [arXiv:0810.3866 [hep-lat]].
- [21] Y. Taniguchi, JHEP **0512** (2005) 037 [arXiv:hep-lat/0412024].
- [22] Y. Taniguchi, JHEP **0610** (2006) 027 [arXiv:hep-lat/0604002].
- [23] S. Takeda, arXiv:0910.2485 [hep-lat], to appear in the proceedings of the 27th International Symposium on Lattice Field Theory (Lattice 2009), Beijing, China, 25-31 July 2009.
- [24] M. Luscher, JHEP **0605** (2006) 042 [arXiv:hep-lat/0603029].

- [25] S. Sint, PoS **LAT2007** (2007) 253.
- [26] A. Bode, U. Wolff and P. Weisz [Alpha Collaboration], Nucl. Phys. B **540** (1999) 491 [arXiv:hep-lat/9809175].
- [27] A. Bode, P. Weisz and U. Wolff [ALPHA collaboration], Nucl. Phys. B **576** (2000) 517 [Erratum-ibid. B **600** (2001) 453] [Erratum-ibid. B **608** (2001) 481] [arXiv:hep-lat/9911018].
- [28] R. Frezzotti and G. C. Rossi, JHEP **0408** (2004) 007 [arXiv:hep-lat/0306014].
- [29] S. Sint, PoS **LAT2005** (2006) 235 [arXiv:hep-lat/0511034].
- [30] S. Sint, proceedings of the workshop “Perspectives in Lattice QCD”, Nara, Japan 31 October - 11 November 2005, Yoshinobu Kuramashi (ed.), World Scientific (2008) [arXiv:hep-lat/0702008].
- [31] M. Lüscher, S. Sint, R. Sommer and P. Weisz, Nucl. Phys. B **478** (1996) 365 [arXiv:hep-lat/9605038].
- [32] K. Symanzik, Nucl. Phys. B **226** (1983) 187.
- [33] J. Balog, F. Niedermayer and P. Weisz, Nucl. Phys. B **824** (2010) 563 [arXiv:0905.1730 [hep-lat]].
- [34] S. Aoki and O. Bär, Phys. Rev. D **74** (2006) 034511 [arXiv:hep-lat/0604018].
- [35] M. Lüscher, Phys. Lett. B **428** (1998) 342 [arXiv:hep-lat/9802011].
- [36] H. Neuberger, Phys. Lett. B **417** (1998) 141 [arXiv:hep-lat/9707022].
- [37] P. H. Ginsparg and K. G. Wilson, Phys. Rev. D **25** (1982) 2649.
- [38] S. Sint and R. Sommer, Nucl. Phys. B **465** (1996) 71 [arXiv:hep-lat/9508012].
- [39] R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz [Alpha collaboration], JHEP **0108** (2001) 058 [arXiv:hep-lat/0101001].
- [40] M. Lüscher and P. Weisz, Nucl. Phys. B **479** (1996) 429 [arXiv:hep-lat/9606016].
- [41] M. Lüscher, R. Sommer, U. Wolff and P. Weisz, Nucl. Phys. B **389** (1993) 247 [arXiv:hep-lat/9207010].
- [42] S. Duane, A. D. Kennedy, B. J. Pendleton and D. Roweth, Phys. Lett. B **195** (1987) 216.

- [43] R. Baron *et al.*, JHEP **1006** (2010) 111 [arXiv:1004.5284 [hep-lat]].
- [44] B. Leder and S. Sint, PoS **LAT2010** (2010) 265; in preparation.
- [45] J. G. Lopez, K. Jansen, D. B. Renner and A. Shindler, PoS **LAT2009** (2009) 199 [arXiv:0910.3760 [hep-lat]].
- [46] M. Jamin and S. Sint, work in progress.
- [47] M. Lüscher, R. Sommer, P. Weisz and U. Wolff, Nucl. Phys. B **413** (1994) 481 [arXiv:hep-lat/9309005].
- [48] M. Lüscher, S. Sint, R. Sommer, P. Weisz and U. Wolff, Nucl. Phys. B **491** (1997) 323 [arXiv:hep-lat/9609035].