Chirally improving Wilson fermions
III. The Schrödinger functional

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Abstract

We show that it is possible to construct a lattice Schrödinger functional for standard Wilson fermions, where the expectation values of $\mathcal{R}_5$-even operators are $O(a)$ improved, up to terms coming from the boundaries.
1 Introduction

It has been shown in ref. [1] that it is possible to improve the approach to the continuum limit of correlation functions in lattice QCD with standard Wilson fermions by taking arithmetic averages (Wilson averages – WA’s) of vacuum expectation values (v.e.v.’s) computed in theories regularized with opposite values of the Wilson parameter, \( r \). Improved energies and matrix elements can be obtained by similarly averaging the corresponding physical quantities separately computed within the two regularizations. The same result can be obtained by replacing the WA with a linear combination of v.e.s.’s computed with the same value of \( r \), but opposite values of the quark mass, \( m_q \) (mass average – MA). In our notations \( m_q = M_0 - M_{cr} \), with \( M_0 \) the bare quark mass parameter and \( M_{cr} \) the critical mass. The relevant coefficient in the linear combination of the MA is the \( R_5 \) parity (see eq. (3.1) below) of the operator, \( O \), whose v.e.v. one is computing. Notice that in taking the limit \( m_q \to 0 \) the two terms of the MA may not be equal if spontaneous chiral symmetry breaking occurs.

To deal with the problems related to the spectrum of the Wilson–Dirac operator [2], twisted-mass lattice QCD (tm-LQCD) [3] should be better used for actual computations. The choice \( \omega = \pm \pi/2 \) for the twisting angle (maximal twist) is particularly interesting, as \( O(a) \) improved estimates of all interesting physical quantities can be obtained even without averaging data from lattice formulations with opposite Wilson terms.

These results are valid both in the quenched approximation and in the full theory. Indeed it was also shown in ref. [4] how one has to deal with the case of mass non-degenerate quark pairs to get \( O(a) \) improvement and at the same time a real and positive quark determinant.

Maximally twisted tm-LQCD can also be shown to be a sufficiently flexible regularization scheme to allow neat solutions [5, 6] of the difficult problem that goes under the name of “wrong chirality mixing” [7], which has up to now prevented a (reliable) lattice evaluation of the \( \Delta I = 1/2 \) non-leptonic kaon decay amplitudes, if Wilson fermions are employed. By coupling the strategy proposed in ref. [4] for the sea quark regularization with suitable ”twistings” of the Wilson terms of the valence quarks of various flavours, one can rigorously prove that it is possible to get rid of all “wrong chirality mixings” in the evaluation of the matrix elements of the CP-conserving \( \Delta S = 1, 2 \) effective weak Hamiltonian.

Striking confirmation of the viability of the approach outlined above and of the remarkable properties of tm-LQCD at \( |\omega| = \pi/2 \) has come from the recent works of refs. [8, 9, 10], where (quenched) studies of the scaling behaviour of the theory were carried out down to rather small values of lattice spacing.
and pion mass. Indeed, lattice results for pion masses as low as $\sim 250$ MeV show surprisingly small cutoff effects from $a \simeq .12$ fm to $a \simeq .05$ fm, if the optimal value of the critical mass [11, 12, 13, 14, 10] is employed. A careful study of the non-trivial phase structure of the unquenched [15, 16, 17] theory was also carried out in refs. [18, 19] with various choices of the gauge action (standard plaquette, DWB2 [20] and tree-level Symanzik improved).

A complementary role has been played by the Schrödinger functional formulation [21, 22] which has proved to be an invaluable tool in applications, especially because it provides a workable scheme for the computation of the running of the gauge coupling constant and the quark masses [21, 23], as well as for the non-perturbative evaluation of renormalization constants [24]. Thus a natural question to ask is whether the sort of $O(a)$ improvement one could get in the infinite volume formulation of lattice QCD can also be obtained in the Schrödinger functional framework.

In this paper we construct a modified Schrödinger functional describing the gauge interactions of a flavour doublet of massless standard Wilson quarks, in which fermions are endowed with a sort of twisted boundary conditions. We shall show that, under the assumption that IR effects are screened by the natural cutoff provided by the finite extension of the time coordinate and up to $O(a)$ (fermionic and gluonic) contributions coming from the boundaries, the arithmetic average of the expectation values of $R_5$-even (multi-local, gauge invariant, multiplicative renormalizable – m.r.) operators, $O$, computed with opposite values of the Wilson parameter (WA’s) are $O(a)$ improved. Like in the infinite volume case, the symmetries of the theory allow to conclude that the WA is indeed unnecessary, because in the massless limit $O(a)$ bulk lattice artifacts are actually absent.

As for the $O(a)$ boundary terms, we will see that there are two types of them: those coming from the action [25] and those coming from the need of improving operators inserted at the boundaries, if there is any such local factor in $O$. Boundary terms of the first type will appear in the action with coefficients that are even in the Wilson parameter, $r$. Their non-perturbative value is not known. In the standard formulation of the Schrödinger functional given by the Alpha-Collaboration they have been computed in perturbation theory up to two-loops [21, 26]. It turns out that this amount of knowledge is numerically adequate for applications. Boundary terms of the second type appear multiplied by coefficients that do not have definite $r$-parity, owing to the breaking of parity (see eq. (3.3) induced by our choice of fermionic boundary conditions (see below).

As we said, in this paper we will limit ourselves to discuss the massless theory, which is enough for the non-perturbative evaluation of fermionic renormalization constants and the computation of the running of the gauge
coupling and quark masses.

2 The construction of the Schrödinger functional

The problem with exporting the philosophy of the approach of ref. [1] to the standard Schrödinger functional formulation [21, 22] is related to the fact that, when the Schrödinger functional is constructed via the iteration of the transfer matrix operator [27] \(^1\), the projectors that define which fermionic components have to be prescribed at the boundaries are completely determined by the form of the transfer matrix and ultimately of the lattice action. For instance, for Wilson fermions the boundary conditions must have the Dirichlet form

\[
P_+ \psi(x,0) = \rho(x), \quad P_- \psi(x,T) = \rho'(x),
\]

\[
\bar{\psi}(x,0) P_- \bar{\rho}(x), \quad \bar{\psi}(x,T) P_+ \bar{\rho}'(x),
\]

with

\[
P_{\pm} = \frac{1}{2}(1 \pm r\gamma_0).
\]

The choice \(|r| = 1\) of the Wilson parameter is compulsory, in order for spin operators, \(P_{\pm}\), to be true projectors (\(P_{\pm}^2 = P_{\pm}\)).

Despite the fact that the finite time lattice action defined in this way can be shown to enjoy the (spurionic) symmetries that in the infinite volume theory were sufficient to guarantee \(O(a)\) improvement of Wilson averages [1], a similar conclusion cannot be drawn here, because upon inverting the sign of \(r\) the expression of the Schrödinger functional will change by \(O(1)\) terms. This operation, in fact, also affects the form of the boundary conditions since \(P_{\pm} \rightarrow P_{\mp}\) under \(r \rightarrow -r\).

The only envisageable way out of this difficulty is to have a formulation where the structure of the Wilson term and the form of the fermionic boundary conditions are not correlated \(^2\). We then propose to change the spin projectors from (2.2) and consider a situation where homogeneous \(\mathcal{R}_5\)-invariant constraints are taken. More precisely, we propose to construct a Schrödinger-like functional where fermions are introduced in pairs and obey the following homogeneous boundary conditions

\[
\Pi_+ \psi(x,0) = 0, \quad \Pi_- \psi(x,T) = 0,
\]

\(^1\)See ref. [28] for other attempts to define the Schrödinger functional in the continuum and on the lattice.

\(^2\)Though developed with the purpose of constructing a lattice Schrödinger functional for overlap fermions, the interesting orbifold construction of ref. [29] was of some inspiration to us. Ideas similar to the ones discussed here were also presented in ref. [30].
$$\bar{\psi}(x,0)\Pi_-=0, \quad \bar{\psi}(x,T)\Pi_+=0,$$

(2.3)

with

$$\Pi_\pm = \frac{1}{2}(1 \pm \tau_3\gamma_5).$$

(2.4)

Although not immediately required for $O(a)$ improvement, we are imagining that quarks are introduced in pairs with opposite chiral boundary projectors for the two flavour components (say, up and down). As we shall see, this is necessary to have a real and positive determinant.

With only the modification (2.3) of the boundary conditions, the improvement of the expectation value of m.r. $R_5$-even operators (up to $O(a)$ contaminations from boundary lattice artifacts) follows from symmetry arguments very similar to those that have been used in the infinite volume theory.

We now wish to give a few more details about our construction. Let us start by writing down the general form of the action of a pair of massless Wilson fermions obeying the boundary conditions (2.3), extended over the finite time interval $[0,T]$. Adapting the analysis of ref. [22] to the present situation and separating out the boundary terms from the rest, we write

$$S_F = S_{\text{bulk}} + S_B^i + S_B^f,$$

(2.5)

$$S_{\text{bulk}} = -\frac{a^3}{2} \sum_x \sum_{t=a}^{T-a} \left[ \bar{\psi}(x,t)U_0(x,t)(r-\gamma_0)\psi(x,t+a) + 
\bar{\psi}(x,t+a)(r+\gamma_0)U_0^\dagger(x,t)\psi(x,t) \right] + 
-\frac{a^4}{2a} \sum_{x,k} \sum_{t=a}^{T-a} \left[ \bar{\psi}(x,t)U_k(x,t)(r-\gamma_k)\psi(x+\hat{k},t) + 
\bar{\psi}(x+\hat{k},t)(r+\gamma_k)U_k^\dagger(x,t)\psi(x,t) \right] + 
+a^4 \sum_x \sum_{t=a}^{T-a} \bar{\psi}(x,t) \left[ M_{ct}(r) + \frac{4r}{a} \right] \psi(x,t),$$

(2.6)

$$S_B^i = -\frac{a^3}{2} \sum_x \left[ \left( \bar{\psi}(x,0)\Pi_+ U_0(x,0)(r-\gamma_0)\psi(x,0) + 
\bar{\psi}(x,0)(r+\gamma_0)U_0^\dagger(x,0)\Pi_-\psi(x,0) \right) + 
\frac{a^3}{2} \sum_{x,k} \bar{\psi}(x,0)\Pi_+\gamma_k \left[ V_k^i(x)\psi(x+\hat{k},0) - V_k^\dagger(x)\psi(x-\hat{k},0) \right],$$

(2.7)
\[ S_B^f = -\frac{a^3}{2} \sum_x \left[ \bar{\psi}(x, T-a)U_0(x, T-a)(r - \gamma_0)\Pi_+ \psi(x, T) + \bar{\psi}(x, T)\Pi_-(r + \gamma_0)U_0^\dagger(x, T-a)\psi(x, T-a) \right] + \alpha^3 \sum_{x, k} \bar{\psi}(x, T)\Pi_\gamma_k \left[ V_k^f(x)\psi(x + \hat{k}, T) - V_k^f\dagger(x)\psi(x - \hat{k}, T) \right]. \] (2.8)

For clarity in eqs. (2.6) to (2.8) we have kept separated spatial vs time components and sums. As usual we are assuming periodicity in space and fix the spatial components of the gauge links at the two time boundaries through

\[ U_k(x, 0) = V_k^f(x), \quad U_k(x, T) = V_k^f(x), \quad k = 1, 2, 3. \] (2.9)

In eq. (2.6) \( M_{cr}(r) \) is the critical fermion mass. We remark that no mass terms for the fermion fields living at the boundaries have been included. We will clarify the reason for that in the next sections.

With the action (2.5) we define a Schrödinger functional through the formula

\[ K_W[V_f; V_i] = \int \mathcal{D}\mu G[U] \int \mathcal{D}\mu_F[\bar{\psi}, \psi] e^{-S_{YM} - S_F}, \] (2.10)

where \( S_{YM} \) is the pure gauge finite time action \[21\] The gauge integration measure, \( \mathcal{D}\mu G[U] \), is as explained in refs. \[21, 22\]. The fermionic integration measure, \( \mathcal{D}\mu_F[\bar{\psi}, \psi] \), is spatially periodic and it is extended in time to all fermionic variables from \( t = a \) to \( t = T - a \) and over the variables \( \Pi_\gamma \bar{\psi}(x, 0), \bar{\psi}(x, 0)\Pi_+ \) and \( \Pi_+ \bar{\psi}(x, T), \bar{\psi}(x, T)\Pi_\gamma \) at the initial and final time, respectively.

It should be noted that this kernel enjoys the usual convolution properties only in the continuum limit, unlike the situation one has in the construction considered in refs. \[21, 22\]. Notice that, since the kernel (2.10) is not the iteration of the transfer matrix, one could even have dropped the terms proportional to \( r \) in eqs. (2.7) and (2.8).

3 Symmetry properties

The key observation of this paper is that the action (2.5) is invariant under a large set of transformations, which leave unaltered the structure of the homogeneous fermionic boundary constraints \[23\]. They are

- \( R_5 \times (r \to -r) \), where

\[ R_5 : \begin{align*}
\psi(x) &\to \psi^f(x) = \gamma_5 \psi(x) \\
\bar{\psi}(x) &\to \bar{\psi}^f(x) = -\bar{\psi}(x)\gamma_5
\end{align*} \] (3.1)
• \( R_5 \times D_d \times P \times (V_k^f \leftrightarrow V_k^i) \), where \((x_D = (-x,T-x_0)\))

\[
D_d : \begin{cases}
\psi(x) \rightarrow e^{3i\pi/2}\psi(x_D) \\
\bar{\psi}(x) \rightarrow e^{3i\pi/2}\bar{\psi}(x_D) \\
U_0(x) \rightarrow U_0^\dagger(x_D - a\hat{0}) \\
U_k(x) \rightarrow U_k^\dagger(x_D - a\hat{k}), \quad k = 1, 2, 3
\end{cases}
\]

(3.2)

and \( P \) is the standard parity operation \((x_P = (-x,x_0))\)

\[
P : \begin{cases}
\psi(x) \rightarrow \gamma_0\psi(x_P) \\
\bar{\psi}(x) \rightarrow \bar{\psi}(x_P)\gamma_0 \\
U_0(x) \rightarrow U_0(x_P), \\
U_k(x) \rightarrow U_k^\dagger(x_P - a\hat{k}), \quad k = 1, 2, 3
\end{cases}
\]

(3.3)

• the product \( CP \), where \( C \) is charge conjugation \((^T \text{ means transposition})\)

\[
C : \begin{cases}
\psi(x) \rightarrow i\gamma_0\gamma_2\bar{\psi}(x)^T \\
\bar{\psi}(x) \rightarrow -\bar{\psi}(x)^T i\gamma_0\gamma_2 \\
U_\mu(x) \rightarrow U_\mu^*(x), \quad \mu = 0, 1, 2, 3
\end{cases}
\]

(3.4)

• time inversion around the mid-point \( T/2, \ T \times (V_k^f \leftrightarrow V_k^i)\), where \((x_T = (x,T-x_0))\)

\[
T : \begin{cases}
\psi(x) \rightarrow \gamma_0\gamma_5\psi(x_T) \\
\bar{\psi}(x) \rightarrow \bar{\psi}(x_T)\gamma_5\gamma_0 \\
U_0(x) \rightarrow U_0^\dagger(x_T - a\hat{0}) , \\
U_k(x) \rightarrow U_k(x_T), \quad k = 1, 2, 3
\end{cases}
\]

(3.5)

• cubic \( H(3) \) group

We explicitly notice that the breaking of \( P, \ C \) and \( R_5 \times D_d \) is entirely due to the boundary action terms \([2.7] \) and \([2.8] \).

Besides the transformations collected above, which are all flavour diagonal, we have also invariance under

• the vector rotation in the iso-spin direction 3

\[
I_3 : \begin{cases}
\psi(x) \rightarrow e^{i\omega \tau_3/2}\psi(x) \\
\bar{\psi}(x) \rightarrow \bar{\psi}(x)e^{-i\omega \tau_3/2}
\end{cases}
\]

(3.6)

• and the four transformations separately acting on only the fermionic fields at the boundaries

\[
A_3^i : \psi(x,0) \rightarrow -\gamma_5\tau_3\psi(x,0), \quad (3.7)
\]

\[
A_3^i : \bar{\psi}(x,0) \rightarrow \bar{\psi}(x,0)\gamma_5\tau_3, \quad (3.8)
\]

\[
A_3^f : \psi(x,T) \rightarrow \gamma_5\tau_3\psi(x,T), \quad (3.9)
\]

\[
A_3^f : \bar{\psi}(x,T) \rightarrow -\bar{\psi}(x,T)\gamma_5\tau_3. \quad (3.10)
\]
Finally we mention the reflection symmetry, $\Theta \times (V^f_k \leftrightarrow V^i_k)$, related to reflection positivity (see e.g. [32, 14]). $\Theta$ is defined to act as follows

$$
\Theta[f(U)\psi(x_1)\ldots\bar{\psi}(x_n)] = 
= f^*(\Theta[U])\Theta[\bar{\psi}(x_n)]\ldots\Theta[\psi(x_1)],
$$

(3.11)

where $f(U)$ is a functional of link variables and for $a \leq x_0 \leq T - a$

$$
\begin{align*}
\Theta_{s/\ell}[\psi(x)] &= \bar{\psi}((s/\ell)x)\gamma_0 \\
\Theta_{s/\ell}[\bar{\psi}(x)] &= \gamma_0\bar{\psi}((s/\ell)x) \\
\Theta_{s/\ell}[U_k(x)] &= U^*_k((s/\ell)x) \\
\Theta_{s/\ell}[U_0(x)] &= U^T_0((s/\ell)x - a\hat{0})
\end{align*}
$$

(3.12)

with

$$
\theta_{s/\ell}(x, x_0) = (x, T - x_0)
$$

(3.12)

to be interpreted as a site ($s$) or link ($\ell$) time-reflection depending on whether $N_T$ ($T = N_T a$) is odd or even, respectively. The action of $\Theta$ on the fields at the boundaries is

$$
\begin{align*}
\Theta_{s/\ell}\Pi_- \psi(x, 0) &= \bar{\psi}(x, T)\Pi_-\gamma_0 \\
\Theta_{s/\ell}\Pi_+ \psi(x, 0)\Pi_+ &= \gamma_0\Pi_+\psi(x, T) \\
\Theta_{s/\ell}\Pi_+ \bar{\psi}(x, T)\Pi_- &= \bar{\psi}(x, 0)\Pi_+\gamma_0 \\
\Theta_{s/\ell}\Pi_- \bar{\psi}(x, T)\Pi_- &= \gamma_0\Pi_-\bar{\psi}(x, 0)
\end{align*}
$$

4 Lattice artifacts

Our aim in this section is to analyze the lattice artifacts affecting the (on-shell) expectation value

$$
\langle O \rangle_T = \int \mathcal{D}\mu_G[U] \int \mathcal{D}\mu_F[\bar{\psi}, \psi] O(\psi, \bar{\psi}, U) e^{-S_{YM} - S_F},
$$

(4.1)

where $O$ is a m.r. (multi-local) operator.

The analysis will be based on the assumption that the approach to the continuum limit of the Schrödinger functional defined in eq. (2.10) can be described by a local effective theory. The latter will be characterized a local effective Lagrangian (LEL) including bulk and boundary terms [25]. In determining the operators contributing to the Symanzik description of the lattice expectation value (4.1) a key role will be naturally played by the symmetries collected in sect. 3. Let us now go through the list of the allowed operators in the order of increasing dimension.

- The basic observation is that no dimension 3 operators can be generated through radiative corrections in the boundary LEL, because operators of the
form $\bar{\psi}\Gamma(\mathbb{1}/\tau_b)\psi$ (with $\Gamma$ any of the 16 independent Dirac matrix and with or without the insertion of an iso-spin matrix) are all forbidden by some of the symmetries above.

- At dimension 4 there is a number of contributions to the boundary LEL. Besides the terms corresponding to the continuum (infinite volume) QCD action, there will be $O(a)$ boundary terms of the form (see eqs. (2.7) and (2.8))

$$\int d\mathbf{x} \bar{\psi}(x,0)\Pi_+ \gamma_k D_k \psi(x,0), \quad \int d\mathbf{x} \bar{\psi}(x,T)\Pi_- \gamma_k D_k \psi(x,T).$$

(4.2)

The temporal analogs of these terms can be ignored in the present analysis, as they can always be traded for the previous ones using the field equations of motion. Because of the symmetry $R_5 \times (r \rightarrow -r)$ the operators (1.2) being even under $R_5$ will intervene multiplied by coefficients that will be even functions of $r$.

There will also be the $O(a)$ pure gauge boundary terms

$$\int d\mathbf{x} \text{tr}(F_{0k} F_{0k})(x,0), \quad \int d\mathbf{x} \text{tr}(F_{jk} F_{jk})(x,0),$$

$$\int d\mathbf{x} \text{tr}(F_{0k} F_{0k})(x,T), \quad \int d\mathbf{x} \text{tr}(F_{jk} F_{jk})(x,T).$$

(4.3)

always with coefficients even in $r$, while the $\bar{F}F$ term is excluded by $CP$.

Notice that, if in the multi-local operator, $O$, there are boundary local factors, i.e. factors, $O_B$, which in the continuum limit are kept at vanishing distance from the boundaries, there may be (if not excluded by the symmetries listed in sect. 3) $O(a)$ terms coming from the collision of $O_B$ with the spatially integrated boundary terms of eqs. (4.2) and (4.3) above.

- At dimension 5 there are $O(a)$ effects in the expectation value $\langle O \rangle_T$ that in the Symanzik language are described by the insertion, together with $O$, of the integrated (dimension 5 and parity even) bulk LEL density $L_5$. Besides these terms there will also appear bulk contact terms, coming from the collision under integration of $L_5$ with the various local bulk factors of $O$. In opposition with the previously mentioned local boundary factors, local bulk factors are (products of local) operators that in the continuum limit are kept at finite distance in physical units from the boundaries.

Because of the symmetries $R_5 \times (r \rightarrow -r)$ and $R_5 \times D_d \times P \times T$, all such $O(a)$ bulk contributions will appear with coefficients odd in $r$. This conclusion follows also here thanks to the fact that in the continuum LEL parity is only broken by boundary terms which are not relevant for bulk operators, while the bulk LEL density $L_5$ is still even under parity and $T$ and consequently odd under $R_5$. Thus just like in the infinite volume formulation,
all O(a) bulk contributions in the Symanzik expansion will cancel out if the expectation value of O computed with r is averaged with its expectation value computed with −r, i.e. in the quantity

$$\langle O \rangle_{T} \bigg|_{WA} = \frac{1}{2} \left[ \langle O \rangle_{T}(r) + \langle O \rangle_{T}(-r) \right].$$  \hspace{1cm} (4.4)

Notice that in order to compute $$\langle O \rangle_{T} \bigg|_{WA}$$ it is not necessary to perform two independent simulations with opposite value of r. It is enough to notice the relation

$$\langle O \rangle_{T}(-r) = (-1)^{P_{5}[O]} \langle O \rangle_{T}(r),$$  \hspace{1cm} (4.5)

where $$P_{5}[O]$$ is the parity of O under the transformation $$R_{5}$$. Introducing eq. (4.5) in (4.4), we conclude that for $$R_{5}$$-even operators O(a) bulk terms are actually absent in the chiral limit and this is why only one simulation is needed to get O(a) bulk improvement. If instead O is an $$R_{5}$$-odd operator, an identically vanishing result is obtained from the WA. In the absence of spontaneous symmetry breaking phenomena affecting the expectation value of O, this is indeed the result we would like to get in the continuum. In fact $$\langle O \rangle_{T}(r)$$ is itself an O(a) quantity.

### 4.1 Boundary operators and O(a) artifacts: an example

As an example, we briefly discuss a possible setting for the non-perturbative computation of the renormalization constant, $$Z_{P}$$, of the pseudoscalar density operator, $$\bar{\psi} \gamma_{5} \tau_{b} \psi$$, where $$b = 1, 2, 3$$ is an isospin index. The knowledge of $$Z_{P}$$ is relevant, for instance, for the study of the running of the quark mass [23].

To extract $$Z_{P}$$ from simulation data it is sufficient to compute the following lattice expectation values (for definiteness we set the isospin index b equal to 1)

$$\langle (\bar{\psi} \gamma_{5} \tau_{1} \psi)(0, T/2) \Phi_{P1S2}^{i} \rangle_{T} \quad \text{and} \quad \langle \Phi_{P1S2}^{f} \Phi_{P1S2}^{i} \rangle_{T},$$  \hspace{1cm} (4.6)

where $$\Phi_{P1S2}^{i}$$ and $$\Phi_{P1S2}^{f}$$ are zero three-momentum operators sitting at the initial ($$x_0 = 0$$) and final ($$x_0 = T$$) times, respectively, given by

$$\Phi_{P1S2}^{i} = a^{3} \sum_{x} \bar{\psi}(x, 0) \Pi_{-} \frac{1}{2} (\gamma_{5} \tau_{1} + i \tau_{2}) \Pi_{-} \psi(x, 0),$$

$$\Phi_{P1S2}^{f} = a^{3} \sum_{x} \bar{\psi}(x, T) \Pi_{-} \frac{1}{2} (\gamma_{5} \tau_{1} - i \tau_{2}) \Pi_{+} \psi(x, T).$$  \hspace{1cm} (4.7)

Notice that $$\Phi_{P1S2}^{i}$$ and $$\Phi_{P1S2}^{f}$$ are defined in terms of the dynamical boundary quark components only. The presence of the projectors $$\Pi_{\pm}$$ implies that the
Dirac-flavour structure necessarily appears in the combinations \( (\gamma_5\tau_1 + i\tau_2) \) and \( (\gamma_5\tau_1 - i\tau_2) \) at \( x_0 = 0 \) and \( x_0 = T \), respectively.

An analysis of the dimension three and four boundary operators compatible with the symmetries listed in sect. 3 shows that the fields renormalize multiplicatively and, once summed over their spatial argument, are free from \( O(a) \) corrections.

Putting this result together with that on the \( O(a) \) bulk improvement reached in sect. 4, one arrives at the conclusion that the calculation of \( Z_P \) carried out with the Schrödinger functional formalism developed in this paper is free from \( O(a) \) discretization errors, except of course for those coming from the boundary gauge link operators in the first column of eq. (4.3), which survive even at vanishing values of the boundary gauge links.

Although the Schrödinger functional setup proposed in this paper allows more freedom (than apparent from the above example) in building fermionic boundary operators \(^3\), the important point we would like to make here is that in several cases it may be possible to choose the boundary operators in \( O \) (those denoted above as \( O_B \)) in such a way that \( \langle O \rangle_T \) is free from \( O(a) \) cutoff effects, once the lattice action has been supplemented with boundary counterterms.

5 Fermion determinant

In this section we want to show that, associated with the fermionic integration defined in eq. (2.10), there is a real and positive determinant. This feature is necessary for the proper interpretation of the fermionic contribution to the functional integral as a well defined weight for the successive gauge integration and the viability of simulations. It is precisely the need to fulfill this requirement that has led us to introduce a flavour doublet of fermions endowed with opposite chirality boundary conditions.

The situation for the fermion integration is very similar to the one discussed in sect. 6 of ref. \(^{22}\). Calling \( u \) and \( d \) the two flavour components of \( \psi \), we can define the two pre-Hilbert spaces \( \mathcal{H}_u \) and \( \mathcal{H}_d \) as the spaces of spinors satisfying the conditions dictated by the eqs. (2.3), namely

\[
\mathcal{H}_u = \{ u \mid (1 + \gamma_5)u(x,0) = 0, (1 - \gamma_5)u(x,T) = 0 \}, \quad \mathcal{H}_d = \{ d \mid (1 - \gamma_5)d(x,0) = 0, (1 + \gamma_5)d(x,T) = 0 \}.
\] (5.1)

With this splitting the action (2.5) can be rewritten in terms of the operator

\[
\mathcal{D} = \begin{pmatrix} 0 & D_u \\ D_d & 0 \end{pmatrix}
\] (5.3)

\(^3\)This interesting matter is left for a future study.
through the formula

\[ S_F = \left( \bar{u} \bar{d} \right) \begin{pmatrix} 0 & D_u \\ D_d & 0 \end{pmatrix} \left( \begin{array}{c} d \\ u \end{array} \right) = \bar{u}D_u u + \bar{d}D_d d. \] (5.4)

One notices that the operator \( D \) admits a well defined eigenvalue problem in the Hilbert space \( \mathcal{H}_u \oplus \mathcal{H}_d \), with the functional integration over the fermionic variables \( u \) and \( d \) giving as a result precisely the determinant of \( D \).

Furthermore we observe that for the purpose of computing the fermionic functional integral in (2.10) we can replace the operator (5.3) with\[ \tilde{D} = \begin{pmatrix} 0 & D_u \\ \gamma_5D_d\gamma_5 & 0 \end{pmatrix}. \] (5.5)

This replacement only amounts to the harmless change of integration variables

\[ d \to \gamma_5d \quad \bar{d} \to \bar{d}\gamma_5. \] (5.6)

The reason for doing so is that in this way one gets an operator, \( \tilde{D} \), which is self-adjoint since\[ \gamma_5D_d\gamma_5 = D_u^\dagger, \] (5.7)
as one can explicitly check with some algebra. Consequently the determinant of \( \tilde{D} \) will be a real number. Actually this number, hence the determinant of \( D \), is also positive.

To prove this statement it is convenient to consider the auxiliary operator\[ \mathcal{M} = \begin{pmatrix} 0 & \Gamma_0 \\ \Gamma_0 & 0 \end{pmatrix} \begin{pmatrix} 0 & D_u \\ D_u^\dagger & 0 \end{pmatrix} = \begin{pmatrix} \Gamma_0D_u^\dagger & 0 \\ 0 & \Gamma_0D_u \end{pmatrix}, \] (5.8)
where \( \Gamma_0 \) is a block diagonal matrix in the time direction with the following structure. All along the diagonal there are \( N_T - 1 \) copies (recall \( T = N_T a \)) of the \( 4 \times 4 \) usual \( \gamma_0 \) Dirac-matrix, except in the upper-left and the lower-right corners where there is a \( 2 \times 2 \) unit matrix. One checks that \( \mathcal{M} \) maps \( \mathcal{H} \) into itself, because

\[ \Gamma_0D_u : \mathcal{H}_u \to \mathcal{H}_u, \]
\[ \Gamma_0D_u^\dagger : \mathcal{H}_d \to \mathcal{H}_d. \] (5.9)

Positivity of \( \det[D] \) then follows from the chain of equalities

\[ \det[D] = \det[\tilde{D}] = \det[\mathcal{M}] = \det[D_u^\dagger\Gamma_0] \det[\Gamma_0D_u] = |\det[\Gamma_0D_u]|^2, \] (5.10)
in which we have used the observation that the determinant of the off-diagonal matrix where \( \Gamma_0 \) intervene in eq. (5.8) is equal to 1.

\(^4\)Not to obscure the argument we have suppressed space-time indices.
6 Conclusions

We have shown in this paper that it is possible to modify the usual definition of the Schrödinger functional in a way that allows to compute expectation values of $\mathcal{R}_5$-even (multi-local) operators having $O(a)$ cutoff effects only coming from the boundaries. Assuming that the latter are under control, either because they are just absent, owing to symmetry reasons, or because known to some order in perturbation theory, this approach provides a viable scheme for the improved computation of the renormalization constants of fermionic operators and the running of QCD parameters.

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