

# The Schrödinger functional in lattice QCD with exact chiral symmetry

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**ABSTRACT:** Similarly to the interaction lagrangian, the possible boundary conditions in quantum field theories on space-time manifolds with boundaries are strongly constrained by the symmetry and scaling properties of the theory. Based on this general insight, a lattice formulation of the QCD Schrödinger functional is proposed for the case where the lattice Dirac operator in the bulk of the lattice coincides with the Neuberger–Dirac operator. The construction satisfies all basic requirements (locality, symmetries, hermiticity) and is suitable for numerical simulations.

**KEYWORDS:** Lattice QCD, Lattice Gauge Field Theories.

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## 1. Introduction

In numerical lattice QCD, the Schrödinger functional mainly serves as a probe in scaling studies of the theory close to the continuum limit [1, 2]. The non-perturbative computation of renormalization factors, for example, is an important case where the Schrödinger functional proved to be very useful (see ref. [3] for an introduction).

In the continuum limit the Schrödinger functional is obtained by restricting the time coordinate  $x_0$  to a finite range,  $0 \leq x_0 \leq T$ , and by imposing Dirichlet boundary conditions on the fields at  $x_0 = 0$  and  $x_0 = T$ . The boundary conditions break chiral symmetry, but the chiral Ward identities remain valid away from the boundaries and thus forbid the mixing of operator insertions belonging to different chiral multiplets, for example, as is the case in the absence of the boundaries.

The symmetry properties of the Schrödinger functional in lattice QCD should ideally be the same if the chosen lattice Dirac operator preserves chiral symmetry on the infinite lattice via the Ginsparg–Wilson relation [4]–[8]. However, in the presence of the boundaries, the Dirac operator and the Ginsparg–Wilson relation must both be modified. Chiral symmetry would otherwise not be broken and the lattice Schrödinger functional could not possibly have the correct continuum limit. The modifications must evidently be local and be linked to the boundary conditions, but without further insight it is difficult to say how to proceed from here.

A theoretically attractive possibility, recently studied by Taniguchi [9], is to define the Schrödinger functional through an orbifold projection. The boundary conditions are determined by the  $\mathbb{Z}_2$  orbifold symmetry in this case, which is taken to be the product of a time reflection and a chiral rotation. As it turns out, however, the latter leads to some technical difficulties on the lattice and one ends up with a lattice Dirac operator whose determinant has a non-trivial phase. Moreover, the construction becomes rather artificial when the masses of the quarks do not vanish.<sup>1</sup>

To a large extent, the solution proposed in this paper is based on universality considerations. Stated somewhat superficially, the idea is that Schrödinger functional boundary conditions do not require any fine-tuning and will thus be satisfied automatically in the continuum limit, as long as the lattice theory in the presence of the boundaries respects locality and the obvious lattice symmetries. The problem then reduces to finding a lattice Dirac operator that has these properties and additionally satisfies the Ginsparg–Wilson relation away from the lattice boundaries.

Starting from the Neuberger–Dirac operator in infinite volume [7], such operators are not too difficult to construct. It may be useful, however, to first recall some basic facts on the quark sector of the Schrödinger functional (section 2) and to address the issue of universality in some detail (section 3). In section 4, Ginsparg–Wilson fermions in one dimension are briefly discussed and it is then only a small step to write down an acceptable lattice Dirac operator in four dimensions (section 5).

## 2. Quark fields and Dirac operator in the continuum theory

In the following, it will be assumed that the reader is familiar with the Schrödinger functional in QCD [1, 2]. Most of the time the SU(3) gauge field will play a spectator rôle

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<sup>1</sup>All these problems disappear if chirally rotated boundary conditions are adopted, as suggested by Sint [10]. The goal here, however, is to define the Schrödinger functional with the standard parity-conserving boundary conditions [2].

and its presence can be largely ignored. In this section some properties of the quark sector in the continuum theory are highlighted. This serves partly to introduce the subject and partly to guide the construction of the lattice theory in the later sections.

## 2.1 Boundary conditions

It suffices to consider a single quark with mass  $m$ , since all formulae and comments trivially extend to the case of several quarks with arbitrary masses. The quark and antiquark fields  $\psi(x)$  and  $\bar{\psi}(x)$  are defined at all times  $x_0 \in [0, T]$  and are required to satisfy<sup>2</sup>

$$P_+\psi(x) = \bar{\psi}(x)P_- = 0 \quad \text{at } x_0 = 0, \tag{2.1}$$

$$P_-\psi(x) = \bar{\psi}(x)P_+ = 0 \quad \text{at } x_0 = T, \tag{2.2}$$

where  $P_{\pm} = \frac{1}{2}(1 \pm \gamma_0)$ . These boundary conditions are invariant under space rotations, parity, time reflections ( $x_0 \rightarrow T - x_0$ ) and charge conjugation.

The quark action in the presence of a gauge field  $A_{\mu}(x)$  is then given by

$$S_F = \int_0^T dx_0 \int d^3\mathbf{x} \bar{\psi}(x) D_m \psi(x), \tag{2.3}$$

$$D_m = \gamma_{\mu} D_{\mu} + m, \quad D_{\mu} = \partial_{\mu} + A_{\mu}. \tag{2.4}$$

Usually the Schrödinger functional is set up with inhomogeneous boundary conditions, where the boundary values serve as sources for the quark field at  $x_0 = 0$  and  $x_0 = T$  [2]. One may, however, just as well adopt homogeneous boundary conditions, as is done here, and introduce the boundary quark fields directly through

$$\zeta(\mathbf{x}) = P_-\psi(x), \quad \bar{\zeta}(\mathbf{x}) = \bar{\psi}(x)P_+ \quad \text{at } x_0 = 0, \tag{2.5}$$

$$\zeta'(\mathbf{x}) = P_+\psi(x), \quad \bar{\zeta}'(\mathbf{x}) = \bar{\psi}(x)P_- \quad \text{at } x_0 = T. \tag{2.6}$$

These are just the non-zero Dirac components of the quark fields at the boundaries.

## 2.2 Spectrum of the Dirac operator

Let  $\mathcal{H}$  be the linear space of all smooth quark fields that satisfy the required boundary conditions. With respect to the natural scalar product in this space,

$$(\psi, \chi) = \int_0^T dx_0 \int d^3\mathbf{x} \psi(x)^{\dagger} \chi(x), \tag{2.7}$$

the operator  $Q_m = \gamma_5 D_m$  is easily shown to be hermitian. Since  $Q_m$  is also elliptic, it follows that this operator has a complete orthonormal set of eigenfunctions  $v_n \in \mathcal{H}$ , labelled by an index  $n = 0, 1, 2, \dots$ , with real eigenvalues  $\lambda_n$ .

For non-negative quark masses  $m$ , the eigenvalues are bounded from below by

$$\lambda_n^2 \geq m^2 + \mu^2, \tag{2.8}$$

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<sup>2</sup>The notation is the one commonly used in lattice QCD. In particular, the space-time metric is euclidean and the Dirac matrices  $\gamma_{\mu}$ ,  $\mu = 0, \dots, 3$ , are taken to be hermitian. The fifth Dirac matrix,  $\gamma_5 = \gamma_0 \gamma_1 \gamma_2 \gamma_3$ , is then also hermitian. Where appropriate, the Einstein summation convention is applied.

where  $\mu$  denotes the spectral gap at  $m = 0$ . This is a straightforward consequence of the identity

$$\lambda_n^2 = \|Q_m v_n\|^2 = m^2 \|v_n\|^2 + \|Q_m|_{m=0} v_n\|^2 + m \int_{x_0=0} d^3\mathbf{x} v_n(x)^\dagger v_n(x) + m \int_{x_0=T} d^3\mathbf{x} v_n(x)^\dagger v_n(x). \quad (2.9)$$

Moreover, using the fact that the current  $v_n(x)^\dagger \gamma_\mu v_n(x)$  is conserved at  $m = \lambda_n = 0$ , it is possible to show that the massless Dirac operator has no zero modes.

Note that the bound (2.8) becomes invalid at  $m < 0$ . The Dirac operator has eigenmodes localized at the boundaries in this case, with eigenvalues that decrease exponentially at large  $|m|T$ . These are just the well-known domain wall fermion modes. The fact that the sign of the quark mass matters is a consequence of the breaking of chiral symmetry through the boundary conditions. This is also why the eigenvalues at non-zero quark masses are not simply related to those at vanishing mass.

### 2.3 Determinant of the Dirac operator

Since there are positive and negative eigenvalues  $\lambda_n$ , the determinant,  $\det Q_m$ , may have a non-trivial phase. However, this is not the case if the standard lattice regularization is employed [2]. Other regularizations may give different results, but the universality of the continuum limit implies that the determinant must always be real after removal of the ultraviolet cutoff, up to some local terms perhaps. These can always be “renormalized away”, and the requirement of a real determinant then becomes part of the definition of the theory.

At non-negative quark masses, the quark determinant actually has a definite sign in this case, because the eigenvalues of  $Q_m$  never pass through zero. In the functional integral, the quark determinant may thus be replaced by its absolute value.

### 2.4 Chiral symmetry properties of the quark propagator at $m = 0$

As a differential operator, the massless Dirac operator anticommutes with  $\gamma_5$  and the local chiral Ward identities are thus not affected by the presence of the boundaries. The quark propagator  $S(x, y)$ , on the other hand, transforms according to

$$\gamma_5 S(x, y) + S(x, y) \gamma_5 = \int_{z_0=0} d^3\mathbf{z} S(x, z) \gamma_5 S(z, y) + \int_{z_0=T} d^3\mathbf{z} S(x, z) \gamma_5 S(z, y). \quad (2.10)$$

This equation is easily established by noting that, as a function of  $x$ , the expression on the left solves the homogenous Dirac equation. The other side of the equation is then obtained by reconstructing the solution from its boundary values at  $x_0 = 0$  and  $x_0 = T$ .

In QCD with more than one massless quark, eq. (2.10) implies the non-singlet chiral Ward identity

$$\begin{aligned} & \langle \lambda^a \gamma_5 \psi(x) \bar{\psi}(y) + \psi(x) \bar{\psi}(y) \lambda^a \gamma_5 \rangle_F \\ &= \int d^3\mathbf{z} \langle \psi(x) \bar{\psi}(y) \{ \bar{\zeta}(\mathbf{z}) \lambda^a \gamma_5 \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \lambda^a \gamma_5 \zeta'(\mathbf{z}) \} \rangle_F, \end{aligned} \quad (2.11)$$

where  $\lambda^a$  is any traceless matrix in flavour space and  $\langle \dots \rangle_F$  denotes the expectation value in the quark sector. The breaking of chiral symmetry through the boundary conditions is made explicit by this formula. Purely from the symmetry point of view, it actually looks as if there were a unit mass term at the boundaries.

### 3. Field theories on lattices with boundaries

In continuum field theories, the notion of smoothness plays a central rôle. Differential operators can only act on smooth functions, for example, and boundary conditions really only make sense when imposed on such functions.

The situation in lattice field theory is quite different. Strictly speaking, boundary conditions are no longer imposed on the fields but instead are encoded in the lattice action. As usual different lattice theories may have the same continuum limit, where now the characterization of the latter must include a specification of the boundary conditions. An important point to note is that the possible boundary conditions are strongly constrained by the requirement of locality, the lattice symmetries and by power-counting arguments. There are then not many more universality classes than there are in the absence of boundaries.

The aim in this section is to make these remarks a bit more concrete, so that they can be applied to the Schrödinger functional in QCD. Eventually, the argumentation is based on Symanzik's work on the renormalization of quantum field theories in the presence of boundaries [11] and also on the theory of boundary critical phenomena in statistical mechanics (see ref. [12] for a review).

#### 3.1 Boundary conditions and the field equations

The concepts that will be developed in the following are best introduced by considering a free scalar field in the half-space  $x_0 \geq 0$  with various boundary conditions at  $x_0 = 0$ . A simple lattice formulation of this theory is obtained by choosing the lattice field  $\phi(x)$  to reside on the sites of a hypercubic lattice with spacing  $a$ . The expression

$$S = a^4 \sum_{x_0 \geq a} \sum_{\mathbf{x}} \frac{1}{2} \{ \partial_\mu \phi(x) \partial_\mu \phi(x) + m^2 \phi(x)^2 \} \tag{3.1}$$

is then a possible choice of the lattice action, where  $\partial_\mu$  denotes the forward nearest-neighbour difference operator in direction  $\mu$  and the mass  $m$  is assumed to be positive. Note that the action depends on the field variables at time  $x_0 = a, 2a, 3a, \dots$  only. These are thus the unconstrained dynamical degrees of freedom of the field which are to be integrated over in the functional integral.

Starting from the action (3.1), the propagator  $\langle \phi(x) \phi(y) \rangle$  can easily be worked out in a time-momentum representation. It then turns out that the propagator satisfies Neumann boundary conditions in the continuum limit. On the other hand, after a slight modification of the action by a boundary term,

$$S \rightarrow S + a^3 \sum_{\mathbf{x}} \frac{c}{2a} \phi(x)^2 \Big|_{x_0=a} , \tag{3.2}$$

the calculation yields a propagator that satisfies Dirichlet boundary conditions in the continuum limit, for any fixed  $c > 0$  (the powers of  $a$  are such that  $c$  is dimensionless).

Some understanding of how a particular boundary condition arises can be achieved by considering the field equation

$$\langle \eta(x)\phi(y) \rangle = a^{-4}\delta_{xy}, \quad \eta(x) = \frac{\delta S}{\delta \phi(x)}. \quad (3.3)$$

A short calculation yields

$$\eta(x) = \{-\partial_\mu^* \partial_\mu + m^2\} \phi(x) \quad \text{at} \quad x_0 > a, \quad (3.4)$$

where  $\partial_\mu^*$  denotes the backward nearest-neighbour difference operator. In the bulk of the lattice, the field equation thus coincides with the lattice Klein–Gordon equation. At  $x_0 = a$ , however, a different equation is obtained,

$$\eta(x) = \frac{c}{a^2} \phi(x) - \frac{1}{a} \partial_0 \phi(x) + \{-\partial_k^* \partial_k + m^2\} \phi(x), \quad (3.5)$$

which depends on the details of the action close to the boundary. Formally, the first term in this expression dominates in the continuum limit and the field equation at the boundary thus implies Dirichlet boundary conditions at  $a = 0$  if  $c > 0$ . On the other hand, the second term dominates if  $c = 0$ , which leads to Neumann boundary conditions in the continuum limit.

### 3.2 Natural boundary conditions

The example considered in the previous subsection illustrates the fact that boundary conditions are a property of the continuum theory which arises dynamically in the continuum limit. In particular, they are not determined by the space of lattice fields alone. Another outcome is that some boundary conditions are obtained generically, while others (Neumann and mixed boundary conditions in the study case) are unstable under perturbations of the lattice action.

In an interacting theory, and also in free theories with complicated lattice actions, the connection between the lattice field equations and the boundary conditions in the continuum limit may not be as transparent as suggested above. It seems plausible, however, that the boundary conditions are always of the form  $\mathcal{O}(x)|_{x_0=0} = 0$ , where  $\mathcal{O}(x)$  is a linear combination of local fields with the appropriate number of components and symmetry properties.

The boundary conditions that are stable under perturbations of the lattice theory, and which thus arise naturally, then correspond to the fields with the lowest possible dimension. Some tuning of the lattice theory will normally be required in all other cases, unless there are some symmetries that protect  $\mathcal{O}(x)$  from mixing with lower dimensional fields.

### 3.3 Are Schrödinger functional boundary conditions natural?

Following Wilson [13], the quark fields are represented on the lattice by Dirac spinors  $\psi(x)$  that reside on the points  $x$  of the lattice. Since QCD is asymptotically free, the scaling dimension of the local fields in this theory coincides with their engineering dimension (up to

logarithms). In particular, the fields of lowest dimension that carry the quantum numbers of the quark fields are the quark fields themselves.

The boundary conditions at  $x_0 = 0$ , which arise naturally in the continuum limit, are thus of the form  $B\psi(x)|_{x_0=0} = 0$ , where  $B$  is a constant matrix in Dirac and colour space. At  $x_0 = T$  the boundary conditions are linked to those at  $x_0 = 0$  by the time reflection symmetry and charge conjugation then determines the boundary conditions for the antiquark field.

If the lattice theory is invariant under gauge transformations, cubic rotations and parity, as will be the case in the following, the boundary conditions must respect these symmetries.<sup>3</sup> Moreover,  $B$  cannot have maximal rank, as otherwise the boundary conditions and the Dirac equation at  $0 < x_0 < T$  would imply a vanishing quark propagator. Up to a normalization constant, the only matrices that are compatible with all these conditions then are  $B = P_+$  and  $B = P_-$ .

Schrödinger functional boundary conditions thus arise naturally and do not require any particular adjustments of the lattice action. There are two classes of lattice theories, which are distinguished by the sign in the boundary condition  $P_{\pm}\psi(x)|_{x_0=0} = 0$ . The difference matters if the quark mass does not vanish, but the sign may easily be determined, in any given case, by studying the free-quark propagator for example.

#### 4. Ginsparg–Wilson quarks in one dimension

In the presence of the boundaries, an acceptable lattice Dirac operator that satisfies the Ginsparg–Wilson relation in the bulk of the lattice still needs to be found. The Wilson–Dirac operator provides a simple solution to this problem in one dimension. This is a somewhat trivial case, but it gives important hints for the construction of the Dirac operator in higher dimensions.

##### 4.1 Lattice Dirac operator

For simplicity the gauge field is omitted in this section. The Wilson–Dirac operator in one dimension then reads

$$D = \frac{1}{2} \{ \gamma_0(\partial_0^* + \partial_0) - a\partial_0^*\partial_0 \} = P_+\partial_0^* - P_-\partial_0. \tag{4.1}$$

In the absence of boundaries, this operator satisfies the Ginsparg–Wilson relation

$$\gamma_5 D + D \gamma_5 = a D \gamma_5 D. \tag{4.2}$$

Moreover, from the definition (4.1) it is immediate that  $\gamma_5 D$  is hermitian and that the quark propagator is given by

$$S(x_0, y_0) = \theta(x_0 \geq y_0) P_+ + \theta(x_0 \leq y_0) P_-, \tag{4.3}$$

where  $\theta(*)$  is equal to 1 if the logical condition in brackets is true and 0 otherwise.

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<sup>3</sup>Gauge transformations include the gauge field variables at the boundaries and are thus a spurious symmetry to some extent. In the present context, this is of no importance, however, since  $B$  does not depend on the gauge field.



Following the standard treatment [2], the dynamical degrees of freedom of the quark fields in the presence of the boundaries at  $x_0 = 0$  and  $x_0 = T$  are taken to be their components at  $x_0 = a, 2a, \dots, T - a$ . It is convenient to assume that the fields are defined at all other times as well, but that they are equal to zero there.

The Dirac operator in the presence of the boundaries (which is also denoted by  $D$ ) maps this space of quark fields into itself. At  $x_0 = a, 2a, \dots, T - a$ , its action is given by eq. (4.1), while at  $x_0 \leq 0$  and  $x_0 \geq T$  the target field is set to zero. With respect to the scalar product

$$(\psi, \chi) = a \sum_{x_0=a}^{T-a} \psi(x_0)^\dagger \chi(x_0), \tag{4.4}$$

the operator  $\gamma_5 D$  is then again hermitian. It is also easy to show that  $D$  has no zero modes and that the associated propagator coincides with the propagator (4.3) on the infinite lattice, at all times in the range  $0 < x_0, y_0 < T$ . In particular, the correct Schrödinger functional boundary conditions are obtained in the continuum limit.

#### 4.2 Modified Ginsparg–Wilson relation

As already pointed out in section 1, the lattice Dirac operator is not expected to satisfy the Ginsparg–Wilson relation in the presence of the boundaries, for general reasons. On the finite lattice, the operator  $D$  introduced above in fact satisfies the modified relation

$$\gamma_5 D + D \gamma_5 = a D \gamma_5 D + \gamma_5 P, \tag{4.5}$$

where  $P$  is a local operator given by

$$P\psi(x_0) = \frac{1}{a} \{ \delta_{x_0 a} P_- \psi(a) + \delta_{x_0 T-a} P_+ \psi(T - a) \}. \tag{4.6}$$

Equation (4.5) is a straightforward consequence of the precise definition of  $D$  in the presence of the boundaries. In particular, the boundary term  $\gamma_5 P$  is obtained when the product  $D \gamma_5 D$  is worked out at  $x_0 = a$  and  $x_0 = T - a$ .

By multiplication of the modified Ginsparg–Wilson relation (4.5) from both sides with the quark propagator, it follows that

$$\begin{aligned} \gamma_5 S(x_0, y_0) + S(x_0, y_0) \gamma_5 &= \gamma_5 \delta_{x_0 y_0} + \\ &S(x_0, a) \gamma_5 P_- S(a, y_0) + S(x_0, T - a) \gamma_5 P_+ S(T - a, y_0). \end{aligned} \tag{4.7}$$

In the continuum limit, the projectors  $P_\pm$  on the right-hand side of this equation can be dropped in view of the boundary conditions satisfied by the propagator. The relation then reduces to the one-dimensional form of the chiral Ward identity (2.10). This shows that the presence of the boundary term in the modified Ginsparg–Wilson relation (4.5) is directly linked to the breaking of chiral symmetry in the continuum theory by the boundary conditions.

## 5. Lattice Dirac operator in four dimensions

Since Schrödinger functional boundary conditions arise naturally, the choice of the lattice Dirac operator is not critical and there are probably many viable constructions. The operator proposed here is a simple modification of the Neuberger–Dirac operator in infinite volume.

### 5.1 Definition

As before the theory is first set up on the infinite lattice. The quark fields are thus assumed to be defined at all sites of the lattice. Although the gauge field continues to play a spectator rôle, it is now included in the formulae. The Wilson–Dirac operator is then given by [13]

$$D_w = \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - a \nabla_\mu^* \nabla_\mu \}, \quad (5.1)$$

where  $\nabla_\mu$  and  $\nabla_\mu^*$  denote the gauge-covariant forward and backward difference operators. As already mentioned, the starting point in this section is the Neuberger–Dirac operator [7]

$$D = \frac{1}{\bar{a}} \left\{ 1 - A \left( A^\dagger A \right)^{-1/2} \right\}, \quad (5.2)$$

$$A = 1 + s - a D_w, \quad \bar{a} = \frac{a}{1 + s}. \quad (5.3)$$

The parameter  $s$  in this formula allows for some optimization and is only relevant in the context of numerical simulations. In practice, it is normally set to a fixed value in the range  $0 \leq s \leq 1/2$ .

In the presence of the boundaries at  $x_0 = 0$  and  $x_0 = T$ , the dynamical degrees of freedom of the quark fields reside on the lattice sites at time  $x_0 = a, 2a, \dots, T - a$ . It is again convenient to assume that the fields are defined at all other points as well and that they are equal to zero there. The Wilson–Dirac operator may be considered to be a linear operator in this space of fields, whose action at  $0 < x_0 < T$  is given by eq. (5.1) (elsewhere the target field is set to zero). This is the lattice Dirac operator that was introduced by Sint [2].

The structure of eq. (5.2) is such that  $D$  satisfies the Ginsparg–Wilson relation (4.2) automatically (with  $a$  replaced by  $\bar{a}$ ) if  $\gamma_5 A$  is hermitian. In the presence of the boundaries, the Dirac operator must therefore be given by a different expression. A formula that works out is

$$D = \frac{1}{\bar{a}} \left\{ 1 - \frac{1}{2} (U + U^\sim) \right\}, \quad (5.4)$$

$$U = A \left( A^\dagger A + caP \right)^{-1/2}, \quad U^\sim = \gamma_5 U^\dagger \gamma_5, \quad (5.5)$$

where  $c \geq 1$  is another tuneable parameter, whose optimal value will turn out to be close to  $1 + s$ . In eq. (5.5), the boundary operator

$$P\psi(x) = \frac{1}{a} \{ \delta_{x_0 a} P_- \psi(x)|_{x_0=a} + \delta_{x_0 T-a} P_+ \psi(x)|_{x_0=T-a} \} \quad (5.6)$$

is the four-dimensional version of the operator  $P$  previously encountered, while  $A$  is again given by eq. (5.3), where  $D_w$  is now the Wilson–Dirac operator in the presence of the boundaries.

The merits of the definition (5.4),(5.5) will be discussed in detail, but before this it may be helpful to note that the operator  $D$  reduces to the Wilson–Dirac operator in the one-dimensional theory if  $s = 0$  and  $c = 1$ . The results reported in section 4 actually imply that  $A^\dagger A + caP = 1$  in this case.

## 5.2 Lattice symmetries, hermiticity and spectral bounds

It is not difficult to check that the Dirac operator  $D$  transforms like the Wilson–Dirac operator under cubic rotations, parity, time-reflections and charge conjugation. The latter interchanges  $U$  with  $U^\sim$ , and having the sum of these two operators in eq. (5.4) also ensures that  $\gamma_5 D$  is hermitian.

Another implication of the form (5.5) is the bound

$$\|U\| = \|U^\sim\| \leq 1. \tag{5.7}$$

To show this, it suffices to note that

$$\|U\psi\|^2 = \left(\chi, A^\dagger A \chi\right) \leq \left(\chi, (A^\dagger A + caP)\chi\right) = \|\psi\|^2, \tag{5.8}$$

for any quark field  $\psi$ , where  $\chi = (A^\dagger A + caP)^{-1/2}\psi$ . The spectrum of  $\bar{a}D$  is thus contained in the unit disk in the complex plane centred at 1. However, one should not expect the spectrum to be on the unit circle, as is the case for Dirac operators satisfying the Ginsparg–Wilson relation.

In the present framework, the natural choice of the massive Dirac operator is [14]

$$D_m = \left(1 - \frac{1}{2}\bar{a}m\right)D + m. \tag{5.9}$$

When the bare quark mass  $m$  is in the range  $0 \leq m \leq 2/\bar{a}$ , as will be assumed in the following, the spectrum of this operator is separated from the origin by a distance of at least  $m$ . The middle term in the expansion

$$(\gamma_5 D_m)^2 = m^2 + m\left(1 - \frac{1}{2}\bar{a}m\right)(D^\dagger + D) + \left(1 - \frac{1}{2}\bar{a}m\right)^2 (\gamma_5 D)^2 \tag{5.10}$$

is in fact non-negative and the eigenvalues  $\lambda_n$  of  $\gamma_5 D_m$  are therefore bounded by

$$\lambda_n^2 \geq m^2 + \left(1 - \frac{1}{2}\bar{a}m\right)^2 \mu^2, \tag{5.11}$$

where  $\mu$  denotes the spectral gap at  $m = 0$ . This bound coincides with the spectral bound (2.8) in the continuum theory, up to corrections of order  $am$ .

An important consequence of these results is that the determinant  $\det D_m$  is real and non-zero at all quark masses  $m > 0$ . Actually,  $\det D_m$  must be positive at these masses, because this is trivially the case at  $m = 2/\bar{a}$  and because the determinant is a continuous function of  $m$ , on any finite lattice.

### 5.3 Locality

In position space, the Dirac operator is represented by a kernel  $D(x, y)$  through

$$D\psi(x) = a^4 \sum_{y_0=a}^{T-a} \sum_y D(x, y)\psi(y), \quad 0 < x_0 < T. \quad (5.12)$$

Locality requires that the bound

$$a^5 \|D(x, y)\| \leq C e^{-\kappa \|x-y\|/a} \quad (5.13)$$

holds for some constants  $C$  and  $\kappa > 0$  that do not depend on  $a$ . Moreover, up to such exponentially small tails,  $D(x, y)$  should be locally constructed and only depend on the gauge field variables in the vicinity of  $x$  and  $y$ .

In infinite volume, a rigorous proof of the locality of the Neuberger–Dirac operator can be given if the gauge field is not too rough on the scale of the lattice spacing [15]. Further studies then suggest that locality holds under far more general conditions, including those typically encountered in numerical lattice QCD at lattice spacings  $a \leq 0.1$  fm [15, 16].

The proof presented in ref. [15] is based on an expansion of the inverse square root in eq. (5.2) in Legendre polynomials. The expansion converges rapidly if  $A^\dagger A \geq \alpha$  for some  $\alpha > 0$ , and the locality of the Dirac operator then follows immediately. In the case of the operator (5.5), the Legendre expansion similarly links its locality properties to the existence of a non-zero lower bound on  $A^\dagger A + caP$ .

As shown in appendix A, the spectral gap of  $A^\dagger A + caP$  is not smaller than that of  $A^\dagger A$  on the infinite lattice, independently of how precisely the gauge field is extended from the time slice  $0 \leq x_0 \leq T$  to all times. The field may be extended through time reflections at the planes  $x_0 = 0 \bmod T$ , for example, which is a good choice in the present context, since the smoothness properties of the field (if any) are preserved. In particular, the estimates of ref. [15] then immediately imply the existence of a spectral gap if the gauge field at  $0 \leq x_0 \leq T$  is sufficiently smooth on the scale of the lattice spacing.

Presumably the locality properties of the Dirac operator (5.4) are thus as good as those of the Neuberger–Dirac operator on lattices with periodic boundary conditions, also when the rigorous arguments of ref. [15] do not apply. However, some numerical studies may still be required to confirm this in the cases of interest.

### 5.4 Chiral symmetry

At a distance  $d$  from the boundaries, the kernel  $D(x, y)$  of the Dirac operator (5.4) coincides with the kernel of the Neuberger–Dirac operator on the infinite lattice, up to terms that decrease exponentially like  $e^{-\kappa d/a}$ . From the expansion in Legendre polynomials mentioned in the previous subsection, for example, this property is evident, taking into account the fact that the operator  $P$  is supported at the boundaries of the lattice. The separation of bulk and boundary terms is actually a direct consequence of the locality of the operators involved (see appendix B).

The remark has two important implications. First of all, it shows that the Schrödinger functional constructed here probes the right theory, i.e. the one where the lattice Dirac operator in the absence of the boundaries is equal to the Neuberger–Dirac operator.

Secondly, it follows that

$$\gamma_5 D + D \gamma_5 = \bar{a} D \gamma_5 D + \Delta_B, \tag{5.14}$$

where  $\Delta_B$  is a local operator with kernel  $\Delta_B(x, y)$  supported in the vicinity of the boundaries (up to the usual exponentially small tails). Correlation functions of local fields at physical distances from the boundaries thus satisfy the same chiral Ward identities as they do on lattices with periodic boundary conditions, for example.

Starting from the definition (5.4),(5.5) of the Dirac operator, or from the formulae in appendix B, the operator  $\Delta_B$  can be worked out explicitly. One may hope to find  $\Delta_B = \gamma_5 P$ , as is the case in one dimension, but the expressions that are obtained are complicated and not very illuminating.

### 5.5 Boundary fields and $O(a)$ improvement

A possible lattice representation of the boundary fields (2.5) at time  $x_0 = 0$  is

$$\zeta(\mathbf{x}) = U(x, 0)|_{x_0=0} P_- \psi(x)|_{x_0=a}, \tag{5.15}$$

$$\bar{\zeta}(\mathbf{x}) = \bar{\psi}(x)|_{x_0=a} P_+ U(x, 0)^{-1}|_{x_0=0}, \tag{5.16}$$

where  $U(x, \mu)$  denotes the link variable at the point  $x$  in direction  $\mu$ . This definition coincides with the one commonly adopted in lattice QCD with Wilson quarks [2]. It should be noted, however, that the normalization of these fields depends on the details of the lattice regularization and may not be the canonical one (cf. subsection 5.6).

Formulations of lattice QCD with Ginsparg–Wilson quarks are automatically on-shell  $O(a)$ -improved [17, 18]. In the presence of the boundaries, this is no longer the case, but the theory can be improved by including a few  $O(a)$  boundary counterterms in the lattice action. The list of terms that must be added was determined in ref. [18]. One of the counterterms amounts to a modification of the lattice Dirac operator, while all others are either pure gauge terms or reduce to contact terms and  $1 + O(am)$  renormalization factors.

These other counterterms can be implemented as in the standard lattice theory [2, 18]. The situation is a bit more tricky in the case of the counterterm that modifies the lattice Dirac operator, because some of the desirable properties of the latter may be compromised (the spectral bound (5.11), for example).

The counterterm at the boundary  $x_0 = 0$  is usually taken to be a straightforward lattice implementation of the boundary action

$$a \int_{x_0=0} d^3 \mathbf{x} \{ \bar{\psi}(x) P_+ D_0 \psi(x) + \bar{\psi}(x) \overleftarrow{D}_0 P_- \psi(x) \}. \tag{5.17}$$

The precise choices that one makes do not matter, since the counterterm is uniquely determined by its symmetries and dimension, up to redundant terms and corrections of higher order in  $a$ . In the present context, the  $O(a)$  improvement can therefore also be achieved by tuning the coefficient  $c$  on which the Dirac operator (5.4),(5.5) depends. Changes of this coefficient actually amount to a modification of the operator in the vicinity of the boundaries by a local term with the correct symmetries. The properties of the Dirac operator discussed in the previous subsections are then preserved.

## 5.6 Free-quark theory

In the absence of the gauge field, it is possible to check explicitly that the lattice theory has the correct continuum limit and that the  $O(a)$  improvement works out in the way described in the previous subsection.

The operator under the square root in eq. (5.5) assumes the form

$$A^\dagger A + caP = (1 + s)^2 + sa^2 \sum_{\mu} \partial_{\mu}^* \partial_{\mu} + \frac{1}{2} a^4 \sum_{\mu < \nu} \partial_{\mu}^* \partial_{\mu} \partial_{\nu}^* \partial_{\nu} + (c - 1)aP \quad (5.18)$$

in the free theory. As explained in subsection 5.1, the operator acts on quark fields in the presence of the boundaries. Its eigenfunctions at  $c = 1$ , for example, are given by

$$\sin(p_0 x_0) e^{i\mathbf{p}\mathbf{x}}, \quad p_0 = \frac{n\pi}{T}, \quad n = 1, 2, \dots, T/a - 1. \quad (5.19)$$

Since the associated eigenvalues are bounded from below by  $(1 - |s|)^2$  if  $|s| \leq 1$ , the locality of the free Dirac operator is guaranteed at all  $|s| < 1$  and  $c \geq 1$ .

In the time-momentum representation, the kernel  $D(x, y)$  of the Dirac operator can be worked out analytically to some extent. The quark propagator, on the other hand, may be difficult to obtain in closed form, but it can be computed numerically on lattices with hundreds of points in each direction, using established techniques (see ref. [19], for example). This allows the lattice propagator to be compared with the continuum propagator in a large range of lattice spacings, spatial momenta and quark masses.

Many checks were then performed, including the following three:

- (1) It was verified that the quark propagator  $\langle \psi(x) \bar{\psi}(y) \rangle$  at non-zero distances from the boundary as well as the boundary-to-bulk propagator  $\langle \zeta(\mathbf{x}) \bar{\psi}(y) \rangle$  have the correct continuum limit (explicit expressions for the continuum propagator can be found in ref. [20]).
- (2) The full spectrum of  $(\gamma_5 D)^2$  was computed and compared with the spectrum in the continuum theory. In particular, the presence of any additional modes that would survive in the continuum limit could be excluded in this way.
- (3) The approach of the propagator to the continuum limit was studied and it was shown that the lattice effects of order  $a$  can be cancelled by tuning the parameter  $c$  of the lattice Dirac operator and the field normalization factors.

The  $O(a)$  improvement is achieved for values of  $c$  close to  $1 + s$ , and the improved, canonically normalized boundary field is given by  $Z(1 + bam)\zeta$  where  $Z \simeq 1 - s/4$  and  $b \simeq -3/4$ . These normalization factors will be rarely needed, but it is reassuring to note that they are in a range that is not uncommon for such factors. Moreover, the observed convergence of the propagators to the continuum limit is quite similar to the one seen in the standard Wilson theory[20].

## 6. Concluding remarks

Lattice Dirac operators that satisfy the Ginsparg–Wilson relation have little in common with the difference operators that are obtained by “discretizing” the classical Dirac equation. Classical concepts can in fact be rather misleading in lattice field theory. In particular, boundary conditions cannot simply be imposed on the lattice fields but arise dynamically in the continuum limit.

Universality considerations gain additional importance in this context, since they apply to any local theory, independently of how complicated it may be. The definition of the Schrödinger functional proposed in this paper heavily builds on such arguments. It is clearly not the only possible construction, but the proposed formulation works out and has many attractive features.

In lattice QCD with Ginsparg–Wilson quarks, the application of domain decomposition methods [21] appeared to be excluded so far, because it was not clear how to restrict the lattice Dirac operator to blocks of lattice points. Following the lines of section 5, it is now straightforward to come up with viable expressions for the block Dirac operators. The boundary operator  $P$ , for example, may be fixed by requiring eq. (A.1) to remain valid when  $R$  is set to the block restriction operator. The locality of the block Dirac operators as well as a number of other desirable properties are then guaranteed.

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## A. Spectral bound on $A^\dagger A + caP$

As explained in subsection 5.3, the locality of the Dirac operator (5.4) can be proved rigorously if  $A^\dagger A + caP \geq \alpha$  for some  $\alpha > 0$ . In this appendix, it is shown that such a bound can be obtained by relating  $A^\dagger A + caP$  to the operator  $A^\dagger A$  on the infinite lattice.

The standard setup of the lattice Schrödinger functional assumes the gauge field variables  $U(x, \mu)$  to be defined at all times  $0 \leq x_0 < T$  if  $\mu = 0$  and additionally at  $x_0 = T$  if  $\mu = 1, 2, 3$ . Evidently, a given field can always be extended to all times by setting the so far undefined link variables to unity, for example.

Exactly which extension is chosen will not matter in the following. Once a definite prescription is adopted, the Wilson–Dirac operator becomes a well-defined, bounded linear operator in the space of all square-summable quark fields on the infinite lattice. The associated operator  $A$  [eq. (5.3)] is denoted by  $\hat{A}$  in order to avoid any confusion with the operator  $A$  that appears in eq. (5.5).

A straightforward calculation, similar to the one that leads to eq. (4.5), now shows that

$$R \left( A^\dagger A + aP \right) R = R \hat{A}^\dagger \hat{A} R, \tag{A.1}$$

where  $R$  projects the quark fields to the physical subspace in the presence of the boundaries. Explicitly,

$$R\psi(x) = \begin{cases} \psi(x) & \text{if } 0 < x_0 < T, \\ 0 & \text{otherwise,} \end{cases} \quad (\text{A.2})$$

for any quark field  $\psi$  on the infinite lattice. Note that the product on the left-hand side of eq. (A.1) is perfectly well-defined, since  $R$  projects the fields to the physical subspace before the operator in brackets (which can only act on quark fields in this space) is applied.

Quark fields in the physical subspace satisfy  $R\psi = \psi$ , and from eq. (A.1) it then follows that

$$(\psi, (A^\dagger A + caP)\psi) = (\psi, \hat{A}^\dagger \hat{A}\psi) + (\psi, (c-1)aP\psi) \geq (\psi, \hat{A}^\dagger \hat{A}\psi), \quad (\text{A.3})$$

where  $c \geq 1$  was used and also the fact that  $aP$  is a projector. Since (A.3) holds for all quark fields in the physical subspace, this shows that the operator  $A^\dagger A + caP$  is bounded from below by the spectral gap of  $\hat{A}^\dagger \hat{A}$ , as asserted in subsection 5.3.

## B. Separation of bulk and boundary terms

Equation (A.1) relates the theory in the presence of the boundaries to the one on the infinite lattice. The goal in the following lines is to work out the relation between the corresponding Dirac operators. Along the way, a separation of bulk and boundary terms is achieved, which allows the position-space kernels of the operators to be compared with each other.

The starting point is the identity

$$R(A^\dagger A + caP)R + (1-R)\hat{A}^\dagger \hat{A}(1-R) = \hat{A}^\dagger \hat{A} + \hat{B}, \quad (\text{B.1})$$

in which

$$\hat{B} = (c-1)RaPR - (1-R)\hat{A}^\dagger \hat{A}R - R\hat{A}^\dagger \hat{A}(1-R) \quad (\text{B.2})$$

denotes an operator supported at the boundaries. Since  $A^\dagger A + caP$  operates in the physical subspace, and since  $R$  is a projector, eq. (B.1) implies

$$R(A^\dagger A + caP)^{-1/2}R = R(\hat{A}^\dagger \hat{A} + \hat{B})^{-1/2}R. \quad (\text{B.3})$$

Using a well-known integral representation, the operator on the right-hand side of this equation can be written in the form

$$(\hat{A}^\dagger \hat{A} + \hat{B})^{-1/2} = (\hat{A}^\dagger \hat{A})^{-1/2} - \int_{-\infty}^{\infty} \frac{dt}{\pi} (\hat{A}^\dagger \hat{A} + t^2)^{-1} \hat{B} (\hat{A}^\dagger \hat{A} + \hat{B} + t^2)^{-1}. \quad (\text{B.4})$$

Taken together, these equations provide a representation of  $(A^\dagger A + caP)^{-1/2}$  (and thus of the Dirac operator in the presence of the boundaries) in terms of the operator  $(\hat{A}^\dagger \hat{A})^{-1/2}$  on the infinite lattice plus another operator localized at the boundaries. Both  $(\hat{A}^\dagger \hat{A} + t^2)^{-1}$  and  $(\hat{A}^\dagger \hat{A} + \hat{B} + t^2)^{-1}$  are in fact expected to be local operators, and the last term in eq. (B.4) is thus supported in the vicinity of the boundaries (up to exponentially small tails).



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