Axial Symmetries in Lattice QCD with Kaplan Fermions

Vadim Furman
School of Physics and Astronomy
Beverly and Raymond Sackler Faculty of Exact Sciences
Tel-Aviv University, Ramat Aviv 69978, ISRAEL

and

Yigal Shamir
Department of Physics
Weizmann Institute of Science, Rehovot 76100, ISRAEL

ABSTRACT

A lattice definition of QCD based on chiral defect fermions is discussed in detail. This formulation involves (infinitely) many heavy regulator fields, realized through the introduction of an unphysical fifth dimension. It is proved that non-singlet axial symmetries become exact in the limit of an infinite fifth dimension, and before the continuum limit is taken.

* Present address: School of Physics and Astronomy, Tel-Aviv University, Ramat Aviv 69978, ISRAEL
1. Introduction

Consistent local regularization methods which preserve gauge invariance must break axial symmetries explicitly. This is a consequence of the well-known axial anomaly \[1\]. However, flavour Non-Singlet Axial Symmetries (NSAS for short) are recovered in renormalized correlation functions to all orders in perturbation theory \[2, 3\]. (For recent progress and references to earlier literature see ref. \[4\]).

Going beyond perturbation theory, the rigorous definition of QCD relies on the lattice regulator. The most popular method to avoid the fermion doubling problem employs Wilson’s prescription for the fermion action \[5\]. The advantage of this method is in its simplicity. But the ensuing breaking of axial symmetries is hard, in the sense that perturbative corrections to quark masses are \(O(1/a)\) where \(a\) is the lattice spacing. Hence, one has to fine tune the bare quark masses in order to recover the correct renormalized masses in the continuum limit.

Using Wilson fermions, it was shown that weak coupling perturbation theory (WCPT) on the lattice reproduces the axial anomaly \[6\], and that NSAS are recovered to all orders in WCPT in the continuum limit \[6, 7\]. These results have in fact some validity beyond the scope of WCPT, and one can discuss the renormalization of gauge invariant composite operators. But, because of the severe fine tuning problem inherent to Wilson fermions, one cannot give a completely general non-perturbative proof of the restoration of NSAS.

Assuming the existence of the chiral limit in the full quantum theory, what one can do in numerical simulations with Wilson fermions is to determine the correct finely tuned values of the bare masses by measuring some correlation functions. Fixing the bare parameters this way, one hopes that NSAS will be recovered in all other correlation functions, thus reproducing for example the results of current algebra \[8\].

This situation is unsatisfactory for several reasons. On the theoretical level, one would like to have a true non-perturbative proof of the restoration of NSAS. Moreover, the construction of a lattice model of QCD where the existence of the chiral limit can (a) be proved and (b) does not require any fine tuning, is important for practical reasons. To elucidate the importance of such framework, we can mention for example the problems involved in measuring weak matrix elements on the lattice with Wilson fermions \[3, 4\]. The fine tuning problem is not over when the bare masses have been fixed. Because of the hard breaking of the axial symmetries, the definition of renormalized four fermion operators which are necessary for the computation of weak decays, involves additional fine-tuning. Moreover, some of the relevant operator mixings receive genuinely non-perturbative contributions, which cannot be
determined even in principle by short distance expansions such as the OPE.

An alternative lattice formulation which does enjoy a certain degree of axial symmetry is the staggered fermions formulation. The staggered fermions action has a $U_V(1) \times U_A(1)$ symmetry, and the exact $U_A(1)$ can be used for a better determination of meson decay constants [10]. However, this formulation also has several drawbacks. The number of flavours must be equal to four, and disentangling spacetime and flavour symmetries is a non-trivial issue. Moreover, in the continuum limit one expect to recover the full $SU(4)$ axial flavour symmetry, but on the lattice only one of the corresponding currents is conserved. The other fourteen currents presumably suffer from the same problems as in the case of Wilson fermions.

In this paper we present a new lattice formulation of QCD with a very mild breaking of all non-singlet axial symmetries. The formulation is based on the introduction of many (in the chiral limit infinitely many) heavy “regulator” fields [11, 12, 13]. More specifically, we use a variant [14] of Kaplan’s proposal [12] to realize light ordinary fermions as zero modes bound to four dimensional defects in a theory of massive five dimensional Dirac fermions [12-21]. The right-handed (RH) and left-handed (LH) components of the physical quark arise as surface states on opposite boundaries of a five dimensional slab with free boundary conditions in the fifth direction. One five dimensional fermion field is needed for every physical quark. The surface fermions scheme has also been discussed recently in ref. [15].

While Kaplan intended to propose a solution to the long-standing problem of defining chiral gauge theories on the lattice, the feasibility of reaching this goal is still unclear [16-19,22]. But the advantages of using chiral defect fermions for lattice QCD are obvious. In particular, one can easily show that, in the limit where the width of the five dimensional slab tends to infinity, quark masses undergo only multiplicative renormalization to all orders in perturbation theory [14].

The reason for the absence of additive $O(1/a)$ corrections to quark masses, is the vanishing of the overlap between the RH and LH components of the quark’s wave function. At tree level, the tail of the RH wave function goes like

$$\left(1 - M_a^s\right)^s.$$  \hspace{1cm} (1.1)

Here $s$ is the fifth coordinate which takes the values $s = 1, \ldots, 2N$. The Dirac mass $M$ that appears in the five dimensional fermion action obeys $0 < M a < 1$. A similar expression applies to the LH component, but with $s$ in eq. (1.1) replaced by $2N - s$. Thus, the perturbative overlap of the LH and RH components vanishes exponentially with increasing $N$.

One can also introduce direct couplings between the LH and RH components of every quark, by adding links that couple the layers $s = 1$ and $s = 2N$. These
couplings are controlled by dimensionful parameters $m_i$, where $i$ is a flavour index. As shown in ref. [14], the $m_i$ play the role of multiplicatively renormalized quark masses.

Taking advantage of the special properties of the model, one can define axial currents whose divergences, for $m_i = 0$, are completely localized on the two middle layers $s = N$ and $s = N + 1$. As a result, the anomalous term in the Ward identities of NSAS is governed by the small tail of the quark’s wave function at the center of the five dimensional slab. On the other hand, the divergence of the singlet axial current can couple to two gluons, giving rise in the limit $N \to \infty$ to the expected axial anomaly [20, 18, 16, 15].

In this paper we extend the investigation of axial properties to include also non-perturbative effects. Our main result is that NSAS become exact in the limit $N \to \infty$. To our knowledge, this is the first non-perturbative proof of the restoration of NSAS.

The restoration of NSAS occurs before the continuum limit is taken. The limiting “$N = \infty$” formalism should be regarded as non-perturbative regularization of QCD which is maximally symmetric under axial transformations. Since the “$N = \infty$” formulation preserves NSAS while reproducing correctly the singlet anomaly, it cannot be a strictly local regulator. The non-locality arises from integrating out infinitely many heavy four-dimensional fields, and we believe that it is mild enough not to jeopardize the consistency of the continuum limit.

This paper is organized as follows. In sect. 2 we give the definition of the model. Apart from the obvious gauge and fermion fields, the model includes a set of massive five dimensional scalar fields. These fields are necessary to cancel out some lattice artifacts of the five dimensional fermions [11, 13]. Such scalar fields have often been called Pauli-Villars (PV) fields in the literature, and we will continue to use this terminology here. But it should be stressed that the scalar action is non-negative, and so the partition function of the PV fields is well-defined. The peculiar property of the PV fields is that, apart from a different choice of boundary conditions, their action is the square of the fermionic action.

In sect. 3 we develop a transfer matrix formalism to represent the fermionic partition function as well as correlation functions. The transfer matrix technique was introduced in the context of chiral defect fermions by Narayanan and Neuberger [16] and it relies on the work of Lüscher [23]. It proves particularly convenient for the investigation of the model. Formulae are given both for finite $N$ and for the limiting case $N \to \infty$.

Sect. 4 contains a discussion of the effective action $S^\infty_{\text{eff}}(U)$ obtained by integrating out the fermion and PV fields and taking the limit $N \to \infty$. An interesting result
is that, while being always real, \( \exp\{-S_{\text{eff}}^\infty(U)\} \) is not necessarily positive. This behaviour can be explained on the basis of familiar instanton results.

The results of sect. 3 and 4 are valid for a fixed background gauge field, provided the hamiltonian \( \mathcal{H} = -\log T \) where \( T \) is the transfer matrix has a unique ground state. In sect. 5 we derive an analytical criterion eq. (5.3) which selects those gauge field configurations where \( \mathcal{H} \) has an exact zero mode and, hence, the ground state is degenerate. Such backgrounds allow for unsuppressed fermionic (and PV) propagation across in the fifth dimension, and they contribute to the anomalous term in non-singlet axial Ward identities. The possibility of having light states inside the five dimensional balk is related to the unconventional relative sign of the mass and Wilson terms in the fermion action. (The hopping parameter is supercritical). A simple example of a configuration which supports anomalously light balk states is the dynamical domain wall.

Sect. 6 contains the main results of this paper. Let \( Z(g_0, L, N) \) be the partition function on a finite five dimensional lattice. The \( N \to \infty \) limit of the partition function is

\[
Z^\infty(g_0, L) = \lim_{N \to \infty} Z(g_0, L, N).
\]

Both the four dimensional lattice \( L^4 \) and the bare coupling \( g_0 \) are kept finite. We prove that

\[
Z^\infty(g_0, L) = \prod_{x, \mu} \int dU_{x, \mu} e^{-S_G(U) - S_{\text{eff}}^\infty(U)}.
\]

(1.3)

\( S_G(U) \) and \( S_{\text{eff}}^\infty(U) \) are defined in eqs. (2.3) and (3.19), respectively. In other words, one can interchange the order of integration over the group variables and the \( N \to \infty \) limit. This result follows from the \( s \)-independence of the gauge field, compactness of the gauge field configuration space and eq. (5.3), which implies that exact zero modes of \( \mathcal{H} \) exist only on a zero measure subspace.

Repeating the same steps for non-singlet axial Ward identities, we prove that the anomalous term in every Ward identity vanishes in the limit \( N \to \infty \), at fixed values of \( L \) and \( g_0 \). As expected, the same analysis gives rise to a non-zero expression for the singlet anomaly. We stress that NSAS are recovered before the continuum limit \( g_0 \to 0 \) is taken. Such a non-trivial result is possible because the size of the unphysical fifth dimension \( N \) is sent to infinity. This is reflected in the operator expression for conserved currents, which contains an infinite sum over the \( s \)-coordinate.

A difficulty with the transfer matrix formalism, it that its efficient implementation in numerical simulations would require the development of new techniques. Instead, one may choose to put the fermions on a finite five dimensional lattice. One should then choose an optimal value for \( N \) subject to the constraints dictated by computer
performance. To this end, it is important to have a realistic estimate of the magnitude of anomalous effects on a finite five dimensional lattice.

We believe that the bounds used in proving the existence of the chiral limit, highly overestimate the true magnitude of anomalous terms. A detailed study of the issue is beyond the scope of this paper. However, we have decided to give in Sect. 7 a short heuristic discussion, which is meant to give the reader some feeling about the plausible magnitude of the anomalous term. As we explain, we believe that the magnitude of anomalous effects may turn out to be numerically very small already for currently accessible five dimensional lattices. Finally, some technical details are relegated to two appendices.

2. Definition of the model

In this section we give the definition of lattice QCD with the surface fermions variant of chiral defect fermions [14]. We also define physical quark operators as well as axial and vector currents [18] appropriate for the model. Most of the ingredients have been introduced previously, and we give them here to make the present exposition self-contained.

For definiteness, we take the physical case of four dimensions. This means that the fermion and Pauli-Villars (PV) fields live on five dimensional lattices, whereas the gluon fields are four dimensional. The ordinary four coordinates, labeled \( x_\mu \), range from 1 to \( L \), whereas the extra coordinate takes the values \( s = 1, \ldots, 2N \) for the fermionic lattice. The PV lattice is only half as big, with \( s \) ranging from 1 to \( N \). The preferred boundary conditions in the four ordinary dimensions are periodic or anti-periodic. Free boundary condition in these directions would result in extra unwanted light states which can propagate along the spatial boundaries.

The above scheme is realized by requiring that the link variables in the fermion and PV action obey \( U_{x,s,5} = 1 \) and \( U_{x,s,\mu} = U_{x,\mu} \) independently of \( s \). The topology of the fifth dimension is taken to be a circle, but the couplings which reside on the links connecting the layers \( s = 2N \) and \( s = 1 \) are proportional to a parameter \( -m_i \) (\( i = 1, \ldots, N_f \) is a flavour index. Also, we henceforth set the lattice spacing to \( a = 1 \)). The case \( m_i = 1 \) corresponds to antiperiodic boundary conditions, where the model supports no light fermionic state. The case \( m_i = 0 \) corresponds to open boundaries, and it should give rise to the physics of QCD with massless quarks by taking first the limit \( N \to \infty \) and then the continuum limit.
The partition function is

\[ Z = Z(g_0, L, N, m_i) = \prod_x \left( \prod_{\mu} \int dU_{x, \mu} \prod_{s=1}^{2N} \int d\bar{\psi}_{x,s} d\psi_{x,s} \prod_{s'=1}^{N} \int d\phi_{x,s'} d\phi_{x,s'} \right) e^{-S}. \] (2.1)

The action is given by:

\[ S = S_G(U) + S_F(\bar{\psi}, \psi, U) + S_{PV}(\phi^\dagger, \phi, U). \] (2.2)

Colour, flavour and Dirac indices will be suppressed throughout this paper unless explicitly stated otherwise. We remind the reader that the PV fields carry the same set of indices as the fermion fields. Also, we will usually write \( DU = \prod dU \) etc. as a shorthand for the corresponding measure.

\( S_G(U) \) is the pure gauge part of the action. The results of this paper generalize to any compact Lie group with a non-negative lattice action, which reduces to the appropriate gauge field action in the classical continuum limit. To avoid irrelevant notational complications, we will assume that the gauge group is \( G = SU(N_c) \). In eq. (2.1), \( dU \) is the normalized, invariant group measure, and \( S_G(U) \) is the usual sum over plaquettes

\[ S_G = \frac{1}{g_0^2} \sum_x \sum_{1 \leq \mu < \nu \leq 4} \text{Re} \text{tr} (I - U_{x,\mu \nu}). \] (2.3)

Here \( U_{x,\mu \nu} \) is the plaquette variable.

The fermion and PV actions contain a sum over all flavours. The only difference between various flavours can be in the mass parameter \( m_i \). We give below the one flavour action. The fermionic part has the following form

\[ S_F(\bar{\psi}, \psi, U) = - \sum_{x,y,s,s'} \bar{\psi}_{x,s} (D_F)_{x,s;y,s'} \psi_{y,s'}, \] (2.4)

where the fermionic matrix is defined by

\[ (D_F)_{x,s;y,s'} = \delta_{s,s'} D_{x,y}^\parallel + \delta_{x,y} D_{s,s'}^\perp, \] (2.5)

\[ D_{x,y}^\parallel = \frac{1}{2} \sum_{\mu} \left( (1 + \gamma_\mu) U_{x,\mu} \delta_{x+\hat{\mu},y} + (1 - \gamma_\mu) U_{y,\mu}^\dagger \delta_{x-\hat{\mu},y} \right) + (M - 4) \delta_{x,y}, \] (2.6)

\[ D_{s,s'}^\perp = \begin{cases} P_R \delta_{2,s'} - m P_L \delta_{2N,s'} - \delta_{1,s'} , & s = 1, \\ P_R \delta_{s+1,s'} + P_L \delta_{s-1,s'} - \delta_{s,s'} , & 1 < s < 2N, \\ -m P_R \delta_{1,s'} + P_L \delta_{2N-1,s'} - \delta_{2N,s'} , & s = 2N. \end{cases} \] (2.7)
and
\[ P_{R,L} = \frac{1}{2} (1 \pm \gamma_5) . \]  

Notice that \( D_{s,s'}^\dagger \) is independent of the gauge field. Also, apart from the unconventional sign of the mass term, \( D_{x,y}^\parallel \) is the usual four dimensional gauge covariant Dirac operator for massive Wilson fermions.

When \( m_i = 0 \) the spectrum of surface states contains one RH Weyl fermion near the boundary \( s = 1 \) and one LH Weyl fermion near the other boundary for every five dimensional fermion field. These Weyl fermions have the same coupling to the gauge field, and so they in fact describe \( N_f \) quarks. If we ignore the exponentially small overlap between the tails of the LH and RH surface states, then these states describe massless quarks. Switching \( m_i \) on, we now mix the RH and LH components of each quark and provide it with a Dirac mass \( \overline{m}_i \) which is proportional to \( m_i \). At tree level one has [14]
\[ \overline{m}_i = M(2 - M)m_i . \]  

The PV fields [11, 13] are needed to cancel the contribution of heavy fermion modes to the effective action \( S_{\text{eff}}(U) \). This contribution, while formally being local in the continuum limit, is proportional to \( N \). (Every five dimensional fermion field describes one light quark field and \( 2N - 1 \) four dimensional fields whose mass is of the order of the cutoff). If one does not subtract the contribution of the massive fields by hand, that lattice artifact will dominate the effective action in the limit \( N \to \infty \).

Let us denote the dependence of the Dirac operator in eq. (2.5) on \( m_i \) and on the number of sites in the \( s \)-direction by \( D_F = D_F(2N, m_i) \). The PV fields live on a five dimensional lattice with \( N \) sites in the \( s \)-direction, and using the above notation, the PV action is
\[ S_{\text{PV}}(\phi^\dagger, \phi, U) = \sum_{x,y,z,s,s',s''} \phi_{x,s}^\dagger D_F^\dagger(N,1)_{x,s,z,s''} D_F(N,1)_{z,s'';y,s'} \phi_{y,s'} . \]  

The second order operator in eq. (2.10) is the square of the Dirac operator on a smaller lattice. The choice \( m_i = 1 \) for the PV fields prevents the appearance of light scalar modes on the layers \( s = 1 \) and \( s = N \). As will be shown below, this choice of \( S_{\text{PV}} \) ensures that \( \exp\{-S_{\text{eff}}\} \) remains finite in the limit \( N \to \infty \).

Let us denote by \( \mathcal{R} \) the reflection relative to the hyper-plane \( s = N + 1/2 \)
\[ \mathcal{R} \psi_{x,s} = \psi_{x,2N+1-s} . \]  

The Dirac operator \( D_F \) of eq. (2.3) satisfies the following identity
\[ \gamma_5 \mathcal{R} D_F \gamma_5 \mathcal{R} = D_F^\dagger . \]
This identity is a generalization of a similar relation obeyed by the four dimensional Dirac operator for Wilson fermions, which reads

\[ \gamma_5 D^\parallel \gamma_5 = (D^\parallel)^\dagger. \] (2.13)

As in the case of Wilson fermions, eq. (2.12) plays an important role in establishing the positivity of pion correlators (see App. B).

Eq. (2.12) implies that the operator \( \gamma_5 \mathcal{R} D_F \) is hermitian. One has \( \det (\gamma_5 \mathcal{R}) = 1 \) trivially, and so

\[ \det (D_F) = \det (\gamma_5 \mathcal{R} D_F). \] (2.14)

As a result, the fermionic determinant is real. However, one cannot conclude that the fermionic determinant is necessarily positive. The fermionic determinant can in fact change sign, due to level crossing of an odd number of states (see below).

We comment in passing that one can use the hermitian operator \( \gamma_5 \mathcal{R} D_F \) in the definition of the fermionic action instead of \( D_F \). This is facilitated by the unitary change of variables (recall that \( \psi \) and \( \overline{\psi} \) are independent variables in euclidean space)

\[ \psi \rightarrow \psi' = \psi, \]
\[ \overline{\psi} \rightarrow \overline{\psi}' = \overline{\psi} \gamma_5 \mathcal{R}. \] (2.15)

A similar definition (involving \( \gamma_5 \) only) has been found useful in the construction of the euclidean partition function of continuum supersymmetric QCD [24]. Notice that the uneven treatment of \( \psi \) and \( \overline{\psi} \) in eq. (2.15) gives rise to unconventional expressions for the axial and vector currents. Since we will not use this formulation any further we do not give the details here.

In the rest of this paper we assume \( m_i = m, \; i = 1, \ldots, N_f \). The five dimensional fermion action is invariant under global \( U(N_f) \) symmetry. The conserved five dimensional current has the following components. For \( \mu = 1, \ldots, 4 \)

\[ j^a_\mu(x, s) = \frac{1}{2} \left( \overline{\psi}_{x,s} (1 + \gamma_\mu) U_{x,\mu} \lambda^a \psi_{x+\hat{\mu},s} - \overline{\psi}_{x+\hat{\mu},s} (1 - \gamma_\mu) U_{x,\mu}^\dagger \lambda^a \psi_{x,s} \right), \; 1 \leq s \leq 2N. \] (2.16)

As for the fifth component, we define

\[ j^a_5(x, s) = \begin{cases} \overline{\psi}_{x,s} P_R \lambda^a \psi_{x,s+1} - \overline{\psi}_{x,s+1} P_L \lambda^a \psi_{x,s}, & 1 \leq s < 2N, \\
\overline{\psi}_{x,2N} P_R \lambda^a \psi_{x,1} - \overline{\psi}_{x,1} P_L \lambda^a \psi_{x,2N}, & s = 2N. \end{cases} \] (2.17)

This five dimensional current satisfies the continuity equation

\[ \sum_\mu \Delta_\mu j^a_\mu(x, s) = \begin{cases} -j^a_5(x, 1) - mj^a_5(x, 2N), & s = 1, \\
-\Delta_5 j^a_5(x, s), & 1 < s < 2N, \\
j^a_5(x, 2N - 1) + mj^a_5(x, 2N), & s = 2N. \end{cases} \] (2.18)
Here
\[ \Delta_\mu f(x, s) = f(x, s) - f(x - \hat{\mu}, s), \quad (2.19) \]
\[ \Delta_\delta f(x, s) = f(x, s) - f(x, s - 1). \quad (2.20) \]

\( \lambda^a \) is a flavour symmetry generator. Notice the special form of the boundary terms in the continuity equation.

We now give the definitions of four dimensional vector and axial currents \[^{18}\].

There is a unique set of conserved vector currents, given by
\[ V_\mu^a(x) = \sum_{s=1}^{2N} j_\mu^a(x, s). \quad (2.21) \]

Conservation of the vector current \( V_\mu^a \) follows from eq. (2.18).

On the other hand, there is a lot of arbitrariness in defining axial transformations in the model. Any transformation which assigns opposite charges to the LH and RH chiral modes will reduce to the familiar axial transformation in the continuum limit.

Here we take advantage of the global separation of the LH and RH modes in the \( s \)-direction. We define our axial transformation to act \( \text{vectorially} \) on a given four dimensional layer, but we assign opposite charges to fermions in the two half-spaces
\[
\delta_A^a \psi_{x,s} = +i q(s) \lambda^a \psi_{x,s},
\]
\[
\delta_A^a \overline{\psi}_{x,s} = -i q(s) \overline{\psi}_{x,s} \lambda^a,
\]
where
\[
q(s) = \begin{cases} 
1, & 1 \leq s \leq N, \\
-1, & N < s \leq 2N.
\end{cases}
\]

The corresponding axial currents are
\[ A_\mu^a(x) = -\sum_{s=1}^{2N} \text{sign}(N - s + \frac{1}{2}) j_\mu^a(x, s). \quad (2.25) \]

For \( m = 0 \), the non-invariance of the action under the transformation (2.22) resides entirely in the coupling between the layers \( s = N \) and \( s = N + 1 \). For \( m \neq 0 \), there is an additional contribution coming from the direct coupling between the layers \( s = 1 \) and \( s = 2N \). As a result, the axial currents satisfy the following divergence equations
\[ \Delta_\mu A_\mu^a(x) = 2m J_5^a(x) + 2J_{5q}^a(x), \quad (2.26) \]
where
\[
J_5^a(x) = j_5^a(x, 2N),
\]
\[
J_{5q}^a(x) = j_5^a(x, N).
\]
In order to understand the physical content of eq. (2.26) let us define quark operators as follows

\[
q_x = P_R \psi_{x,1} + P_L \psi_{x,2N},
\]

\[
\bar{q}_x = \bar{\psi}_{x,2N} P_R + \bar{\psi}_{x,1} P_L.
\] (2.29)

These operators have a finite overlap with the surface states in the chiral limit \(N \to \infty\), and so they can play the role of bare quark fields. There are of course many other operators which are localized near the boundaries and, hence, can interpolate quark states. Our choice eq. (2.29) is the simplest possible one, and it leads to considerable simplification of the expressions for correlation functions.

In terms of the quark fields, \(J^a_5\) takes the familiar form

\[
J^a_5(x) = \bar{q}_x \gamma_5 \lambda^a q_x.
\] (2.30)

Thus, up to the finite normalization factor in eq. (2.3), the \(J^a_5\) term on the r.h.s. of eq. (2.26) is the expected contribution from a classical mass term. \(J^a_{5q}\) represents an additional, quantum breaking term. Below we will be interested in axial Ward identities of the general form

\[
\Delta_\mu \langle A^a_\mu(x) O(y_1, y_2, \ldots) \rangle = 2m \langle J^a_5(x) O(y_1, y_2, \ldots) \rangle + 2 \langle J^a_{5q}(x) O(y_1, y_2, \ldots) \rangle + i \langle \delta^a_A O(y_1, y_2, \ldots) \rangle,
\] (2.31)

where \(A^a_\mu\) is a non-singlet axial current. Our aim is to show that, if \(O(y_1, y_2, \ldots)\) involves only the quark operators of eq. (2.29) then the anomalous term

\[
\langle J^a_{5q}(x) O(y_1, y_2, \ldots) \rangle
\] (2.32)

vanishes in the limit \(N \to \infty\). An especially important case is when the operator \(O\) is itself a pseudo-scalar density \(O = J^b_5(y)\). The corresponding Ward identity

\[
\Delta_\mu \langle A^a_\mu(x) J^b_5(y) \rangle = 2m \langle J^a_5(x) J^b_5(y) \rangle + 2 \langle J^a_{5q}(x) J^b_5(y) \rangle - \delta_{x,y} \langle \bar{q}_y \{\lambda^a, \lambda^b\} q_y \rangle
\] (2.33)

governs the pion mass.
3. Transfer matrix formalism

It is convenient to discuss non-perturbative effects using the transfer matrix formalism. This technique was adapted to domain wall fermions in ref. [16]. Here we in fact have a constant five dimensional mass \( M \), and the only deviation compared to ref. [23] is in the \( m_i \)-dependent value of the couplings on the links connecting the layers \( s = 1 \) and \( s = 2N \). In this section and the next one we will assume that the background gauge field \( U_{x,\mu} \) is fixed.

A simple generalization of the result of ref. [23] gives rise to the following second quantized expression for the Grassmann path integral

\[
\det D_F(2N, m) = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_F(\bar{\psi}, \psi, U)} = (\det B)^{2N} \text{tr} T^{2N} \mathcal{O}(m). \tag{3.1}
\]

The second quantized transfer matrix \( T \) acts in a Fock space spanned by the action of fermionic creation operators \( \hat{a}_x^\dagger \) on a vacuum state \( |0\rangle \) annihilated by \( \hat{a}_x \). The operators \( \hat{a}_x \) and \( \hat{a}_x^\dagger \) satisfy canonical anticommutation relations. They live on the sites \( x_\mu \) of a four dimensional lattice of size \( L^4 \), and they also carry Dirac, colour and flavour indices which we have suppressed. The decomposition of \( \hat{a}_x \) into RH and LH components is

\[
\hat{a} = \begin{pmatrix} \hat{c} \\ \hat{d}^\dagger \end{pmatrix} \tag{3.2}
\]

The transfer matrix is defined by

\[
T = e^{-\hat{a}^\dagger H \hat{a}}, \tag{3.3}
\]

where

\[
e^{-H} = \begin{pmatrix} B^{-1} & B^{-1}C \\ C^+ B^{-1} & C^+ B^{-1}C + B \end{pmatrix} \tag{3.4}
\]

\[
B_{x,y} = (5 - M) \delta_{x,y} - \frac{1}{2} \sum_\mu \left[ \delta_{x+\mu,y} U_{x,\mu} + \delta_{x-\mu,y} U_{y,\mu}^\dagger \right], \tag{3.5}
\]

\[
C_{x,y} = \frac{1}{2} \sum_\mu \left[ \delta_{x+\mu,y} U_{x,\mu} - \delta_{x-\mu,y} U_{y,\mu}^\dagger \right] \sigma_\mu, \tag{3.6}
\]

and \( \sigma_\mu = (i, \vec{\sigma}) \). An important identity is

\[
e^{-H} = K K^\dagger, \tag{3.7}
\]

where

\[
K = \begin{pmatrix} B^{-1/2} & 0 \\ C^+ B^{-1/2} & B^{1/2} \end{pmatrix}. \tag{3.8}
\]
The last equation implies that the matrix operator $H$ is well-defined. Notice also that $D^\parallel$ can be expressed in terms of $B$ and $C$ as follows:

$$D^\parallel = \begin{pmatrix} 1 - B & C \\ -C^\dagger & 1 - B \end{pmatrix}. \tag{3.9}$$

The operator $\mathcal{O}(m)$ contains all the $m$-dependence, and it is given by

$$\mathcal{O}(m) = \prod_n (\hat{c}_n\hat{c}_n^\dagger + m\hat{c}_n\hat{c}_n^\dagger)(\hat{d}_n\hat{d}_n^\dagger + m\hat{d}_n\hat{d}_n^\dagger). \tag{3.10}$$

In this equation, $n$ is a generic name for all indices. The special cases $m = 0$ and $m = 1$ deserve special attention. For $m = 1$, $\mathcal{O}(m)$ becomes the identity operator, whereas for $m = 0$ it is a projection operator on a different ground state $|0'\rangle$ annihilated by all the $\hat{c}$-s and $\hat{d}$-s. The relation between $|0\rangle$ and $|0'\rangle$ is

$$|0\rangle = \prod_n \hat{d}_n^\dagger |0'\rangle. \tag{3.11}$$

Both $|0\rangle$ and $|0'\rangle$ are “kinematical” ground states which can serve as convenient reference states in the construction of the Fock space. But none of them play a special role dynamically. Since we use creation and annihilation operators in the coordinate basis, both $|0\rangle$ and $|0'\rangle$ are very different from the filled Dirac sea even in the case of free fermions.

Like $D^\parallel$, the hermitian operator $H$ is a $N_t \times N_t$ matrix, where $N_t = 4N_cN_fL^4$. Let $R$ be the unitary matrix which diagonalizes $H$

$$\sum_i H_{mi}R_{in} = E_nR_{mn}. \tag{3.12}$$

Corresponding to the splitting into two-by-two matrices in Dirac space in eq. (3.4), we write $R$ as two $\frac{1}{2}N_t \times N_t$ matrices $P$ and $Q$. We will assume that the columns of $R$ are ordered according to their eigenvalues, with the negative eigenvalues on the left. Accordingly, we further decomposed $P$ and $Q$ into submatrices which contain the positive and negative eigenvectors

$$R = \begin{pmatrix} P^- & P^+ \\ Q^- & Q^+ \end{pmatrix}. \tag{3.13}$$

$P^\pm$ and $Q^\pm$ are $\frac{1}{2}N_t \times N^\pm$ matrices, where $N^+ + N^- = N_t$.

The ground state of of the second quantized operator $\mathcal{H} = \hat{a}^\dagger H\hat{a}$ is obtained by filling all negative energy states

$$|0_H\rangle = \prod_{i=1}^{N^-} (\hat{c}^\dagger_{i,-} P_{i,-}^- + \hat{d}^\dagger_{i,-} Q_{i,-}^-)|0\rangle. \tag{3.14}$$
In the limit $N \to \infty$, $T^{2N}$ is proportional to a projector on the ground state of $\mathcal{H}$

$$T^{2N} \to \left| 0_{H} \right\rangle \lambda_{\text{max}}^{2N} \left\langle 0_{H} \right|, \quad N \to \infty,$$  \hspace{1cm} (3.15)

where

$$\lambda_{\text{max}} = \exp \left\{ - \sum_{i=1}^{N^{-}} E_{i} \right\}. \hspace{1cm} (3.16)$$

We now turn to the scalar PV fields. The action is bilinear in these fields, and so

$$\int \mathcal{D}\phi \mathcal{D}\phi^{\dagger} e^{-S_{\text{PV}}(\phi^{\dagger},\phi,U)} = \det^{-1} \left( D_{F}^{\dagger}(N,1) D_{F}(N,1) \right)$$

$$= (\det B)^{-2N} \left( \text{tr} T^{N} \right)^{-2}. \hspace{1cm} (3.17)$$

In going from the first to the second row we have used eq. (3.1) and substituted $m = 1$.

The effective action $S_{\text{eff}}(U)$ is defined by integrating out both fermion and PV fields. Using eqs. (3.1) and (3.17) we find

$$\exp \{-S_{\text{eff}}\} = \frac{\text{tr} T^{2N} \mathcal{O}(m)}{(\text{tr} T^{N})^{2}}. \hspace{1cm} (3.18)$$

In the limit $N \to \infty$ the effective action becomes

$$\exp \{-S_{\text{eff}}^{\infty}\} \equiv \lim_{N \to \infty} \exp \{-S_{\text{eff}}\}$$

$$= \left\langle 0_{H} \right| \mathcal{O}(m) \left| 0_{H} \right\rangle. \hspace{1cm} (3.19)$$

Eq. (3.19) is valid for a fixed background field provided the ground state of $\mathcal{H}$ is non-degenerate. The limiting expression eq. (3.19) is completely well defined here, and it is free of any subtleties of the kind encountered in trying to define chiral gauge theories on the lattice using chiral defect fermions [18].

4. The effective action

As a first step, we want to study the behaviour of $\left\langle 0_{H} \right| \mathcal{O}(m) \left| 0_{H} \right\rangle$ under various conditions. The physically interesting case is $m \ll 1$. In the case $m = 1$ one has $\left\langle 0_{H} \right| \mathcal{O}(1) \left| 0_{H} \right\rangle = 1$. The reason for this trivial result is the subtraction of the balk effect through the PV fields. By contrast, in the opposite limit $m = 0$ one has

$$\exp \{-S_{\text{eff}}^{\infty}\} = \left| \left\langle 0_{H} \right| 0' \right\rangle \right|^{2}, \quad m = 0. \hspace{1cm} (4.1)$$

Thus, in a model of massless chiral defect fermions, the physical information is not in the trace of the transfer matrix but, rather, in the overlap of its ground state with
some other state. This was first found by Narayanan and Neuberger for domain wall fermions, where the overlap formula reads \[16\]

$$
\exp\{-S^\infty_{\text{eff}}(\text{domain wall})\} = \left| \langle 0_{H^+} | 0_{H^-} \rangle \right|^2.
$$

(4.2)

Here \(H^\pm\) are the hamiltonians corresponding to the two sides of the domain wall. Hence, one has to compare two dynamical ground states. But all the non-trivial dynamics of the model is contained in the \(H^+\) hamiltonian. In the continuum limit, eqs. (4.1) and (4.2) should describe the same physics. It is therefore advantageous to work with the surface fermion scheme, where one has to calculate the overlap of \(|0_H\rangle\) with a fixed reference state \(|0'\rangle\).

An explicit expression for the \(m = 0\) overlap eq. (4.1) can be easily written down \[16\]. We first comment that for free fermions, as well as for perturbative gauge field configurations, the numbers of positive and negative eigenvalues of \(H\) are equal \(N^\mp = \frac{1}{2}N_t\). In this case \(P^\mp\) and \(Q^\mp\) are square matrices. Using eq. (3.11) it follows that only the \(\tilde{d}\)-dependent terms in eq. (3.14) contribute to the overlap eq. (4.1). Taking into account the anticommuting character of the fermionic operators one arrives at

$$
\langle 0_{H} | 0' \rangle = \det Q^-.
$$

(4.3)

The phase ambiguity in defining the columns of \(Q^-\) is irrelevant, because only the modulus of \(\det Q^-\) enters eq. (4.1).

For non-perturbative configurations there may be level crossing, resulting in \(N^\mp \neq \frac{1}{2}N_t\). In this case the \(m = 0\) overlap vanishes identically. As discussed in ref. \[16\] this is a welcomed phenomenon, which signals that the chiral defect fermion model can reproduce instanton effects.

We now want to generalize the explicit expression for \(\langle 0_{H} | \mathcal{O}(m) | 0_{H} \rangle\) to \(m \neq 0\). We first notice that \(\mathcal{O}(m)\) can be expanded as

$$
\mathcal{O}(m) = \sum_{k=0}^{N_t} m^k \sum_{l+n=k} \frac{1}{n!} \hat{c}_{i_1}^\dagger \cdots \hat{c}_{i_l}^\dagger \hat{d}_{j_1}^\dagger \cdots \hat{d}_{j_n}^\dagger |0'\rangle \langle 0'| \hat{c}_{i_1} \cdots \hat{c}_{i_l} \hat{d}_{j_1} \cdots \hat{d}_{j_n}.
$$

(4.4)

In eq. (4.4), \(m^k\) multiplies a sum over orthogonal projection operators whose number grows like \(N^k_t/k!\). Recall that \(N_t\) is proportional to the four-volume \(V = L^4\). In calculating the \(m\)-expansion of the effective action, at the \(k\)-th order we will therefore encounter \(O(V^k/k!\})\) terms, where the magnitude of each term is bounded by \(m^k\). This is in agreement with the anticipated behaviour of a system which undergoes spontaneous symmetry breaking. The finite volume partition function is analytic in \(m\), but in the infinite volume limit singularities may appear because the product \(mV\) diverges.

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Returning to the calculation of \( \langle 0_H | \mathcal{O}(m) | 0_H \rangle \), let us denote
\[
\Delta = \frac{1}{2} N_t - N^- .
\] (4.5)

The first term in the expansion eq. (4.4) which contributes to \( \langle 0_H | \mathcal{O}(m) | 0_H \rangle \) is the term with \( k = \Delta \). This immediately implies that
\[
\langle 0_H | \mathcal{O}(m) | 0_H \rangle = O(m^{\Delta}) .
\] (4.6)

Moreover, for sufficiently small \( m \), the sign of \( \langle 0_H | \mathcal{O}(m) | 0_H \rangle \) is determined by the sign of \( m^{\Delta} \). Hence, \( \langle 0_H | \mathcal{O}(m) | 0_H \rangle \) will be negative for \( m < 0 \) and odd \( \Delta \). For example, in the one flavour case \( \langle 0_H | \mathcal{O}(m) | 0_H \rangle \) is negative for \( m < 0 \) if an odd number of level crossing took place.

This behaviour is not unexpected and, in fact, it is in agreement with the familiar instanton result [25]. In the one flavour case, the fermionic determinant in an instanton background is proportional to \( m \), and so it changes sign if \( m \) does. The gauge field’s effective measure \( \exp \{-S_G - S_{\text{eff}}^\infty \} \) is therefore real, but not always positive. We still expect the partition function to be strictly positive when one approaches the continuum limit, because configurations with a non-zero topological charge are rare. But we are unable to prove the positivity of the partition function in a completely general way. Special cases where \( \exp \{-S_{\text{eff}}^\infty \} \) is strictly positive include \( m > 0 \), or \( m \neq 0 \) and even \( N_f \).

An explicit expression for \( \langle 0_H | \mathcal{O}(m) | 0_H \rangle \) is more easily obtained using the definition eq. (3.10). Straightforward application of the canonical anticommutation relations gives rise to
\[
\mathcal{O}(m)|0_H\rangle = m^{\frac{1}{2} N_t} \prod_{i=1}^{N^-} (m c_{i,i}^+ P_{i,i}^- + m^{-1} d_{i,i} Q_{i,i}^-) |0\rangle .
\] (4.7)

Introducing the \( N_t \times N^- \) matrix
\[
R^-(m) = m^{\frac{1}{2} N_t} \begin{pmatrix} m P^- \\ m^{-1} Q^- \end{pmatrix} ,
\] (4.8)
we find
\[
\langle 0_H | \mathcal{O}(m) | 0_H \rangle = \det R^-(1) R^-(m) .
\] (4.9)

In the case \( m > 0 \) one can use the relation \( \mathcal{O}(m) = \mathcal{O}(m^{\frac{1}{2}}) \mathcal{O}(m^{\frac{1}{2}}) \) to write
\[
\langle 0_H | \mathcal{O}(m) | 0_H \rangle = \det R^-(m^{\frac{1}{2}}) R^-(m^{\frac{1}{2}}) ,
\] (4.10)
which is manifestly positive.
The transfer matrix formalism can also be used to write down expressions for correlation functions. The correlation functions for the quark operators \(2.29\) take a particularly simple form. The rules for their construction, as well as some explicit examples, are given in Appendix A. The transfer matrix formula for axial Ward identities is discussed also in Sect. 6.

5. The dynamical domain wall

In the previous section we discussed some properties of the effective action under the assumption that the ground state of \(\mathcal{H}\) is non-degenerate. The ground state will be degenerate if \(\mathcal{H}\) has an exact zero mode or, equivalently, if the matrix \(e^{-\mathcal{H}}\) has a unit eigenvalue

\[ e^{-\mathcal{H}}\psi_0 = \psi_0. \]  

(5.1)

If eq. (5.1) holds for a particular background field we expect strong correlations across the five dimensional slab. In particular, the anomalous term in NSAS Ward identities receives its dominant contribution from such configurations. It is therefore important to identify these configurations and to understand their properties.

The matrix operator \(e^{-\mathcal{H}}\) is non-local, and to understand better the physical content of eq. (5.1) we want to find a simpler equation satisfied by the zero mode \(\psi_0\). Using eqs. (3.7), (3.8) and (3.9) it is straightforward to show that

\[ 0 = (K^\dagger - K^{-1})\psi_0 = B^{-1/2}\gamma_5 D^\parallel \psi_0. \]  

(5.2)

Since \(B\) is a positive definite operator, we conclude that \(\psi_0\) is a zero mode of the hermitian operator \(\gamma_5 D^\parallel\). Therefore, a necessary and sufficient condition for the existence of a zero mode is

\[ \det (\gamma_5 D^\parallel) = 0. \]  

(5.3)

Notice that the l.h.s. of eq. (5.3) is a polynomial in the group variables \(U_{x,\mu}\).

Since \(D^\parallel\) is a massive lattice Dirac operator, one may ask whether eq. (5.1) has any non-trivial solutions at all. An indirect way to argue that such solutions should exist, is to observe that this is a necessary condition for \(\langle 0_H | O(m) | 0_H \rangle\) to reproduce the instanton results. The vanishing of this expectation value for \(m = 0\) requires that level crossing should occur in the spectrum of \(\mathcal{H}\). At the crossing point one has a solution of eq. (5.1). This observation was made by Narayanan and Neuberger [16], who also found numerically solutions of eq. (5.1).
The reason why solutions to eq. (5.1) exist in spite of the mass term present in $D^\parallel = D^\parallel(M)$, is the unconventional sign of that mass term. For comparison, the conventional Dirac operator for a massive Wilson fermion is $D^\parallel(-M)$ in our notation. The “wrong” sign of the mass term relative to the Wilson term, implies that the sum of the two terms is not a positive definite operator. As a result, Vafa-Witten bounds [26] cannot be established here. On the other hand, if one were to choose the conventional relative sign, then a Vafa-Witten bound could be establish for the propagation of fermions in all directions. This, in turn, would imply the absence of any light states in the model. Indeed, one can easily check that the massless surface modes disappear for $M < 0$. We comment that in the domain wall case, too, all the non-trivial dynamics occurs on that side of the wall where one has the “wrong” relative sign.

In the absence of gauge fields, as well as in perturbation theory, the only zero modes of the five dimensional Dirac operator $D_F$ are the ones discussed in refs. [12, 21, 14]. But with dynamical gauge fields, other zero modes can exist. Since the gauge field is $s$-independent, any zero mode of the four dimensional operator $D^\parallel$ will also be a zero mode of the five dimensional operator $D_F$. This is true up to boundary effects, which can be ignored here because the new type of zero modes in not localized in the $s$-direction.

An interesting example is provided by the dynamical domain wall. For simplicity we consider here a $U(1)$ gauge group. (The same configuration exists also for $SU(2)$. For general $SU(N)$ one can simply embed the below configuration in some $SU(2)$ subgroup). We consider the following configuration of link variables. We let $U_{x,\mu} = 1$ for $\mu = 1, 3, 4$. For $U_{x,2}$ we take

$$U_{x,2} = \begin{cases} 
 1, & x_1 < x_1^0, \\
 -1, & x_1 \geq x_1^0. 
\end{cases}$$

(5.4)

Notice that this is essentially a two dimensional configuration. Eq. (5.4) describes a wall of magnetic flux, with one unit of flux going through each plaquette to the left of the hyperplane $x_1 = x_1^0$.

We now consider the ansatz

$$\psi_0 = \frac{1}{2} (1 - \gamma_1) \Psi_0(x_1).$$

(5.5)

One can easily check that the following is a zero mode of $D^\parallel$

$$\Psi_0(x_1) = \begin{cases} 
 (1 - M)x_1^0 - x_1, & x_1 < x_1^0, \\
 (3 - M)x_1^0 - x_1, & x_1 \geq x_1^0. 
\end{cases}$$

(5.6)
This is the simplest case of a dynamically generated zero mode. Other gauge field configurations with a topological character may also support zero modes of $D_{\parallel}$. These include for example lattice analogs of the static string-like singularity discussed in ref. [27]. The zero modes observed in ref. [16] are actually of that type.

Finally, we recall the close relationship between the fermionic and PV action. Whenever the hermitian operator $\gamma_5 D_{\parallel}$ has light states, the same will be true for the PV fields. Therefore, anomalously strong correlations in the $s$-direction arise simultaneously for the fermions and the PV fields. However, the two contributions to the anomalous term do not cancel each other in general.

In the Ward identity eq. (2.33) which governs the pion mass, the anomalous term is the correlator of two pseudoscalar densities. As a generalization of similar results for Wilson fermions, one can prove in the present model the positivity of a whole family of correlators of pseudoscalar densities. The details can be found in App. B. As a result, the anomalous term in eq. (2.33) is strictly positive for finite values of $N$ and $g_0$. The vanishing of the anomalous term in the limit $N \to \infty$ can only arise from the vanishing of its absolute value on almost the entire gauge field configuration space.

6. The chiral limit

The characterization (5.3) of gauge field configurations which support exact fermionic zero modes, allows us to prove the following important result (see eq. (1.2))

$$\lim_{N \to \infty} Z(g_0, L, N, m) = \int \mathcal{D}U e^{-S_G(U)} \langle 0_H | O(m) | 0_H \rangle.$$  

In technical terms, eq. (6.1) means that we can interchange the order of the $N \to \infty$ limit and the integration over the group variables. As we discuss below, the physical content of eq. (6.1) is that correlation functions obey clustering in the $s$-direction.

Let us first introduce some terminology. The gauge field configuration space is $\mathcal{G} = (SU(N_c))^{4L^4}$. An element of $\mathcal{G}$, i.e. a particular configuration of link variables will be denoted by $U = \{U_{x,\mu}\}$. We let $\mathcal{G}_0 \subset \mathcal{G}$ be the subspace of all configurations which satisfy condition (5.3).

In this section we make the technical assumption $0 \leq m \leq 1$. (The reader should not confuse this condition with the similarly looking one $0 < M < 1$, which we enforce for entirely different reasons). The condition $m \geq 0$ ensures the positivity of $\langle 0_H | O(m) | 0_H \rangle$. In the continuum limit we expect to recover the symmetry under $m \to -m$, and so choosing a non-negative $m$ should not lead to any restrictions on the physical content of the model. The condition $|m| \leq 1$ implies $\|O(m)\| \leq 1$. This
gives rise to less cumbersome expressions for some of the bounds below. As we have already explained, the physically interesting case is $|m| \ll 1$.

The proof of eq. (6.1) is simple, and it relies on the following ingredients. (a) The gauge field is $s$-independent, and the configuration space $\mathcal{G}$ is compact. (b) According to standard results in calculus, the subspace $\mathcal{G}_0$ has a zero measure.

Consider an element $U \in \mathcal{G} - \mathcal{G}_0$, and let $E_n$ be the eigenvalues of $H(U)$. We define

$$E_0(U) = \min \{ |E_n| \} .$$

(6.2)

Since $H(U)$ is a finite dimensional matrix, $E_0(U)$ is well-defined, and since $U \in \mathcal{G} - \mathcal{G}_0$, one has $E_0(U) > 0$.

We use this information to put a bound on the difference between the r.h.s. of eq. (3.18) and the r.h.s. of eq. (3.19). Separating the ground state contribution from the rest we find

$$\left| \left| \left| \text{tr} T^{2N} \mathcal{O}(m) / \left( \text{tr} T^N \right)^2 - \langle 0_H | \mathcal{O}(m) | 0_H \rangle \right| \right| \right| \leq \lambda_{\max}^{-2N} \text{tr}' T^{2N} + \left| \lambda_{\max}^{2N} (\text{tr} T^N)^{-2} - 1 \right| \leq 2^{Nt} \left[ e^{-2N E_0(U)} + e^{-2N E_0(U)} (2 + 2^{Nt} e^{-N E_0(U)}) \right] .$$

(6.3a)

The notation $\text{tr}'$ means that the ground state contribution is excluded. Notice that $2^{Nt}$ is the dimensionality of the fermionic Fock space. The last row of the above inequality highly overestimates its first row. Nevertheless, it will be sufficient for our purpose, because it implies that expression (6.3a) vanishes in the limit $N \to \infty$ for $E_0(U) > 0$.

We now have to show that for arbitrary $\epsilon > 0$, there exist $N_\epsilon$ such that

$$\left| Z(g_0, L, N, m) - \int_{\mathcal{G}} DU e^{-S_{\mathcal{O}}(U)} \langle 0_H | \mathcal{O}(m) | 0_H \rangle \right| \leq \epsilon ,$$

(6.4)

for every $N \geq N_\epsilon$. To this end, we divide the group integration into two parts

$$\int_{\mathcal{G}} DU = \int_{\mathcal{G}_\epsilon} DU + \int_{\mathcal{G} - \mathcal{G}_\epsilon} DU .$$

(6.5)

$\mathcal{G}_\epsilon$ is an open covering of $\mathcal{G}_0$ whose volume is less than $\epsilon/4$. Such an open covering can always be found. Furthermore, the r.h.s. of both eqs. (3.18) and (3.19) is always bounded by one. Hence, the contribution to the l.h.s. of inequality (6.4) coming from the integration over $\mathcal{G}_\epsilon$ is bounded by $\epsilon/2$.

Now let us denote

$$E_0 = \min \{ E_0(U) \mid U \in \mathcal{G} - \mathcal{G}_\epsilon \} .$$

(6.6)
Since $\mathcal{G} - \mathcal{G}_c$ is compact, the minimum exists and satisfies $E_0 > 0$. It now follows that the contribution to the l.h.s. of inequality (6.4) coming from the integration over $\mathcal{G} - \mathcal{G}_c$ is bounded by expression (6.3c) with $E_0(U)$ replaced by $\bar{E}_0$. The existence of $N_\varepsilon$ such that inequality (6.4) holds now follows from that fact that $\bar{E}_0 > 0$. This completes the proof of eq. (6.1).

Similar results can be established for correlation functions. In order to prove the restoration of NSAS in the limit $N \to \infty$, we have to show that the anomalous term (2.32) in the Ward identity eq. (2.31) vanishes for any operator $O(y_1, y_2, \ldots)$ which is constructed solely out of the quark operators in eq. (2.29).

Consider first a fixed background field $U \in \mathcal{G} - \mathcal{G}_0$. Suppressing the coordinates $y_1, y_2, \ldots$ we find in the limit $N \to \infty$

$$\lim_{N \to \infty} \langle J_a^5(x) O \rangle_{U,N} = \langle 0_H | \hat{O}_L O(m) \hat{O}_R | 0_H \rangle \langle 0_H | \check{J}_5^a(x) | 0_H \rangle .$$

(6.7)

The subscript $U$ indicates the we have given the expression for the correlator in a fixed background. Here

$$\check{J}_5^a(x) = \hat{c}_x^\dagger \lambda^a \hat{c}_x - \hat{d}_x^\dagger \lambda^a \hat{d}_x .$$

(6.8)

The operator expressions for $\hat{O}_L$ and $\hat{O}_R$ can be found using the rules of App. A. For finite $N$, the difference between the expressions on the l.h.s. and the r.h.s. of eq. (6.7) obeys a bound analogous to inequality (6.3). The crucial observation is that the matrix element $\langle 0_H | \check{J}_5^a(x) | 0_H \rangle$ is proportional to $\text{tr} \lambda^a$, and so it vanishes identically for a non-singlet pseudo-scalar density. Hence

$$\left| \langle J_a^5(x) O \rangle_{U,N} \right| \leq c 2^{2N_\varepsilon} e^{-NE_0(U)} .$$

(6.9)

The constant $c$ is the product of the operator norms $\| \hat{O}_L \hat{O}_R \|$ and $\| \check{J}_5^a \|$. Integrating over the group variables and following the same reasoning as before we conclude that

$$\lim_{N \to \infty} \langle J_a^5(x) O \rangle_N = 0 .$$

(6.10)

This proves the restoration of NSAS in the chiral limit $N \to \infty$. As an example, the explicit expression for the $N \to \infty$ limit of the ward identity (2.33) is given in App. A.

We conclude this section with two comments. For the singlet current, $\text{tr} I \neq 0$, and the matrix element $\langle 0_H | \check{J}_5^a(x) | 0_H \rangle$ is in general non-zero. As was shown in refs. [20, 18, 16, 15] the axial anomaly is reproduced correctly in the continuum limit.

Our second comment concerns the factorized form of the r.h.s. of eq. (6.7). In the limit $N \to \infty$, factorization of the expectation value of an operator product occurs whenever the limiting s-separation between two factors in the product tends
to infinity. This means that correlation functions obey clustering in the s-direction. Now, clustering is by itself a rather weak condition, which we normally expect to hold even if massless particles can propagate between two points. As is often the case with rigorous bounds, we believe that the actual damping of correlations in the s-direction is much stronger, and that the correlation length in the s-direction is finite in physical units, if not in lattice units. A heuristic discussion of the actual magnitude of anomalous effects for finite $N$ is given in the concluding section.

7. Conclusions

In this paper we discussed in detail a new formulation of lattice QCD which is based on the surface fermions scheme. Our main result is that non-singlet axial symmetries become exact in the chiral limit. The chiral limit is defined to be the limit of an infinite fifth direction, at fixed finite values of the bare coupling and the size of the four dimensional lattice. The vanishing of the anomalous term in all NSAS Ward identities implies in particular that non-singlet axial currents do not undergo any renormalization in the chiral limit, as should be the case for truly conserved currents.

As was shown in previous works [20, 18, 16], the singlet axial anomaly is correctly reproduced if one takes first the limit $N \to \infty$ and then the continuum limit $g_0 \to 0$. For finite $g_0$, the limiting “$N = \infty$” formulation is therefore a new non-perturbative regulator of QCD which is maximally symmetric under axial transformations. This new regularization scheme is mildly non-local because we have integrated out an infinite number of heavy four-dimensional fields. We believe that the mild non-locality does not jeopardize the consistency of the continuum limit, but we have not investigated every possible aspect of this issue.

The non-singlet currents defined in eq. (2.25) are exactly conserved in the limit $N \to \infty$ regardless of the value of $g_0$. Thus, they will be conserved not only in the continuum limit, but also in the strong coupling limit. However, it is not necessarily true that in the strong coupling limit, these currents retain the physical significance of axial current. We do not rule out that for sufficiently strong coupling, some or all of the doubler modes reappear. The likely consequence would be that the currents of eq. (2.25) become vectorial with respect to the new massless spectrum. In this case, the singlet current would become vectorial too, and it will be conserved in the strong coupling phase.

Returning to the physically interesting limit $g_0 \ll 1$, the biggest advantage of the new formulation is that fine tuning is no longer needed in the fermion sector. For
example, the theoretical values of current masses are determined using weak coupling perturbation theory, and they involve only multiplicative renormalization. Likewise, operator mixing are restricted by the naive transformation properties under nonsinglet axial symmetries, and meson decay constants can be inferred directly from the corresponding Ward identities.

All the above properties become exact in the limit $N \to \infty$. Looking forward to the implementation of the surface fermions scheme in numerical simulations, it is important to have a realistic estimate of the magnitude of anomalous effects on a finite five dimensional lattice. While sufficient for proving the restoration of NSAS in the limit, we believe that the rigorous bounds used in Sect. 6 represent a gross overestimation on the actual magnitude of anomalous effects. We have decide to include here a short heuristic discussion of this issue, mainly because we believe that the true picture is much more promising. A more detailed study is relegated to a separate publication.

Our central observation is the following. As we noted previously, the naive continuum limit of the lattice operator $D^\parallel$ is a massive Dirac operator. This does not rule out the existence of (exact or approximate) zero modes of $D^\parallel$ for certain gauge field configurations. But it does indicate that the relevant configurations cannot in any sense be the discretized approximation of smooth continuum gauge fields. It may therefore be possible to prove the following conjecture: if a given lattice gauge field is the discretized approximation of a smooth continuum gauge field, then there is an $O(1)$ gap in the spectrum of the (hermitian) operator $\gamma_5D^\parallel$. We have intentionally omitted here a precise definition of what we mean by a “lattice approximation of a smooth continuum gauge field”. Basically what we have in mind is a condition which states that the gauge field’s action density is very small everywhere. However, there may be other definitions that have the same physical content, and which are more convenient from a mathematical point of view.

The above conjecture receives circumstantial evidence from the two known examples of zero modes of $D^\parallel$. These are the singular fluxon of ref. [16], and the singular dynamical domain wall of Sect. 5. Both are characterize by an action density which is $O(1)$ on some $n$-dimensional subspace, where $n = 2$ and $n = 3$ respectively for a fluxon and for a domain wall. Now, if we want the configuration to support an approximate zero mode whose energy is $E_0 \ll 1$, then its longitudinal extension should be at least $O(1/E_0)$. This implies that the total gauge field action for such configurations should be bounded from below by $S_G \sim C/(\alpha_0^2 E_0^n)$. Here $C$ is some $O(1)$ constant.

Typically, a single extended configuration supports a single (approximate) zero
mode, up to symmetry factors. In other words, level crossing in the spectrum of $\mathcal{H}$ occurs one at a time, and all other eigenstates are separated by a finite gap in the vicinity of the crossing point. Assuming this to be true in general, all factors of $2^N$ (which count the total number of eigenstates) in the inequalities of Sect. 6 can be dropped. Putting everything together, this suggests that the magnitude of the anomalous term for a given background should be

$$\exp\left\{-\frac{C}{(g_0^2 E_0^5)} - NE_0\right\}. \quad (7.1)$$

To complete the estimate of the anomalous term, it is necessary to determine what are the most important singular configurations. If all configurations have $n > 0$, the most important effect should be the need to increase the longitudinal extension of the singular configuration with decreasing $E_0$. The dominant configurations, as well as the magnitude of the resulting anomalous term, can then be determined by a saddle point approximation. If, on the other hand, there exist point-like four dimensional configurations which support (approximate) zero modes of $\gamma_5 D^\parallel$, then a more refined analysis would be needed, and one would have to estimate the phase space for such configurations as a function of $g_0$. We believe that, either way, the correlation length in the $s$-direction should turn out to be finite. If it is found that, moreover, the correlation length in the $s$-direction remains finite in lattice units, then we may hope to obtain good results already on five dimensional lattices which can be simulated today.

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A. Correlation functions in the $N = \infty$ limit

In this appendix we give the transfer matrix formulae for various correlation functions. The correlation functions for the quark operators $(2.29)$ take a particularly simple form in the limit $N = \infty$. For example, the expression for the quark condensate is

$$\langle \bar{q}q \rangle_U = -\langle 0_H | \hat{c}^\dagger \mathcal{O}(m) \hat{c} | 0_H \rangle - \langle 0_H | \hat{d}^\dagger \mathcal{O}(m) \hat{d} | 0_H \rangle.$$ \quad (A.1)

The subscript $U$ indicates that we give the expression for the correlator in a fixed background field. Another example is the two pion correlator

$$\langle \pi^-(x) \pi^+(y) \rangle_U = -\langle 0_H | \hat{c}^\dagger_{x\uparrow} \hat{c}^\dagger_{y\uparrow} \mathcal{O}(m) \hat{c}_{y\uparrow} \hat{c}_{x\uparrow} | 0_H \rangle.$$
\[
+ \left\langle 0_H \left| \hat{c}_x^\dagger \hat{d}_y^\dagger O(m) \hat{d}_y \hat{c}_x \right| 0_H \rightangle
+ \left\langle 0_H \left| \hat{d}_x^\dagger \hat{c}_y^\dagger O(m) \hat{c}_y \hat{d}_x \right| 0_H \rightangle
- \left\langle 0_H \left| \hat{d}_x^\dagger \hat{d}_y^\dagger O(m) \hat{d}_y \hat{d}_x \right| 0_H \rightangle.
\]

(A.2)

Here

\[
\pi^- = i \bar{q}_L \gamma_5 q_L,
\]
\[
\pi^+ = i \bar{q}_L \gamma_5 q_R.
\]

(A.3)

The arrows denote isospin. Notice that the pion operators are special cases of the pseudoscalar densities eq. (2.27).

The general prescription for correlation functions of the quark operators eq. (2.29) is the following. Considering \( q_{R,L} \) and \( \bar{q}_{R,L} \) as Grassmann variables, one first reorder each product of quark operators such that \( q_L \) and \( \bar{q}_L \) occur to the left of all \( q_R \) and \( \bar{q}_R \). This step may result in a minus sign. One then translates the result into a matrix element of the form

\[
\left\langle 0_H \left| \cdots O(m) \cdots \right| 0_H \right\rangle.
\]

(A.4)

The operators to the left of \( O(m) \) are obtained from the ordered product of \( q_L \)-s and \( \bar{q}_L \)-s by the substitution

\[
\bar{q}_L \rightarrow \hat{c}^\dagger,
q_L \rightarrow \hat{d}^\dagger.
\]

(A.5)

Similarly, on the right of \( O(m) \) one makes the substitution

\[
\bar{q}_R \rightarrow \hat{d},
q_R \rightarrow -\hat{c}.
\]

(A.6)

All indices are left unchanged in this substitution. (The transition from the Grassmann path integral to operator language involves a non-local transformation at an intermediate step \[23, 16\]. But this non-locality cancels out in the final expression).

Apart from quark operators, we may also be interested in the transfer matrix formulae for correlation functions that involve vector or axial currents. As an example, for finite \( N \), the correlator on the l.h.s. of eq. (2.31) becomes

\[
\left\langle A^a_\mu(x) O(y_1, y_2, \ldots) \right\rangle_{l,t} = \sum_{s=0}^{2N-1} \text{sign}(N - s - \frac{1}{2}) \frac{\text{tr} T^{2N} \hat{O}_L O(m) \hat{O}_R \hat{j}^a_\mu(x, s)}{\left(\text{tr} T^N\right)^2}
\]

(A.7)

where

\[
\hat{j}^a_\mu(x, s) = T^s \hat{j}^a_\mu(x) T^{-s}.
\]

(A.8)
To obtain an explicit expression for $\hat{j}_\mu^a(x)$, the different terms in eq. (2.16) are translated according to the following rules

$$
\begin{align*}
\bar{\psi}_{L,x} \psi_{R,y} & \rightarrow -\hat{c}_y T \hat{c}_x T^{-1} \\
\bar{\psi}_{R,x} \psi_{L,y} & \rightarrow -\hat{d}_x T \hat{d}_y T^{-1} \\
\bar{\psi}_{L,x} \psi_{L,y} & \rightarrow -T \hat{c}_x \hat{d}_y T^{-1} \\
\bar{\psi}_{R,x} \psi_{R,y} & \rightarrow -\hat{d}_x \hat{c}_y
\end{align*}
$$

(A.9)

The somewhat unexpected appearance of the transfer matrix $T$ in these rules is due to our definition of $\exp\{-H\}$ eq. (3.4). If instead we decided to use $\exp\{-H'\} = K^\dagger K$ and the corresponding transfer matrix $T'$, then there would be no factors of $T'$ in resulting expression for $\hat{j}_\mu^a(x)$. On the other hand, the expressions for quark correlators would become more cumbersome.

Convergence of the infinite sum on the l.h.s. of every Ward identity is guaranteed by the finiteness of the r.h.s. We comment that, if a slightly stronger form of clustering than the one proved in Sect. 6 holds, then

$$
\lim_{N \to \infty} \left\langle A^a_\mu(x) \mathcal{O}(y_1, y_2, \ldots) \right\rangle_U = \sum_{s=0}^{\infty} \langle 0_H | \hat{O}_L \mathcal{O}(m) \hat{O}_R \hat{j}_\mu^a(x, s) | 0_H \rangle \\
- \sum_{s=-\infty}^{-1} \langle 0_H | \hat{j}_\mu^a(x, s) \hat{O}_L \mathcal{O}(m) \hat{O}_R | 0_H \rangle .
$$

(A.10)

This equation is in particular valid if, as we have every reason to believe, the correlation length in the $s$-direction is finite.

**B. Inequalities**

Eq. (2.12) implies an analogous identity for fermion propagator, considered as a matrix. Writing the coordinates explicitly one has

$$
\gamma_5 G(x, s; y, s') \gamma_5 = G^\dagger(y, 2N + 1 - s'; x, 2N + 1 - s).
$$

(B.1)

Here the dagger refers only to the the suppressed internal indices. We will use this identity to prove the positivity of correlators of the following pseudoscalar densities

$$
K^a(x, t) = i\bar{\psi}(x, N + t) P_R \lambda^a \psi(x, N + 1 - t) \\
- i\bar{\psi}(x, N + 1 - t) P_L \lambda^a \psi(x, N + t).
$$

(B.2)

Notice the special cases

$$
K^a(x, 0) = iJ_{5q}^a(x),
$$

(B.3)
Using eq. (B.1) and inserting a minus sign for the closed fermion loop we now obtain
\[ \langle K^a(x, t) K^b(y, t') \rangle = \delta^{ab} Z^{-1} \int DU e^{-S(U)} (\det D_F(U))^N_I (U; x, t; y, t'), \] (B.5)

where
\[ I = \text{tr} \left\{ P_R G(y, N + t'; x, N + 1 - t) P_R G^\dagger(y, N + t'; x, N + 1 - t) \right. \\
+ P_R G(y, N + 1 - t'; x, N + 1 - t) P_L G^\dagger(y, N + t'; x, N + t) \\
+ P_L G(y, N + 1 - t'; x, N + t) P_R G^\dagger(y, N + 1 - t'; x, N + t) \left. \right\}. \] (B.6)

For even \( N_f \) or for \( m > 0 \), the factor \( (\det D_F(U))^N_I \) is positive. We assume that one of these conditions is satisfied. It is now straightforward to prove the positivity of each term in eq. (B.6). Consider the second row as an example. Independently of the values of \( x \) and \( y \), it has the generic form
\[ \text{tr} \left\{ P_R A P_L A^\dagger \right\} = \text{tr} \left\{ P_R^2 A P_L^2 A^\dagger \right\} = \text{tr} \left\{ (P_R A P_L) (P_R A P_L)^\dagger \right\}. \] (B.7)
The last row is manifestly positive.

Consider now the Ward identity (2.33) which determines the pion mass. Notice that
\[ \pi^a(y) = K^a(x, N). \] (B.8)
Using eq. (B.3) the anomalous term in this Ward identity can be written as
\[ \langle K^a(x, 0) K^a(x, N) \rangle, \] (B.9)
which is positive according to the previous discussion. The same reasoning proves the positivity of the two-pion correlator.

The positivity of the two-pion correlator can also be established directly from the \( N = \infty \) formula eq. (A.2). One should notice that the Fock space is a direct product of the Up and Down Fock spaces. Thanks to factorization of \( \mathcal{O}(m) = \mathcal{O}_\uparrow(m) \mathcal{O}_\downarrow(m) \), each matrix element in eq. (A.2) becomes the product of two complex conjugate matrix elements, one in the Up Fock space and one in the Down Fock space.
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