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Theoretical Foundation for the Index Theorem on the Lattice with Staggered Fermions

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A way to identify the would-be zero modes of staggered lattice fermions away from the continuum limit is presented. Our approach also identifies the chiralities of these modes, and their index is seen to be determined by gauge field topology in accordance with the index theorem. The key idea is to consider the spectral flow of a certain Hermitian version of the staggered Dirac operator. The staggered fermion index thus obtained can be used as a new way to assign the topological charge of lattice gauge fields. In a numerical study in U(1) backgrounds in two dimensions it is found to perform as well as the Wilson index while being computationally more efficient. It can also be expressed as the index of an overlap Dirac operator with a new staggered fermion kernel.

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The computational efficiency and other attractive features of the staggered lattice fermion formulation made possible the first high-precision lattice simulations of quantum chromodynamics (QCD) [1], and it continues to be widely used. However, this formulation has long been perceived as disadvantaged compared to Wilson fermions—the other traditional lattice fermion formulation—regarding topological aspects of QCD. This concerns, in particular, the index theorem [2] relating gauge field topological charge to fermionic zero modes, which is needed to explain the large mass of the $\eta'$ meson [3]. A field-theoretic approach to the staggered fermion index was developed and used by Smit and Vink [4,5]; however, it does not give an integer value for the index from the beginning and requires a renormalization that depends on the full ensemble of lattice gauge fields. In contrast, for Wilson fermions, an integer-valued index is obtained without any need for renormalization. This is because Wilson fermions have identifiable would-be zero modes with definite chirality, provided the lattice gauge field is not too rough, from which the index can be defined. The Wilson fermion index [4,6,7], calculated from its equivalent description as the index of the overlap Dirac operator [8], is currently widely used for issues such as calculation of the topological susceptibility [9] and investigations of topological structure in the QCD vacuum—see, e.g., [10]. But for staggered fermions it has not been known how to identify the would-be zero modes and their chiralities in nonsmooth gauge field backgrounds; they were only seen to emerge in simulations with improved actions that are sufficiently close to the continuum [11].

In this Letter we show how the would-be chiral zero modes of staggered fermions can be identified away from the continuum limit when the background gauge field is not too rough, thus determining an integer-valued index. A theoretical foundation for the index theorem for staggered fermions is established, placing them on the same footing as Wilson fermions in this regard.

Our new approach in the staggered case parallels the spectral flow approach to the index theorem for continuum and Wilson lattice fermions [6,7], which we begin by briefly reviewing in the following. Spacetime is taken to be a Euclidean box with periodic boundary conditions (the setting in which Lattice QCD simulations are performed) with even dimension $d$. Besides the physically relevant case $d = 4$ we will also consider $d = 2$ for illustrative purposes. From the Hermitian Dirac gamma matrices $\{\gamma_{\mu}\}_{\mu=1,...,d}$ the chirality matrix $\gamma_5 = -(i)^{d/2} \gamma_1 \cdots \gamma_d$ is defined. It has the properties $\gamma_5^2 = \gamma_5$, $\gamma_5^2 = 1$, $\{\gamma_5, \gamma_{\mu}\} = 0$ and $\{\gamma_5, D\} = 0$ where $D = \gamma_{\mu} (\partial_{\mu} + A_{\mu})$ is the continuum massless Dirac operator on spinor fields coupled to a gauge field $A$. Consequently, the vector space of zero modes of $D$ (i.e., solutions to $D \psi = 0$) decomposes into $\pm$ chirality subspaces on which $\gamma_5 = \pm 1$. The index of $D$ is the difference between the numbers $n_+$ of independent $\pm$ chirality zero modes, and is fixed by topology: Gauge fields with smooth field tensor $F_{\mu\nu}(x)$ have an integer topological charge $Q$, and the index theorem in this setting states

$$n_+ - n_- = (-1)^{d/2} Q.$$ \hspace{1cm} (1)

The spectral flow perspective on the index arises by considering the eigenvalues $\{\lambda(m)\}$ of the Hermitian operator

$$H(m) = \gamma_5 (D - m)$$ \hspace{1cm} (2)

as a function of the parameter $m$. Note that a zero mode $\psi$ of $D$ with $\pm$ chirality is also an eigenmode of $H(m)$ with eigenvalue $\lambda(m) = \mp m$, crossing the origin with slope $\mp 1$ at $m = 0$. Furthermore, from the property

$$H(m)^2 = D^\dagger D + m^2$$ \hspace{1cm} (3)

we see that these are the only eigenvalues of $H(m)$ that cross the origin at any value of $m$. It follows that the spectral flow of $H(m)$, defined as the net number of eigenvalues $\lambda(m)$ of $H(m)$ that cross the origin, counted with
sign \( \pm \) depending on the slope of the crossing, comes entirely from eigenvalue crossings at \( m = 0 \) and equals \( n_+ - n_- \), i.e., minus the index.

In the lattice setting with Wilson fermions, the would-be zero modes can be identified as the low-lying real eigenvalues of the Wilson-Dirac operator \( D_W \) [4,12]. The spectral flow perspective [6,7] is based on the Hermitian lattice analogue of (2):

\[
H_W(m) = \gamma_5 (D_W - m).
\]  

(4)

Regarding the spectral flows \( H_W(m) \psi(m) = \lambda(m) \psi(m) \), note that \( \lambda(m_0) = 0 \Leftrightarrow D_W \psi(m_0) = m_0 \psi(m_0) \). Thus eigenvalue crossings of \( H_W(m) \) are in one-to-one correspondence with real eigenvalues of \( D_W \). Furthermore, after normalizing eigenmodes such that \( \psi^\dagger \psi = 1 \) one easily finds \( \lambda'(m) = - \psi(m)^\dagger \gamma_5 \psi(m) \) [6]. Thus the sign of the slope of \( \lambda(m) \) at a low-lying crossing value \( m_0 \) is minus the chirality of the corresponding would-be zero mode \( \psi(m_0) \) for \( D_W \). It follows that the index of \( D_W \) is minus the spectral flow of \( H_W(m) \) coming from the eigenvalues which cross the origin at low-lying values of \( m \). Numerical results illustrating this can be found, e.g., in [6]. An illustration in the \( d = 2 \) case is given in Fig. 4 below.

Turning now to staggered lattice fermions, where the lattice field \( \chi(x) \) is scalar (rather than spinor) and describes \( \delta^{d/2} \) degenerate continuum fermion species (called quark tastes), the massless staggered Dirac operator is

\[
D_{st} = \eta_{\mu} \nabla_{\mu},
\]  

(5)

where \( \nabla_{\mu} \) is the usual lattice finite difference operator coupled to the lattice gauge field and \( \eta_{\mu} \chi(x) = (-1)^{n_1 + \ldots + n_d} \chi(x) \) where \( x = (n_1, \ldots, n_d) \) runs over the lattice sites. \( D_{st} \) is anti-Hermitian and therefore has purely imaginary spectrum. Consequently, the identification of would-be zero modes in the Wilson case does not carry over to the staggered case since it relied crucially on the role of nonzero real eigenvalues. For the same reason it is clear that an index of \( D_{st} \) cannot be obtained from spectral flow of a staggered version of \( H_W(m) \). In fact the staggered analogue of (4), \( \Gamma_5 (D_{st} - m) \), is not even Hermitian. However, there is an alternative spectral flow approach which we now discuss, and which turns out to be perfectly suited to the staggered case.

Return momentarily to the continuum setting and note that \( H(m) \) in (2) is not the only Hermitian operator that can be used for the spectral flow perspective on the index. We could just as well use \( H(m) = iD - m \gamma_5 \). Its spectral flow is equal to minus the index of \( D \) just as before, since the previous argument, including the property (3), holds verbatim for this operator. But now the analogue in the staggered case,

\[
H_{st}(m) = iD_{st} - m \Gamma_5
\]  

(6)

is also Hermitian, so we can consider its spectral flow as well. Here \( \Gamma_5 \) is the analogue of \( \gamma_5 \) in the staggered formulation; it is Hermitian and corresponds up to \( O(a) \) discretization errors to \( \gamma_5 \otimes 1 \) in the spin-flavor interpretation [13]. Note that \( H_{st}(0) = iD_{st} \) so the eigenvalues of \( D_{st} \) are \( \{ -i \lambda(0) \} \) where \( \{ \lambda(m) \} \) are the eigenvalue flows of \( H_{st}(m) \). This fact allows us to identify the would-be zero modes of \( D_{st} \); as shown below, they are the eigenmodes with eigenvalues \( -i \lambda = -i \lambda(0) \) for which the associated flow \( \lambda(m) \) crosses zero at a low-lying value of \( m \). Furthermore, the sign of the slope of the crossing is minus the chirality of the would-be zero mode, and hence the index is minus the spectral flow of \( H_{st}(m) \) coming from the crossings at low-lying values of \( m \).

To see this, consider first the situation in a smooth continuumlike gauge field background: The eigenvalues \( -i \lambda \) of the would-be zero modes \( \chi \) of \( D_{st} \) separate out from the rest of the spectrum; they are almost zero and have approximately definite chirality \( \chi^\dagger \Gamma_5 \chi = \pm 1 \). For the corresponding eigenvalue flows \( \lambda(m) \) of \( H_{st}(m) \) we have \( \lambda'(m) = - \chi(m)^\dagger \Gamma_5 \chi(m) \) just as in the Wilson case. Since \( \chi = \chi(0) \) it follows that \( \lambda(0) = \mp 1 \), and since \( \lambda = \lambda(0) \) is almost zero it then follows that \( \lambda(m) \) crosses the origin at a very small (in magnitude) value \( m_0 \) of \( m \). Whether \( m_0 \) is positive or negative depends on the chirality and sign of \( \lambda(0) \), but in either case the sign of the slope of the crossing is the same as that of \( \lambda'(0) \), i.e., minus the chirality. Under a roughening of the gauge field the location of a crossing will move, but it cannot disappear until it meets another crossing with opposite slope. Hence the would-be zero modes remain identifiable with unchanged chiralities and index.

To illustrate the identification of the staggered would-be zero modes and their index we present results of a numerical study in U(1) backgrounds in two dimensions. Following [4] we start from specific smooth lattice gauge fields with topological charge \( Q \) and roughen them by multiplying the link variables by random phase factors: \( U_{\mu}(x) \rightarrow e^{i \delta_{\mu}(x) \delta} U_{\mu}(x) \) with each \( r_{\mu}(x) \) randomly chosen in \([ -\pi, \pi] \); the parameter \( \delta \) controls the roughness. Our numerical computations were all on the \( 12 \times 12 \) lattice (as in [4]) and done using ARPACK [14]. The code was checked by reproducing the results in Table 1 of [4].

Figure 1 shows low-magnitude eigenvalues of \( H_{st}(m) \) versus \( m \) (horizontal axis) in a \( Q = 1 \) background of moderate roughness \( \delta = 0.33 \). The low-magnitude eigenvalues of \( iD_{st} \) are the eigenvalues at \( m = 0 \) in the figure. There is no clear separation in their magnitudes. Nor is there a clear separation in the magnitudes of the chiralities as measured by \( \chi^\dagger \Gamma_5 \chi \); numerical calculation of this quantity for the 3 pairs of eigenmodes with lowest-magnitude eigenvalues gives \(-0.28, +0.17, +0.13 \). Nevertheless, the would-be zero modes can now be identified among these low-magnitude modes: as discussed above, they are precisely the eigenmodes whose eigenvalues \( \lambda = \lambda(0) \) belong to eigenvalue flows \( \lambda(m) \) which cross zero at a low-lying value of \( m \). From the figure we see that there are two of these, both with positive slope, corresponding to negative chirality. Thus the index is \(-2 \). This
is in accordance with the index theorem, since in the staggered fermion case (1) becomes

$$\text{index}(D_\alpha) = 2^{d/2}(-1)^{d/2}Q.$$  \hfill (7)

As a second illustration, Fig. 2 shows the eigenvalue flow in a $Q = -2$ background of the same roughness level $\delta = 0.33$. From the eigenvalues at $m = 0$ we see that $iD_\alpha = H_{\text{st}}(0)$ has one eigenvalue pair of much smaller magnitude than the others. Numerical calculation of $\chi^T \Gamma_5 \chi$ for these gives +0.34 compared to +0.21, +0.13 for the eigenmode pairs with the next two lowest-magnitude eigenvalues. Hence we would naively expect the first pair to be the would-be zero modes, giving index +2. However, from the eigenvalue flows we see that there is in fact one more pair of would-be zero modes of $D_\alpha$, also with positive chirality, giving index +4 in accordance with the index theorem (7).

A crucial property that would-be zero modes of a lattice fermion formulation should have is robustness: they should not disappear under small deformations of the gauge field. This is assured in the present case if there is a clear separation between low- and high-lying crossing regions. Figure 3 shows the eigenvalue flow of $H_{\text{st}}(m)$ in the same background as Fig. 1 but over a larger $m$ range. We see that the eigenvalue crossings only occur in a localized region around $m = 0$ and in high-lying regions, $|m| \approx 9$ in this case. The large separation between low-lying and high-lying crossings illustrates the robustness of the would-be zero modes and index for staggered fermions. For comparison, Fig. 4 shows the eigenvalue flow of the Hermitian Wilson operator $H_W(m)$ in the same gauge field background. It has one low-lying positive-slope crossing in accordance with the index theorem, and the high-lying crossings are localized around $m = 2$ and $m = 4$ as expected on theoretical grounds [6,15].

As in the Wilson case [15], separation between low- and high-lying crossing regions can be proved analytically when the plaquette variables of the lattice gauge field satisfy the approximate smoothness condition $||1 - U_{\mu \nu}(x)|| < \epsilon$ for sufficiently small $\epsilon$ [16]: We derive in [17] a bound of the form

$$H_{\text{st}}(m)^2 \geq \begin{cases} m^2 - K(m,d)\epsilon & \text{for } |m| \leq 1 \\ 1 - K(m,d)\epsilon & \text{for } |m| \geq 1 \end{cases}$$  \hfill (8)

(which is found to be saturated in the free field case where $\epsilon = 0$). The precise form of $K(m,d)$ is not important here, only the fact that it depends continuously on $m$, which ensures that $K_0$ defined in the following is finite. For any $b_1$, $b_2$ with $0 < b_1 < b_2$, set $K_0 = \max\{K(m,d)||m| \leq b_2\}$ and $\epsilon_0 = b_1^2/K_0$, then the bound (8) implies $H_{\text{st}}(m)^2 > 0$ for $b_1 \leq |m| \leq b_2$ when $\epsilon < \epsilon_0$ in the plaquette condition. This shows that the separation between low-lying ($|m| < b_1$) and high-lying ($|m| > b_2$) eigenvalue crossing regions can be made arbitrarily large by taking $\epsilon > 0$ to be sufficiently small.

The performance of the staggered index compared to the Wilson index was investigated in the numerical study with $Q = 1$. For each randomly generated $\{r_{\mu}(x)\}$ we examined the would-be zero modes and index as the roughness increases.

FIG. 1. Staggered spectral flow in a $Q = 1$ background.

FIG. 2. Staggered spectral flow in a $Q = -2$ background.

FIG. 3. Staggered spectral flow over a larger $m$ range in same background as Fig. 1.

FIG. 4. Wilson spectral flow in same background as Figs. 1 and 3.
parameter \( \delta \) is increased. In both the staggered and Wilson cases they were found to remain identifiable up to roughness levels \( 0.33 \leq \delta \leq 0.41 \) (which easily exceeds the limit \( \delta = 0.25 \) at which the field-theoretic approach to the staggered fermion index was found to break down in [4]). Furthermore, in all the backgrounds considered, the breakdown value of \( \delta \) for staggered was found to be the same as for Wilson up to differences \( \Delta \delta = \pm 0.02 \) (which favored staggered as often as Wilson). This suggests that the staggered and Wilson indexes are accessing the same topological content of the lattice gauge field. However, the computational cost was roughly twice as much in the Wilson case. This is as expected since \( d = 2 \) Wilson fermions have two spinor components.

Finally, we show that, analogously to the Wilson case, the staggered fermion index can be obtained as the index of the exact zero modes of an overlap Dirac operator \( D_{ov} \). This is of practical as well as theoretical interest since the Wilson fermion index is usually calculated in practice as \( \text{index}(D_{ov}) \). The role of \( \gamma_5 \) in the overlap construction [8] is not to be played by \( \Gamma_5 \) here since it violates the required property \( \gamma_5^2 = 1 \) by an \( O(\alpha) \) term. Instead we use

\[
\Gamma_{55} \chi(x) = (-1)^{n_1 + \cdots + n_D} \chi(x),
\]

which corresponds to \( \gamma_5 \otimes \gamma_5 \) in the spin-flavor interpretation [13]. We define the overlap Dirac operator with staggered fermion kernel by

\[
D_{ov} = \frac{1}{\alpha} \left( 1 + \Gamma_{55} \frac{H_m(m_0)}{\sqrt{H_m(m_0)^2}} \right),
\]

As in the Wilson case [8] \( D_{ov} \) has exact zero modes, with definite chirality with respect to \( \Gamma_{55} \), and satisfying an index formula

\[
\text{index}(D_{ov}) = -\frac{1}{2} \text{Tr} \left( \frac{H_m(m_0)}{\sqrt{H_m(m_0)^2}} \right),
\]

which also follows from the general index formula in [18] after noting that \( (10) \) satisfies the Ginsparg-Wilson relation [18] with \( \gamma_5 \rightarrow \Gamma_{55} \). As in the Wilson case we take \( m_0 \) to be in the region in between the positive low-lying and high-lying eigenvalue crossings of \( H_m(m) \), then (11) gives

\[
\text{index}(D_{ov}) = \frac{1}{2} \text{index}(D_m).
\]

To see this, note that \( H_m(m) \Gamma_{55} = -\Gamma_{55} H_m(-m) \), which implies a symmetry in the eigenvalue flow: \( H_m(m) \) and \( -H_m(-m) \) have the same spectrum (as seen in Figs. 1–3). It follows that \( H_m(0) \) has symmetric spectrum; therefore (11) is minus the spectral flow from \( m = 0 \) to \( m = m_0 \), which in turn is minus half the spectral flow from \( -m_0 \) to \( m_0 \), i.e., half of index(\( D_m \)).

The staggered overlap operator introduced here is of independent interest as a new fermion formulation for Lattice QCD, and will be studied in a separate paper [17]. It has the remarkable feature of reducing the number of staggered fermion tastes by half [as reflected in the factor 1/2 in (12)]. The physical fields turn out to correspond to the two continuum tastes with positive flavor chirality under \( 1 \otimes \gamma_5 \), so that \( \gamma_5 \otimes \gamma_5 \) chirality is the same as the physical \( \gamma_5 \otimes 1 \) for them. A new staggered version of domain wall fermions is also obtained [17].

In summary, staggered lattice fermions do maintain the important index theorem connection between gauge field topology and fermionic zero modes, but in a way that was not realized previously. In the present \( d = 2 \) study it was seen to perform as well as the Wilson index, but with greater numerical efficiency. Future work should investigate the performance of the index for improved staggered fermions versus Wilson index in backgrounds generated in current Lattice QCD simulations in four dimensions.

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[16] As a practical illustration, \( \text{max}_x |1 - U_m(x)| \) for the backgrounds of Figs. 1 and 2 is 1.949 and 1.950, respectively, which is very close to the maximum possible value 2.