Remnant index theorem and low-lying eigenmodes for twisted mass fermions

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Abstract

We analyze the low-lying spectrum and eigenmodes of lattice Dirac operators with a twisted mass term. The twist term expels the eigenvalues from a strip in the complex plane and all eigenmodes obtain a non-vanishing matrix element with $\gamma_5$. For a twisted Ginsparg-Wilson operator the spectrum is located on two arcs in the complex plane. Modes due to non-trivial topological charge of the underlying gauge field have their eigenvalues at the edges of these arcs and obey a remnant index theorem. For configurations in the confined phase we find that the twist mainly affects the zero modes, while the bulk of the spectrum is essentially unchanged.

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Lattice fermions with a twisted mass term have gained a lot of attention recently \cite{1, 2, 3, 4}. Particularly appealing for numerical simulations is the fact that a twisted mass term cures the notorious problem with exceptional configurations at a very low cost. This allows for simulations with relatively small pion mass close to the physical point \cite{4}.

For small pion masses the role of topological configurations of the gauge field and the corresponding dynamics of low-lying modes of the Dirac operator become more important for QCD phenomenology. Of particular interest is the index theorem \cite{5} and its manifestation on the lattice. While for chiral lattice Dirac operators, obeying the Ginsparg-Wilson equation \cite{6}, an exact index theorem holds \cite{7}, for other formulations only an approximate realization of the index theorem can be expected. For Wilson and staggered fermions this has been studied numerically \cite{8, 9}. For twisted mass fermions the interplay of topology and low-lying Dirac eigenmodes has not yet been analyzed. In this letter we close this gap, combining analytical arguments and numerical results.

The twisted mass Dirac operator $D$ for two mass-degenerate flavors of fermions, $u$ and $d$, has the form

$$D = (D_0 + m) 1_2 + i \mu \gamma_5 \tau_3 \ , \ \tau_3 = \text{diag} \ (1, -1),$$

with $1_2$ and $\tau_3$ acting in flavor space. Alternatively one can define the Dirac operators for $u$ and $d$ separately by $D_u = D(\mu)$ and $D_d = D(-\mu)$ with

$$D(\mu) = D_0 + m + i \mu \gamma_5 .$$

(1)

$D_0$ is a standard lattice Dirac operator and for the numerical results presented here is chosen to be Wilson’s Dirac operator. $\mu$ is the twisted mass parameter and $m$ the regular mass. In our notation we assume $\mu \geq 0$. In this work the mass parameter $m$ is adjusted such that for $\mu = 0$ massless quarks are described (“maximal twist”). We remark, however, that for the study of eigenvalues and eigenvectors $m$ is an irrelevant parameter, since it only shifts the whole spectrum in the complex plane.

As remarked, QCD with a twisted mass term is particularly interesting for lattice simulations since exceptional configurations are avoided because

$$\det[D_u] \det[D_d] = \det[D(\mu)] \det[D(-\mu)] = \det[\gamma_5 D(\mu) \gamma_5] \det[D(-\mu)] = \det[(D_0^\dagger + m + i \mu \gamma_5)(D_0 + m - i \mu \gamma_5)] = \det[(D_0 + m)^\dagger (D_0 + m) + \mu^2] ,$$

(2)

showing that the determinant for two flavors is strictly positive. For staggered fermions the regular mass term already excludes exceptional configurations. For Wilson fermions fluctuations of real eigenvalues can become
large and only for relatively high values of the regular mass are exceptional
configurations ruled out. When using the Wilson operator as input in the
overlap projection, these fluctuations can also make the evaluation of the
square root problematic.

In the second line of Eq. (2) we have used the $\gamma_5$-hermiticity of the Dirac
operator $D_0$,\[ \gamma_5 D_0 \gamma_5 = D_0^\dagger. \]

In passing we note that for non-vanishing twist parameter $\mu$ this equation
is replaced by the generalized $\gamma_5$-hermiticity relation [10]\[ \gamma_5 D(\mu) \gamma_5 = D(-\mu)^\dagger. \]

Since the similarity transformation on the l.h.s. leaves the eigenvalues in-
vvariant, we conclude from (3) that the spectrum of $D(\mu)$ is the complex
conjugate of the spectrum of $D(\mu)$. This property is reflected in the fact,
that the product of determinants in (2) is real.

Let us begin our analysis of the twisted mass Dirac operator $D(\mu)$ by com-
paring the spectrum with and without twist. In Fig. 1 we show the low-lying
eigenvalues for $\mu = 0$ (l.h.s. plot) and $\mu = 0.02$ (r.h.s.) on the same quenched
configuration, generated with the Lüscher-Weisz action [11] on a 16$^4$ lattice
at $\beta = 8.45$. The lattice spacing is $a = 0.094$ fm as determined from the
Sommer parameter in [12]. The eigenvalues $\lambda$ were computed with the im-
plicitly restarted Arnoldi method [13]. In the plots the numbers next to
the symbols representing the eigenvalues $\lambda$ are the chiralities of the corre-
sponding eigenvectors $\psi_\lambda$, i.e., the matrix elements $(\psi_\lambda, \gamma_5 \psi_\lambda)$. The plots are
representative for a larger ensemble of configurations we studied at several
values of $\mu$, ranging from $\mu = 0.01$ to $\mu = 0.1$.

We first discuss the spectrum for zero twist (l.h.s. plot). The configu-
ration we consider has topological charge $Q = +1$ and thus we find a real
eigenvalue near the origin. This “topological eigenvalue” is represented by
a filled circle, while for the other eigenvalues we use open diamonds. For a
lattice Dirac operator obeying the Ginsparg-Wilson equation the topologi-
cal eigenvalue would be exactly at the origin. For Wilson’s Dirac operator
$\gamma_5$-hermiticity implies that real eigenvalues near the origin take over the role
of the zero-modes, since only for real eigenvalues $\tau$ the corresponding eigen-
vector has non-trivial chirality, $(\psi_\tau, \gamma_5 \psi_\tau) \neq 0$. This is evident from the $\gamma_5$
matrix elements displayed next to the symbols for the eigenvalues.

Upon turning on the twist parameter the spectrum changes considerably
(r.h.s. plot). The eigenvalues are expelled from a strip along the real axis
Figure 1: Spectrum of the Wilson Dirac operator in the complex plane for vanishing twist (l.h.s. plot) and $\mu = 0.02$ (r.h.s.). For both plots the same quenched charge $Q = +1$ configuration was used. The filled circle is used for the topological mode (zero-mode), while open diamonds represent bulk modes. The numbers next to the lowest eigenvalues are the values of the $\gamma_5$ matrix elements (chirality) for the corresponding eigenvectors.

excluding eigenvalues $\lambda$ with $|\text{Im}\lambda| < \mu$. Also the topological mode is shifted outside the “forbidden strip.” It is shifted downwards since, according to the index theorem, it has negative chirality for our $Q = +1$ configuration. The eigenvalues of topological modes with positive chirality are shifted upwards. This demonstrates that for $\mu \neq 0$ the spectrum is not symmetric with respect to reflection at the real axis. We stress that this holds not only for the topological eigenvalue, but also the other eigenvalues do not come in complex conjugate pairs. For $\mu = 0$ the spectrum is symmetric as a consequence of \[3\]. Another drastic change is the fact that for $\mu \neq 0$ all eigenvectors acquire non-vanishing chirality. They have positive chirality for eigenvalues in the upper half and negative chirality in the lower half (for positive $\mu$). The absolute value of the $\gamma_5$ matrix element decreases with increasing distance from the real axis.

Let us now try to understand these observations analytically. The $\gamma_5$ matrix element of an eigenvector $\psi_\lambda$ can be transformed as

$$
\lambda(\psi_\lambda, \gamma_5 \psi_\lambda) = (\psi_\lambda, \gamma_5 D(\mu) \psi_\lambda) = (\psi_\lambda, D(-\mu)^\dagger \gamma_5 \psi_\lambda) = (D(-\mu) \psi_\lambda, \gamma_5 \psi_\lambda) =
$$

$$
([D(\mu) - i2\mu \gamma_5] \psi_\lambda, \gamma_5 \psi_\lambda) = \lambda^*(\psi_\lambda, \gamma_5 \psi_\lambda) + i2\mu(\psi_\lambda, \psi_\lambda) = \lambda^*(\psi_\lambda, \gamma_5 \psi_\lambda) + i2\mu.
$$

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In the second step we have used (4) and in the last step that the eigenvectors are normalized to 1. From this equation follows

\[
\langle \psi_\lambda, \gamma_5 \psi_\lambda \rangle = \frac{\mu}{\text{Im} \lambda},
\]

establishing that all eigenvectors have non-vanishing chirality which decreases monotonically with \(\text{Im} \lambda\). Using the fact that \(\gamma_5\) is bounded, i.e., \(|\langle \psi_\lambda, \gamma_5 \psi_\lambda \rangle| \leq 1\), we find \((\mu \geq 0)\)

\[
|\text{Im} \lambda| \geq \mu.
\]

This result for the imaginary part is of course equivalent to the lower bound for the determinant in Eq. (2).

We remark that the fluctuations of the real part of the eigenvalues are not reduced by the twisted mass term. This is obvious from comparing the scatter of the eigenvalues in horizontal direction for the two plots in Fig. 11 and was observed also on the larger sample of configurations we analyzed. For \(\mu = 0\) the range of these fluctuations is related to the Aoki phase. The fact that the horizontal spread of the eigenvalues is essentially unchanged, indicates qualitatively that also for twisted Wilson fermions with small \(\mu\) an Aoki phase has to be expected (compare [3]).

It is interesting to analyze the case of a twisted chiral operator, i.e., we now demand that the lattice Dirac operator \(D_0\) obeys the Ginsparg-Wilson equation [6]

\[
\gamma_5 D_0 + D_0 \gamma_5 = a D_0 \gamma_5 D_0 .
\]

Since a chiral \(D_0\) has exact zero modes \(\psi_0^\pm\) with definite chirality \(\gamma_5 \psi_0^\pm = \pm \psi_0^\pm\), it is more suitable for analyzing the interplay between the twisted mass and topology. A twisted chiral Dirac operator provides a clean setting for such an analysis and the twisted Wilson Dirac operator is expected to approximate the chiral behavior for sufficiently smooth gauge fields.

It is straightforward, that adding a twisted mass term to a chiral \(D_0\) turns \(\psi_0^\pm\) into an eigenmode of \(D(\mu)\) with eigenvalue \(\lambda = \pm i \mu\). However, more information can be extracted from the Ginsparg-Wilson equation. Using the definition (11) one has \(D_0 = D(\mu) - i \mu \gamma_5\). Inserting this expression into (7) one finds after a few lines of algebra (use (4) and \(D(-\mu) = D(\mu) - i 2 \mu \gamma_5\)),

\[
D(\mu) + D(\mu)^\dagger = a D(\mu) D(\mu)^\dagger - a \mu^2 .
\]

Multiplying this equation with an eigenvector \(\psi_\lambda\) from the right and with \(\psi_\lambda^\dagger\) from the left, it turns into an equation for the eigenvalue \(\lambda\),

\[
\lambda + \lambda^* = a \lambda \lambda^* - a \mu^2 .
\]
Setting $\lambda = x + iy$ one finds that this is the equation for a circle in the complex plane. This “stretched Ginsparg-Wilson circle” has center $1/a$ and radius $\sqrt{1/a^2 + \mu^2}$. Thus, in addition to obeying the bound $|\psi, \gamma_5 \psi| \leq 1$, the eigenvalues of a twisted chiral Dirac operator are restricted to the stretched Ginsparg-Wilson circle.

Our results for the spectrum of twisted chiral fermions are represented in the l.h.s. plot of Fig. 2. The eigenvalues are restricted to the two arcs drawn as full curves. The zero-modes of the untwisted chiral operator are mapped to the edges $\pm i\mu$ of the arcs (the doublers of the zero modes end up at the other edges at $2/a \pm i\mu$). The index theorem for zero twist turns into a “remnant index theorem” for the edge modes,

$$Q = N_- - N_+,$$

where $N_\pm$ is the number of eigenvalues $\lambda = \pm i\mu$. The corresponding eigenvectors have chiralities $\pm 1$.

The largest imaginary parts that can be reached by the eigenvalues restricted to the arcs are $\text{Im} \lambda = \pm \sqrt{1/a^2 + \mu^2}$. According to (5), this implies a lower bound for the $\gamma_5$ matrix element, and we conclude

$$\frac{\mu}{\sqrt{1/a^2 + \mu^2}} \leq |(\psi, \gamma_5 \psi)| \leq 1.$$

The upper bound is reached only by the topological edge-modes (and their
Analyzing the case of a twisted chiral fermion, we have seen that topology plays an important role for the spectrum also for finite $\mu$. In particular the topological edge modes are protected by chiral symmetry and are unchanged when varying $\mu$. However, Wilson fermions are not chiral and one expects that the connection between topology, low-lying spectrum and chirality of eigenmodes is only approximate. An instance of this approximate realization is apparent in the fact that the topological mode in the r.h.s. plot of Fig. 1 is indeed the eigenvalue closest to the real axis. It is, however, not located at exactly $-i\mu$, as would be the case for a twisted chiral Dirac operator.

In order to study the behavior of the edge modes we computed the spectrum and eigenvectors of twisted Wilson fermions in the background of a discretized smooth instanton with radius $\rho = 4a$ on a $16^4$ lattice (see [14] for details of the discretization). In Fig. 3 we show, as a function of $\mu$, the eigenvalue of the edge mode (l.h.s. plot), its chirality (center), and its inverse participation ratio (r.h.s.). The inverse participation ratio is defined as $16^4 \sum_x (\psi^\dagger(x)\psi(x))^2$. It is a measure for the localization of the eigenmode with large values corresponding to localized modes while small values indicate spread-out modes. In all three plots the symbols are the numerical data, while the dotted lines are the analytical results for twisted chiral fermions. The plots show a clear difference between the data and the expectation for chiral fermions. This indicates that twisted Wilson fermions
do not give rise to a clear separation of topological modes and bulk modes, which is only restored in the limit $\mu \to 0$. Repeating the same analysis with the chirally improved Dirac operator \[15\], we found that there the data points fall on the chiral lines, demonstrating that for this case the topological edge mode is essentially protected by chiral symmetry. We remark, that since the chirally improved Dirac operator is only an approximate solution of the Ginsparg-Wilson equation, in this case the protection of the edge mode is also only approximate.

A final question which we address in this letter is the role of the twisted mass term for configurations in the deconfined phase. There the spectrum acquires a gap near the origin and, according to the Banks-Casher formula \[16\], the chiral condensate vanishes. In Fig. 4 we show the effect of the twist term by comparing spectra with $\mu = 0$ and $\mu = 0.02$ for quenched configurations in the deconfined phase (L"uscher Weisz action, $\beta = 8.45, 20^3 \times 6$). The l.h.s. pair of spectra is for a configuration with real Polyakov loop where a larger gap opens up \[17\], while the right-hand side is for a configuration with complex Polyakov loop. The plots show that in both cases, at least for moderately small $\mu$, the twisted mass term affects only the topological mode, while the bulk of the spectrum is essentially unchanged.
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