Low-lying Eigenvalues of the improved Wilson-Dirac Operator in QCD *

Hubert Simma¹, Douglas Smith²
(UKQCD collaboration)

¹ DESY-Zeuthen, Platanenallee 6, D-15738 Zeuthen, Germany
² Dept. of Physics and Astronomy, University of Edinburgh,
Edinburgh EH9 3JZ, Scotland

Abstract

The spectral flow of the low-lying eigenvalues of the improved and unimproved Wilson-Dirac operator is studied on instanton-like configurations and on thermalized quenched configurations at various β-values and lattice sizes. We also investigate the space-time localisation and chirality of the corresponding eigenvectors.

1 Introduction

The spectrum of the Dirac operator in QCD around zero is of particular physical interest, because in the continuum it is directly related to topological concepts and to the phenomenon of spontaneous breaking of chiral symmetry.

The topological charge of a smooth classical gauge field is related by the Atiyah-Singer index theorem to the difference between the number of right- and left-handed exact zero modes of the massless Dirac operator in that gauge background. After performing the ensemble average of the path integral and in the limit of an infinite volume, the Banks-Casher formula relates the chiral condensate \( \langle \bar{\psi} \psi \rangle \) to the spectral density for zero eigenvalues of the Dirac operator \([1]\). Moreover, in the framework of an effective chiral Lagrangian one finds sum rules for moments of the spectral density in individual topological sectors, and the derivative of the spectral density at zero can be related to the decay constant of the pion \([4]\).

The situation is substantially more complicated in numerical simulations of QCD on finite discrete lattices. Besides the restriction to a finite volume and the difficulties

---

*Talk presented at the 31st International Symposium Ahrenshoop on the Theory of Elementary Particles, Buckow, September 2-6, 1997
of defining a topological charge, the use of the Wilson action explicitly breaks chiral symmetry.

In numerical simulations the low-lying eigenvalues of the Wilson-Dirac operator are also crucial from a practical point of view. In the quenched approximation (almost-)zero modes are believed to be the origin of “exceptional” configurations, on which the numerical computation of light quark propagators is difficult and expensive, and which lead to large statistical errors of hadronic quantities at small quark masses \[3\]. In simulations with dynamical fermions the eigenvalues of the Wilson-Dirac operator play a central rôle for the performance of the algorithms and their scaling behaviour when approaching the chiral limit \[4\].

In this work we investigate the appearance and space-time localisation of zero and low-lying modes of the hermitian Wilson-Dirac operator \(\gamma_5 M\). In particular, we are interested in the effects of the Sheikholeslami-Wohlert (SW) improvement term, the variation of the zero-mode distribution with the gauge coupling, and the connection between the eigenmodes and topological properties of the underlying gauge field.

This contribution is organised as follows: After the discussion of general properties of the spectra of \(M\) and \(\gamma_5 M\) in the next section, we investigate in sect. 3 the zero modes on simple, instanton-like gauge configurations, before and after heating, and with and without improvement. In sect. 4, we present numerical data for thermalized quenched configurations on \(16^4\) lattices, and discuss our results in sect. 5.

## 2 Properties of the Eigenmodes of \(\gamma_5 M\)

The (improved) Wilson-Dirac matrix is given by

\[
M = 1 - \kappa (H + \frac{i}{2} c_{SW} F_{\mu \nu} \sigma_{\mu \nu}) ,
\]

where \(H\) is the usual hopping term, and \(\kappa\) is related to the bare quark mass \(m_0\) by \(\kappa = (8 + 2m_0)^{-1}\). The boundary conditions for the fermion fields are anti-periodic in time direction and periodic in the space directions. The SW improvement term contains the usual clover combination \(F_{\mu \nu}\) of the SU(3) gauge links.

Due to the \(\gamma_5\)-hermiticity, \(M^\dagger = \gamma_5 M \gamma_5\), the eigenvalues of \(M\) come in complex conjugate pairs \(\mu\) and \(\mu^*\). In addition, for \(c_{SW} = 0\) the spectrum on even lattices is also reflection symmetric along the line \(\text{Re}\mu = 1\), i.e.

\[
Mr = (1 - \kappa \rho) r \quad \Leftrightarrow \quad Ms = (1 + \kappa \rho) s ,
\]

with the eigenvectors related by the stagger transformation \(s(x) = (-1)^{\sum_{\mu} x_{\mu}} r(x)\).

The elementary relation, \(\mu_i^* - \mu_i \cdot r_i^\dagger \gamma_5 r_i = 0\), between eigenvalues \(\mu_i\) and corresponding right eigenvectors \(r_i\) of \(M\), suggests to distinguish two classes of eigenmodes:

- “bulk” modes with \(\mu \notin \mathbf{R}\) and vanishing chirality \((r, \gamma_5 r)\)
- real modes with \(\mu \in \mathbf{R}\) and possibly non-zero chirality
All eigenvalues lie within the disk \( \{ \mu = 1 + \kappa \rho : |\rho| \leq 8 \} \). On configurations with increasing \( \beta \)-values, the bulk modes depopulate the vicinity of the real axis except for five regions corresponding to the different corners of the Brillouin zone where the quark propagator has poles.

One may expect that some of the real modes are related to topological properties of the gauge field by an approximate lattice remnant of the index theorem, but of course also topologically trivial gauge fields can have real modes (e.g. \( U_4(x) = \text{diag}(1,-1,-1) \) on one time slice and all other \( U_\mu(x) = 1 \)).

In the following we shall investigate eigenmodes of the *hermitian* operator

\[
Q = \gamma_5 M / (1 + 8 \kappa) .
\]

The normalisation is such that the eigenvalues \( \lambda(\kappa) \) of \( Q \) satisfy \( 0 \leq \lambda^2 \leq 1 \), and we refer to the part of the spectrum closest to zero as the “low-lying” eigenvalues. They can be computed in an efficient and reliable way by using an accelerated conjugate gradient algorithm \([5]\), which also provides approximate eigenvectors and is viable for large lattice sizes.

Recalling the relation \( M^{-1} = Q^{-1} \gamma_5 / (1 + 8 \kappa) \), we note that all hadronic propagators can be constructed from \( Q^{-1} \), which has a simple spectral representation in terms of the orthonormal eigenvectors of \( Q \).

The eigenmodes (eigenvalues and corresponding eigenvectors) of \( Q(\kappa) \) have a non-trivial \( \kappa \)-dependence. The real modes, \( \mu = 1 - \kappa \rho \in \mathbb{R} \), of \( M \) are equivalent to zero-modes of \( Q \) at \( \kappa \)-values \( \kappa_0 = 1/\rho \). In general, the spectral flow \( Q(\kappa) \) provides indirect information about the complex spectrum of \( M \), and in particular the flow of the low-lying eigenvalues \( \lambda(\kappa) \) probes the spectrum of \( M \) close to the real axis. The five regions, where bulk modes of \( M \) populate the vicinity of the real axis, correspond to minima of the low-lying eigenvalues of \( Q(\kappa) \) at \( \kappa \)-values roughly of the order of \( 0.125, 0.25, \pm \infty, -0.25, \) and \(-0.125 \). In the special case of a flat gauge field each eigenvalue \( \mu = 1 - \kappa \rho \) of \( M \) corresponds to an extremal value in the spectral flow of \( \lambda = \lambda \cdot (1 + 8 \kappa)/\kappa \) at \( \kappa = 1/\Re \rho \).

The chiralities of the eigenvectors of \( Q \)

\[
\chi_i \equiv (u_i, \gamma_5 u_i)
\]

are related to the spectral flow of \( \bar{\lambda}_i(\kappa) \) by the identity

\[
\chi_i(\kappa) = \frac{d \bar{\lambda}_i}{d(1/\kappa)} ,
\]

i.e. the zeroes of the chirality correspond to extrema in the spectral flow of \( \gamma_5 M / \kappa \). Eq. \([4]\) yields the first order \( \kappa \)-dependence of \( \lambda(\kappa) \), and from the flow of a zero modes close to the position \( \kappa_0 \), where \( \lambda \) vanishes, one can thus estimate \( \kappa_0 \) as

\[
\kappa_0 \approx \kappa \cdot \left( 1 + \frac{\chi}{\bar{\lambda} - \chi} \right) ,
\]

which is very helpful for an efficient iterative search for possible zero modes.
3 Instanton-like Configurations

We first investigate to what approximation the index theorem holds for Wilson fermions on simple instanton-like configurations. These are set up on even lattice sizes in the singular gauge as described in [6], followed by a few cooling sweeps to reduce boundary mismatches. We consider configurations with up to two well-separated instantons or anti-instantons in the same SU(2) subgroup and a net topological charge $\nu = 0, \pm 1, \pm 2$.

In the physical $\kappa$-region we find $n_+ = \nu$ zero modes with chiralities of the same sign as $\nu$, and $n_- = 0$ with opposite sign chiralities. On multiple-instanton configurations their positions are split depending on the size and distance of the instantons. In the four unphysical regions one has $(n_+, n_-) = (0, 4\nu), (6\nu, 0), (0, 4\nu)$, and $(\nu, 0)$, respectively. In the following we consider only the physical region $0.1 \leq \kappa \leq 0.2$.

The spectral flow of the low-lying bulk modes on cold instanton-like configurations is characterised by a value of $\kappa_\chi$ which is close to the free-case value of 1/8 and essentially independent of the instanton size $\rho$. On the other hand, the position $\kappa_0$ and the chirality $\chi_0(\kappa_0)$ of the zero mode seem to be sensitive to discretisation effects and are strongly $\rho$-dependent. The following table shows the values for single instantons on a $16^4$ lattice:

| $\rho$ | $c_{SW} = 0$ | $c_{SW} = 1$ |
|-------|--------------|--------------|
|       | $\kappa_0$  | $\chi_0(\kappa_0)$ | $\kappa_0$  | $\chi_0(\kappa_0)$ |
| 2     | .135         | .66          | .1258       | .986          |
| 4     | .127         | .90          | .1250       | .999          |
| 8     | .126         | .99          | .1250       | .999          |

We note the clear effect of the improvement term (using the tree-level value $c_{SW} = 1$): It significantly rises the chirality $\chi(\kappa_0)$ of the zero mode and moves the position $\kappa_0$ towards lower values and closer to $\kappa_\chi$.

When the instanton-like configurations are heated by a moderate number of update sweeps, the zero-mode remains, but the position $\kappa_0$ changes and fluctuates for different heating trajectories. The heating also moves the positions $\kappa_\chi$, where the chiralities of the lowest bulk modes vanish, to values around $\kappa_{crit}(\beta)$, where $\beta$ is the value at which the heating was performed. For the improved operator the variation of $\kappa_0$ is much smaller, and the central value is lower and significantly closer to $\kappa_\chi$ than for $c_{SW} = 0$.

Also on the heated configurations the eigenvectors are centered on the instantons (except for $\kappa \ll \kappa_\chi$), but the space-time extension of the eigenvector density at $\kappa_0$ is not as clearly scaling with the size of the instanton as in the cold case.

4 Quenched Configurations

To study the spectrum of the Wilson-Dirac operator on quenched configurations, we used 10 thermalized $16^4$ configurations for each of the gauge couplings, $\beta = 5.9, 6.0,$
The distribution of the zero modes for the improved operator at $\beta = 6.0$ is shown in Fig. 1. The peak of the distribution around $\kappa_{\text{crit}}$ is more pronounced in the improved case than for $c_{SW} = 0$. The typical behaviour of the chiralities on one of these configurations is illustrated in Fig. 2. The circles denote the lowest (zero) modes and the lines connect points from the same bulk modes to guide the eye. One notices that the chiralities of the low-lying bulk modes vanish around the same value $\kappa_{\chi} \approx \kappa_{\text{crit}}(\beta)$.

The space-time localisation of the low-lying eigenmodes for the unimproved case, is known to change around $\kappa_{\text{crit}}$ from a typically exponential decay of the eigenvector density to an even stronger, almost point-like, localisation [8]. For the improved operator we find in the region $\kappa \ll \kappa_{\chi}$ a somewhat stronger localisation of the lowest-lying modes than for $c_{SW} = 0$, but this difference tends to disappear towards $\kappa_{\chi}$. Above $\kappa_{\chi}$ a sharp drop of the “participation ratio” indicates again a very strong (almost point-like) localisation similar to the unimproved case. The $\kappa$-dependence of the localisation strength is the same for the lowest-lying bulk modes and for the flow of zero modes. Thus, zero modes appearing at very low $\kappa_{0} \leq \kappa_{\chi}$ are in general weaker localised than those at higher $\kappa_{0}$.

To investigate the localisation of the zero modes in relation to topological properties of the underlying gauge field, we approximate the charge density of the cooled gauge configurations by a superposition of single-instanton charge distributions [9]. We find that the peaks closest to the maximum of the eigenvector density are in average significantly higher (i.e. correspond to smaller instantons) than the average value of the configuration. There also seems to exist a weak correlation between the chirality of the eigenmode and the sign of the topological charge of the closest peak.
5 Discussion

On simple instanton-like configurations we confirmed that the improved and unimproved Wilson-Dirac operator approximately satisfy an index theorem similar to the case of staggered fermions or QED$_2$ \[10\]. The presence of the zero modes is rather stable under the effect of roughening the gauge fields by heating.

Inclusion of the SW improvement term significantly increases the chirality of the zero modes and moves $\kappa_0$ closer to $\kappa_{\text{crit}}$. On thermalized quenched configurations the improvement term renders the zero mode distribution stronger peaked around $\kappa_{\text{crit}}$. This is in accordance with the picture that in the continuum limit the $\kappa$-region with vanishing mass gap (i.e. with zero modes of $Q$) shrinks to a point \[11\].

The number of zero modes found on the $16^4$ lattices clearly decreases with increasing $\beta$-values. This, and the much lower abundance of zero modes on $8^4$ lattices, indicates that the number of zero modes grows with the physical volume.

The eigenvectors of the improved operator are somewhat stronger localised than in the unimproved case, and their positions tend to lie close to peaks of the topological charge density of the (cooled) gauge field. The width of these peaks is typically smaller than the average for the configuration.

On the four exceptional configurations encountered by UKQCD at $\beta = 6.0$ on $16^348$ and $32^364$ lattices we verified the presence of a zero mode at a near $\kappa$-value $\kappa_0 < \kappa_{\text{crit}}$. In all cases the eigenvector is localised close to or on a narrow peak in the topological charge density, and the chirality has the same sign as the charge of the peak, but is not correlated with the overall topological charge of the configuration.

The spectral flow of $Q(\kappa)$ can also provide instructive information about the complex spectrum of $M$. For instance, the position $\kappa_{\chi}$ of the chirality zeroes of the lowest bulk modes approximately coincides with $\kappa_{\text{crit}}$ (defined as an ensemble quantity, e.g. from the pion mass), and may be an interesting quantity to characterise the “critical” $\kappa$-value for individual gauge configurations.

Further details and numerical data shall be presented elsewhere \[12\].

Thanks are due to the organisers for an interesting and pleasant Symposium. We thank M. Bäker, K. Jansen, M. Lüscher and S. Pickles for helpful discussions, and R. Petronzio for generous computing time on the APE at Tor Vergata. Part of the numerical computations was also performed at DESY-Zeuthen, at the University of Edinburgh, and at the APE Lab, and we are grateful for their hospitality and support.

References

[1] T. Banks and A. Casher, *Nucl. Phys.* B169 (1980) 103;
   E. Marinari, G. Parisi, and C. Rebbi, *Phys. Rev. Lett.* 37 (1981) 1795

[2] H. Leutwyler, and A. Smilga, *Phys. Rev.* D46 (1992) 5607;
   A. Smilga, hep-th/9503049
[3] W. Bardeen, et al., [hep-lat/9710084] and [hep-lat/9705002]

[4] K. Jansen, *Nucl. Phys. B* (Proc. Suppl.) 53 (1997) 262

[5] T. Kalkreuter and H. Simma, *Comp. Phys. Comm.* 93 (1996) 33.

[6] D.J.R. Pugh and M. Teper, *Phys. Lett.* B212 (1989) 326;
   M. Laursen, J. Smit, and J. Vink, *Nucl. Phys.* B343 (1990) 522

[7] M. Lüscher, et al., *Nucl. Phys.* B491 (1997) 323

[8] K. Jansen, et al. *Nucl. Phys.* B (Proc. Suppl.) 53 (1997) 262

[9] D. Smith and M. Teper (UKQCD Collaboration), [hep-lat/9801008]

[10] I. Barbour, and M. Teper, *Phys. Lett.* B175 (1986) 445;
    S. Itoh, Y. Iwasaki, and T. Yoshié, *Phys. Rev.* D36 (1987) 527;
    J. Smit, and J. Vink, *Nucl. Phys.* B286 (1987) 485;
    C. Gattringer, I. Hipp, and C. Lang, *Nucl. Phys.* B508 (1997) 329, and [hep-lat/9712013]

[11] R.G. Edwards, U.M. Heller, R. Narayanan, R.L. Singleton, [hep-lat/9711029]

[12] H. Simma, in preparation