Clover improvement, spectrum and Atiyah-Singer index theorem for the Dirac operator on the lattice

Christof Gattringer
Department of Physics and Astronomy,
University of British Columbia, Vancouver B.C., Canada

Ivan Hip
Institut für Theoretische Physik
Universität Graz, A-8010 Graz, Austria

Abstract

We study the role of the $O(a)$-improving clover term for the spectrum of the lattice Dirac operator using cooled and thermalized SU(2) gauge field configurations. For cooled configurations we observe improvement of the spectral properties when adding the clover term. For the thermalized case ($12^4, \beta = 2.4$) without clover term we find a rather bad separation of physical and doubler branches making a probabilistic interpretation of the Atiyah-Singer index theorem on the lattice questionable for this $\beta$ and lattice size. Adding the clover term leads to the creation of additional real eigenvalues which come in pairs of opposite chirality thus further worsening the situation for the index theorem.

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1. Introduction

In the last few years the spectrum of the Dirac operator on the lattice has seen a lot of attention. This is partly motivated by the hope that a lattice-regularized gauge theory could put the idea of decomposing the fully quantized path integral into topological sectors on a conceptually sound basis. In the continuum gauge fields can be classified with respect to their topological charge when they are smooth and obey certain boundary conditions. On the other hand the fields which carry the measure in a continuum path integral do not obey these conditions. The topological arguments thus can only be implemented on a semi-classical level. Lattice regularization might provide the framework to set up the topological concepts in a fully quantized theory. Up to so-called exceptional configurations lattice gauge fields can be assigned a topological charge and the exceptional configurations are expected to die out in the continuum limit. A complete decomposition of the path integral into topological sectors could become possible.

In the continuum the Atiyah-Singer index theorem [1] relates the topological charge of classical gauge field configurations to the numbers of left- and right-handed zero modes of the Dirac operator. This gives rise to semi-classical results for fermionic observables. Again, these results can not be implemented in the fully quantized model since the gauge fields in the path integral are too rough.

On the lattice there is no analytic result for the Atiyah-Singer index theorem, but it has been conjectured [2]-[17] that on the lattice, at least for sufficiently smooth configurations, it is realized in a probabilistic sense. The question however arises if for the parameters where current simulations are done the gauge fields are sufficiently smooth so that the spectrum of the Dirac operator can be interpreted in the sense of the index theorem.

For completely smooth configurations such as lattice approximations to continuum instantons there can be no doubt, that the topological interpretation of the spectrum makes sense [3]-[8]. Also for fully quantized QED, it has been established [9]-[11], that the index theorem governs the behavior of the spectrum when approaching the continuum limit.

For thermalized lattice gauge theories in four dimensions the picture is less conclusive. Older results by Itoh, Iwasaki and Yoshié [2] report a rather poor manifestation of the index theorem and also the distinction of physical and doubler modes turned out to be difficult. More recent studies [12, 13] (compare also [3, 14]-[17] for results on the spectrum for thermalized gauge fields) of a fermionic definition of the topological charge, which is based on a lattice manifestation of the index theorem, are more optimistic. However,
only sampled data but no detailed analysis of the index theorem for single thermalized configurations was presented.

One of the motivations for this contribution is to carefully analyze the idea of interpreting the spectrum of the lattice Dirac operator in terms of a probabilistic manifestation of the Atiyah-Singer index theorem. This is done for a sample of thermalized SU(2) configurations on $12^4$ lattices at $\beta = 2.4$ taken from the quenched simulation [18] (sample 1b). The authors of [18] were so kind to provide us also with their cooled data obtained using the improved cooling method (compare also [14]) based on the over-improved action given in [20]. This allows to compare the spectra for the thermalized configurations with the cooled counterparts on a one by one basis. One can check if a fermionic definition of the topological charge based on the index theorem, if possible at all, agrees with the cooling procedure. Our results presented here indicate however, that for SU(2) quenched configurations on $12^4$ lattices at $\beta = 2.4$ most of the configurations give rise to a spectrum where no clear separation of physical and doubler modes can be established. An interpretation of the spectrum in terms of the index theorem is questionable.

In the last few years it was realized that improvement is a powerful if not essential tool when numerically analyzing lattice field theories (see e.g. [21] for an introductory overview). For the fermion action the $O(a)$-improvement is governed by the clover term. Adding this extra term to the lattice Dirac operator certainly alters its spectral properties.

The second motivation for this study of the eigensystem of the lattice Dirac operator is to see how the clover term changes the spectrum. Does it improve the spectral properties similar to the behavior which was observed in QED$_2$ [22] using perfect actions [23]? Again we address this question by analyzing spectra for the thermalized, quenched sample on $12^4$ lattices at $\beta = 2.4$ and also for the corresponding cooled configurations. In addition we analyze the effect of the clover term for complete spectra using smooth toy configurations (constant plaquette configurations + small fluctuations) on $4^4$ lattices.

The article is organized as follows: In the next section we will set our notation and briefly discuss the framework for the Atiyah-Singer index theorem on the lattice. Section 3 presents our results for the effect of the clover term on complete spectra using toy configurations on $4^4$ lattices. Section 4 contains the study of spectra for cooled configurations on $12^4$ lattices. The index theorem and the effects of the clover term are discussed. In Section 5 we present our results for thermalized configurations on $12^4$ lattices at
\( \beta = 2.4 \). We analyze in detail the mechanism for the proliferation of real eigenvalues caused by the clover term using perturbative arguments. In Section 6 we assess the possibility for the interpretation of the spectrum in the sense of the index theorem. The article closes with a discussion.

2. Notation and basic properties of the lattice Dirac operator

We consider the following, \( \mathcal{O}(a) \)-improved fermion action

\[
S = \sum_{x,y} \bar{\psi}(x) D(x,y) \psi(y) ,
\]

where the lattice Dirac operator \( D \) (fermion matrix) consists of three parts

\[
D = (4 + m) \mathbb{1} - K , \quad K = Q - c_{sw} C ,
\]

with \( m \) denoting the bare quark mass. For later convenience we introduced the abbreviation \( K \) for the non-trivial part of the fermion matrix. The Wilson hopping matrix \( Q \) and the clover term \( C \) are given by

\[
Q(x,y) = \frac{1}{2} \sum_{\mu} \left\{ [1 - \gamma_{\mu}] U_{\mu}(x) \delta_{x+\mu,y} + [1 + \gamma_{\mu}] U_{\mu}(x - \mu)^{\dagger} \delta_{x-\mu,y} \right\} ,
\]

\[
C(x,y) = \sum_{\mu,\nu} \frac{i}{4} \sigma_{\mu\nu} F_{\mu\nu}(x) \delta_{x,y} .
\]

Here \( \sigma_{\mu\nu} = i/2[\gamma_\mu, \gamma_\nu] \) and \( F_{\mu\nu} \) is some lattice discretization of the continuum field strength tensor. We use the standard (clover) discretization which can e.g. be found in [24]. For a proper choice of the Sheikholeslami-Wohlert coefficient \( c_{sw} \) in [4], the counter-term [4], first given in [23], removes \( \mathcal{O}(a) \) cutoff effects. For SU(2) the one loop perturbative expansion gives [23, 24]

\[
c_{sw} = 1 + 0.155(1) \ g_0^2 \ + \ O(g_0^4) ,
\]

where \( g_0 \) is the bare coupling, related to \( \beta \) used below via \( \beta = 4/g_0^2 \). As in the case without improvement, the matrix \( K \) (or equivalently \( D \)) is neither hermitian nor anti-hermitian, but hermitian conjugation is implemented as a similarity transformation

\[
\gamma_5 K \gamma_5 = K^{\dagger} .
\]

This equation implies that the eigenvalues of \( K \) (or \( D \)) come in complex conjugate pairs or are real. The staggered transformation which transforms
$Q$ into $-Q$ (see e.g. [27]) leaves the clover term $C$ invariant. Thus for $c_{sw} \neq 0$ the symmetry of the spectrum of $K$ under reflection at the imaginary axis is lost.

Besides leading to symmetry of the spectrum under complex conjugation, (6) also has an interesting implication [2] for the chiral properties of the eigenvectors of $K$: Only eigenvectors $\psi_\lambda$ of $K$ ($D$), where the eigenvalue $\lambda$ is real can have non-vanishing pseudoscalar matrix elements

$$
(\psi_\lambda, \gamma_5 \psi_\lambda) \neq 0 \text{ only for } \lambda \in \mathbb{R}.
$$

For the Dirac operator in the continuum the only eigenstates with non-vanishing pseudoscalar matrix elements are zero modes. Thus the eigenvectors $\psi_\lambda$ of the non-hermitian matrix $K$ (or $D$) which have real eigenvalues $\lambda$ should be interpreted as the "lattice zero modes" [2, 3, 4].

Based on this interpretation of the eigenvectors with real eigenvalues as the lattice zero modes, one can formulate a lattice version of the Atiyah-Singer index theorem [1] which is expected to hold for sufficiently smooth gauge fields

$$
\nu[U] = R_- - R_+.
$$

Here $R_+$ and $R_-$ are the numbers of real eigenvalues in the physical branch of the spectrum with positive and negative chirality. The chirality is defined as the sign of the pseudoscalar matrix element $(\psi, \gamma_5 \psi)$ of the corresponding eigenvectors $\psi$. $\nu[U]$ denotes the topological charge of the lattice gauge field configuration.

### 3. Complete spectra for test configurations on small lattices

Relatively few is known about the role of the clover term for the spectrum of the lattice Dirac operator (for some results see [14, 15, 17]). To gain some basic insight on the role of the clover term $C$ for all eigenvalues of $K$ we computed several complete spectra of $K$ on $4^4$ lattices. These computations were also performed to test the correct implementation of the fermion matrix by checking the linear and quadratic sum rules for the eigenvalues which are obtained by expressing the trace of $K$ and $K^2$ as a functional of the gauge field. Both sum rules are obeyed with excellent numerical accuracy. The computations in this section were done using standard routines for general complex matrices from the LAPACK package.

The gauge fields were constructed from constant field strength configurations where we added some fluctuations. For the details of the preparation
of the gauge field see [7]. In Fig. 1 we show spectra of \( K \) for different values of \( c_{\text{sw}} \). The background field \( U \) has topological charge \( \nu[U] = 2 \) and is relatively smooth (in the notation of [7]: \( s = t = 1, \, \varepsilon = 0.1, \, n_r = 15 \)).

We show the spectra for values of the Sheikholeslami-Wohler t coefficient \( c_{\text{sw}} = 0.0, 1.0, 1.5 \) and 2.5. We remark, that the gauge fields used for this computation are static background fields which cannot be assigned an inverse squared coupling \( \beta \) and here the perturbative formula (5) can only give an idea about the order of magnitude of \( c_{\text{sw}} \).

Figure 1: Dependence of the complete spectrum of \( K \) on \( c_{\text{sw}} \). We plot all eigenvalues of \( K \) in the complex plane for a relatively smooth gauge field with topological charge \( \nu[U] = 2 \). The coefficient \( c_{\text{sw}} \) was chosen to be \( c_{\text{sw}} = 0.0, 1.0, 1.5 \) and 2.5. There are two real eigenvalues with negative chirality in the physical branch (in the vicinity of 4 on the real axis), in accordance with [5].
The first plot in Fig. 1 shows the spectrum of the un-improved \((c_{sw} = 0)\) operator \(K\) in the complex plane. It displays the well known features of the spectrum for a rather smooth background gauge field with topological charge \(\nu = 2\). The spectrum is symmetric with respect to reflection at real and imaginary axis. There is a bulk of complex eigenvalues, well separated from the real axis and several real eigenvalues clustering in small regions, corresponding to the physical and doubler branches. The physical branch (right edge of the spectrum) is well pronounced for this rather smooth gauge field configuration. There are no problems distinguishing the real eigenvalues in the physical branch of the spectrum from the doublers. The two real eigenvalues in the physical branch have negative chirality in accordance with (8).

When the Sheikholeslami-Wohlert coefficient \(c_{sw}\) is chosen equal to 1 the spectrum changes. The symmetry under reflection at the imaginary axis is lost, since the clover term \(C\) is even under the staggered transformation, while the standard hopping term \(Q\) is odd (compare the discussion above). However the symmetry under reflection at the real axis, which is due to (6) remains. The whole physical branch is shifted towards larger real parts (compare also the perturbative analysis in Section 5), and the complex eigenvalues in the physical branch seem to cluster more along a single curve. The discussed deformation of the spectrum becomes more pronounced when increasing \(c_{sw}\) to \(c_{sw} = 1.5\) and 2.5.

It is remarkable, that for this rather smooth gauge field configuration the two real eigenmodes, relevant for the index theorem, remain rather unperturbed when increasing \(c_{sw}\). We will later demonstrate that for thermalized configurations the changes of the spectrum caused by the clover term are much more dramatic.

We end this section with remarking, that from the last plot it is obvious that the bound known at \(c_{sw} = 0\) for the eigenvalues \(\lambda\) of \(K\): \(|\lambda| < 4\), or more general \(|\lambda| < D\) where \(D\) is the dimension, does not apply at \(c_{sw} > 0\). The standard strategy [28] for proving this bound cannot be implemented for \(c_{sw} \neq 0\), and in fact the plot shows that the bound is violated already for not too large \(c_{sw}\).

4. The physical branch of the spectrum - cooled configurations

In this section we study in more detail the role of the improvement term for the physical branch of the spectrum in smooth gauge field configurations. In particular we use cooled configurations obtained from thermalized configurations from a quenched simulation of SU(2) gauge theory [18].
To analyze the physical branch of the spectrum we use the Implicitly Restarted Arnoldi/Lanczos Method [29] which allows to compute a few eigenvalues with user specified properties for large, general matrices. We set up the algorithm such that the 128 eigenvalues with the largest real parts are computed first. This gives the eigenvalues in the physical branch of the spectrum we are interested in. In Fig. 2 we compare the physical branch of the spectrum of $K$ for $c_{sw} = 0$ and $c_{sw} = 1$ for two cooled configurations from [18], one with $\nu[U] = -1$ (left hand side plot) and one with $\nu[U] = 2$ (right hand side plot). The value $c_{sw} = 0$ is the case without $O(a)$-improvement and $c_{sw} = 1$ is the perturbative result (5) for smooth configurations ($g_0 = 0$).

![Figure 2: Plots of 128 eigenvalues in the physical branch of the spectrum of $K$ for cooled gauge field configurations with $\nu[U] = -1$ (left hand side plot) and $\nu[U] = 2$ (right hand side plot). For both configurations we show the spectra for $c_{sw} = 0$ (no improvement) and $c_{sw} = 1$ (perturbative value for smooth fields). The dashed curve is the ellipse centered at the origin of the complex plane with width 8 and height 4. We remark, that in the right-most plot the two real eigenvalues are very close to each other, such that the two symbols appear as one.](image)

The plots show, that already without improvement the complex eigenvalues in the physical branch are concentrated in a small band along the
ellipse with width 8 and height 4 centered at the origin (dashed curve in Fig. 2). When adding the improvement term this alignment along the ellipse is further enhanced.

For the real eigenvalues the situation is different. Without improvement they are considerably shifted away from the limiting curve, while the clover term brings them very close to the ellipse, i.e. close to the origin when looking at the spectrum of $D$. Thus the real eigenvalues become exact poles of the improved massless propagator in smooth background fields. The number of real eigenvalues and their chirality is in accordance with (8). The value of the pseudoscalar matrix element is considerably improved by the clover term, i.e. much closer to ±1 (compare also [17]). As an example we give the values for the $\nu = -1$ configuration (left hand side plot) where we obtain 0.8009 for the matrix element without improvement and 0.9984 at $c_{sw} = 1$.

We analyzed several more cooled configurations from sample 1b of [18] and found the above results for cooled configurations confirmed. The number of real eigenvalues in the physical branch and their chirality are properly described by (8) both for $c_{sw} = 0$ and $c_{sw} = 1$. The clover term improves the alignment of the complex eigenvalues along the ellipse, shifts the real eigenvalues and leads to pseudoscalar matrix elements very close to ±1. This improvement of the spectral properties for smooth configurations when adding the clover term is somewhat surprising for a term which was designed for improving on-shell quantities. It is a little bit reminiscent of the results obtained for the spectrum of the perfect lattice Dirac operator in QED$_2$ [22].

5. Thermalized configurations
The literature [5]-[8], [17] as well as the above results for the cooled configurations and the test configurations in Section 3 show, that the lattice index theorem (8) holds perfectly well for the spectrum in smooth gauge field configurations. For the case of thermalized configurations the situation is less clear [2],[12]-[17].

In this section we carefully analyze the role of $c_{sw}$ for the spectrum for thermalized configurations from sample 1b in [18], i.e. quenched SU(2) gauge field configurations at $\beta = 2.4$ on a $12^4$ lattice. We compare these results to the results for the cooled counterparts obtained in the last section.

Again we use the Implicitly Restarted Arnoldi/Lanczos Method to compute 200 complex eigenvalues with largest real part, i.e. eigenvalues in the physical branch of the spectrum. In addition we compute eigenvalues on the real axis using the method of counting level crossings of the hermitian modification of the fermion matrix. This method was first described in [4]
and brought to further perfection and used for analyzing the real spectrum of the Dirac operator \([4, 8, 12, 13, 14, 17]\). It is now also known as "overlap method".

Whenever \(K\) has a real eigenvalue \(r\), then the operator \(\rho I - K\) has a zero eigenvalue at \(\rho = r\). This implies furthermore \([2]\), that the auxiliary matrix

\[
H(\rho) \equiv \gamma_5[\rho I - K], \tag{9}
\]

has a zero eigenvalue at \(\rho = r\) if and only if \(r\) is a real eigenvalue of \(K\). Thus one can trace the flow of small eigenvalues \(\mu(\rho)\) of \(H(\rho)\) as \(\rho\) is varied. Whenever the flow crosses zero at some \(\rho = r\), then this \(r\) is a real eigenvalue of \(K\). From the definition (9) for the auxiliary operator \(H(\rho)\) it is also obvious that the pseudoscalar matrix element corresponding to \(r\) is given by the slope of the flow for the eigenvalue \(\mu(\rho)\) which crosses zero at \(r\) \([2]\)

\[
(\psi_r, \gamma_5\psi_r) = \left. \frac{d}{d\rho} \mu(\rho) \right|_{\rho = r}. \tag{10}
\]

Thus the chirality assigned to \(r\) is given by the sign of the slope. The auxiliary operator \(H(\rho)\) is hermitian due to (6) and thus much simpler to deal with numerically. A more detailed discussion and technical remarks on the implementation of the level crossing algorithm can be found in the literature \([2, 1, 8, 12, 13, 14, 17]\).

Here we search for the real spectrum between 1.8 and 4. Real eigenvalues in the vicinity of 2 are associated with the 4 doubler modes from the \((\pi, 0, 0, 0)\)-type corners of the Brillouin zone. In order to make sure that we find all real eigenvalues in the physical branch and at least some of the doublers we start our search at 1.8.

In Fig. 3 we show our results for the spectrum of \(K\) (200 complex eigenvalues and all real eigenvalues larger than 1.8) in a thermalized background configuration from \([18]\) (\(12^4\) lattice, SU(2), \(\beta = 2.4\)). We remark that this is the thermalized configuration which corresponds to the cooled configuration used for the left plot in Fig. 2 (after cooling this configuration has \(\nu = -1\)). We display the spectra for \(c_{sw} = 0.0\) (no improvement), \(c_{sw} = 1.258\) (perturbative value) and \(c_{sw} = 1.4\) and 1.7. The last two values were chosen because one expects the non-perturbative value of \(c_{sw}\) to be larger than the perturbative result similar to the case of SU(3) where non-perturbative results for \(c_{sw}\) are known \([30]\).
Figure 3: Plots of 200 complex eigenvalues in the physical branch of the spectrum and all real eigenvalues larger than 1.8 for the matrix $K$ in a thermalized gauge field configuration ($12^4$ lattice, $\beta = 2.4$). We show the results for $c_{sw} = 0.0$ (no improvement), $c_{sw} = 1.258$ (perturbative value at $\beta = 2.4$), for $c_{sw} = 1.4$ and for $c_{sw} = 1.7$.

An interesting feature of the plots is the strong shift of the eigenvalues in the physical branch of the spectrum towards larger real parts as $c_{sw}$ is increased (compare also the perturbative arguments below). This is equivalent to the known shift of the critical $\kappa$ when increasing $c_{sw}$ (compare e.g. the first article listed in [R]). We furthermore find that the eigenvalues tend to cluster more in a narrow band, although the improvement of the spectral
properties (= eigenvalues lined up along a single curve) is not as strong as for the cooled configurations.

For the manifestation of the index theorem on the lattice and also other ideas such as the modified quenched approximation [15] the most important feature of the clover term is however the generation of additional real eigenvalues. This property can be seen clearly from the four plots in Fig. 3. In particular we found, that the additional eigenvectors with real eigenvalues are generated in pairs of opposite chirality. This fact can be understood by analyzing how the spectral flow \( \mu(\rho) \) for the auxiliary problem \( H(\rho) \) changes with \( c_{sw} \): Increasing \( c_{sw} \) can cause a flow line \( \mu(\rho) \), which had no zero crossing at \( c_{sw} = 0 \), to develop a local maximum (or minimum) which eventually crosses zero from below (above) as \( c_{sw} \) is increased further. Two new crossings appear, one with positive and one with negative slope. Thus, due to [10], this gives rise to two real eigenvalues with eigenvectors having opposite chirality. We remark that the discussed mechanism is the only way that additional zero crossings, i.e. real eigenvalues of \( K(D) \) can emerge, since the total number of zero crossings is even. This follows from the continuity of the flow lines in \( \rho \) and the simple limiting behavior of \( H(\rho) \). For \( \rho \to \pm \infty \) one has \( H(\rho) \to \pm \gamma_5 \mathbb{I}_{volume \times N_{color}} \), and the limiting matrices both have \( 2 \times volume \times N_{color} \) eigenvalues of \( +\rho \) and \( 2 \times volume \times N_{color} \) eigenvalues \( -\rho \). The flow lines connect the eigenvalues of the limiting cases and thus only an even number of zero crossings can emerge. Hence the above discussed mechanism for the creation of zero crossings is the only possibility to create new crossings, implying that the additional real eigenvalues of \( K(D) \) are always created in pairs of opposite chirality.

In order to demonstrate this mechanism we isolated the flow \( \mu(\rho) \) of a single small eigenvalue of \( H(\rho) \) which exhibits the discussed phenomenon and present this plot in Fig. 3. We show how a particular flow line creates two new zero crossings as \( c_{sw} \) is increased from the perturbative value \( c_{sw} = 1.258 \) to \( c_{sw} = 1.4 \). We also show the flow for the intermediate values \( c_{sw} = 1.3 \) and \( c_{sw} = 1.35 \). For \( c_{sw} = 1.258 \) the flow has no crossing of zero. When increasing the coefficient to \( c_{sw} = 1.3 \) we find that a clear minimum has developed and the flow line is almost touching zero. At \( c_{sw} = 1.35 \) it has moved further down giving rise to two crossings of zero, i.e. two additional real eigenvalues of \( K(D) \). At \( c_{sw} = 1.4 \) the crossings of zero have moved a little and are now at approximately 2.35 (negative slope, i.e. negative chirality) and at 2.9 (positive chirality).

To further study the phenomenon of proliferation of real eigenvalues
when increasing $c_{sw}$ we numerically evaluated some of the matrix elements which occur in first and second order perturbation theory (in $c_{sw}$) for eigenvalues $\lambda(c_{sw})$ of the operator $K = Q - c_{sw} C$

$$\lambda(c_{sw}) = \lambda(0) - c_{sw} \psi_{\lambda(0)} \dagger C \psi_{\lambda(0)} + c_{sw}^2 \sum_{\mu \neq \lambda(0)} \frac{|\psi_{\lambda(0)} \dagger C \psi_{\mu}|^2}{\lambda(0) - \mu} + O(c_{sw}^3).$$

(11)

Here $\lambda(0)$ is the eigenvalue of $K$ without improvement ($c_{sw} = 0$) and $\psi_{\lambda(0)}$ is the corresponding eigenvector. Since $C$ is a hermitian matrix it is clear that the first order term is real and simply shifts the eigenvalues parallel to the real axis. Already existing real eigenvalues remain real. This linear term seems to be the main contribution for the shift of the spectrum towards larger real parts which was already discussed for Figs.1, 2 and 3.

When analyzing the second order term for some real eigenvalue $r$ we find $|\psi_r \dagger C \psi_{\mu}|^2 = |\psi_{r} \dagger C \psi_{\mu}|^2$. Since both, $\mu$ and $\mu$ occur in the sum for the second order term the imaginary parts cancel and we find that the real eigenvalue $r$ is only shifted along the real axis. Again we see that existing real eigenvalues remain real. For complex eigenvalues $\lambda$ we found that the second order term
leads to a shift essentially parallel to the imaginary axis and always directed towards the real axis. Thus in second order complex eigenvalues can move closer to the real axis and eventually become real eigenvalues.

To summarize this section we find that for thermalized gauge fields the clover term leads to a proliferation of real eigenvalues. The above given argument, based on the spectral flow for the eigenvalues of the auxiliary problem, shows that the eigenvalues are generated in pairs and the corresponding eigenvectors have opposite chirality. A perturbative analysis up to second order in $c_{sw}$ shows that existing real eigenvalues remain real, but complex eigenvalues tend to move towards the real axis.

6. Index theorem and fermionic definition of the topological charge
The fact that the additional real eigenvalues come in pairs with opposite chirality means that in principle they cancel each other in the lattice version ([S]) of the index theorem. However it is also obvious from Fig. 3 that already for $c_{sw} = 0$ the separation of physical and doubler branches is not very pronounced and the additional real eigenvalues make this situation worse for $c_{sw} > 0$. In this section we concentrate on the real spectrum and address the question if the separation of physical and doubler branches is large enough so that one can speak of a probabilistic lattice manifestation of the index theorem in a meaningful way.

Fig. 5 shows our results for 10 thermalized configurations which for further reference were numbered (#1 - #10). We also quote the topological charges that were assigned to these configurations after cooling in [18]. The figure shows the real spectra for $c_{sw} = 0$ and $c_{sw} = 1.4$. For both cases we computed all real eigenvalues larger than 1.8 in order to see at least a few of the real eigenvalues in the doubler branch. In the plot we also encode the chirality of the corresponding eigenstates. An upward pointing triangle means positive and a downward pointing triangle indicates negative chirality.

Let’s first discuss the spectra for the case without clover term. From the arbitrarily chosen sample we show here it is obvious, that the real eigenvalues are rather evenly distributed and only for configuration # 5 one can speak of a reasonably separated physical branch. For the other configurations it is unclear where to set the threshold for the physical modes.

We conclude that for this particular setting (SU(2), $12^4$, $\beta = 2.4$) the naive approach to a probabilistic lattice interpretation of the Atiyah-Singer index theorem by simply counting the real eigenvalues in the physical branch seems problematic.
config. | real spectrum at $c_{sw} = 0.0$ | real spectrum at $c_{sw} = 1.4$
---|---|---
#1: $\nu = -1$ | ![Spectrum 1](image1.png) | ![Spectrum 2](image2.png)
#2: $\nu = 2$ |  |  
#3: $\nu = 0$ |  |  
#4: $\nu = 2$ |  |  
#5: $\nu = 2$ |  |  
#6: $\nu = 0$ |  |  
#7: $\nu = -2$ |  |  
#8: $\nu = 0$ |  |  
#9: $\nu = -1$ |  |  
#10: $\nu = -2$ |  |  

Figure 5: Real eigenvalues larger than 1.8 for 10 thermalized gauge field configurations. The value of $\nu$ given on the right hand side of the plot was assigned after cooling [18]. An upward pointing triangle is the symbol for an eigenvalue with positive chirality while a downward pointing triangle indicates negative chirality.

In this context it is interesting to remark, that Narayanan and Vranas [12] obtained a surprising result using the fermionic overlap definition of the topological charge and averaging over large samples of quenched gauge field configurations (also for SU(2), $12^4$, $\beta = 2.4$). Narayanan and Vranas take into account all real eigenvalues larger than 3 and discard the smaller ones as doublers. From our plots it is clear that even if one is willing to define 3 to be the boundary between physical modes and doublers this definition disagrees in several cases (#2, #6, #7, #8, #10) with the cooling results and is not justified on a one by one basis. However after sampling 140 configurations [18], the result for the distribution of the topological sectors [18] from improved cooling is reproduced with good accuracy. This comparison of the averaged result with the analysis of single configurations indicates that there might be a mechanism which averages the results from counting the eigenvalues such that the distribution of the topological charge matches the outcome of the improved cooling analysis.

As already discussed in Section 5, the clover term does not improve the situation for the lattice index theorem. For a larger sample this is now demonstrated on the right hand side of Fig. 3 where we show the 10 real spectra now at Sheikholeslami-Wohlert coefficient $c_{sw} = 1.4$. Although the
additional real eigenvalues come in pairs of opposite chirality and thus in principle cancel in (8), from a technical point of view the extra real eigenvalues are very unpleasant since the idea of dividing the eigenvalues into physical and doubler modes becomes even more unrealistic than at $c_{sw} = 0$. However, also for $c_{sw} > 0$ a phenomenon similar to the $c_{sw} = 0$ case might occur, which would give the correct distribution of the topological charge when averaging large samples. It would be interesting to study and understand such a possibility in more detail.

7. Discussion
In this article we have studied the spectrum of the lattice Dirac operator and investigated the interplay between topological charge and spectral properties. The effects of the $O(a)$-improving clover term were analyzed.

For relatively smooth toy configurations (constant plaquette fields + small fluctuations) on $4^4$ lattices we find that the clover term leaves the physical branch of the spectrum rather unchanged while the bulk of the eigenvalues is slightly deformed. For the smooth toy configurations the lattice realization of the Atiyah-Singer index theorem is not affected by the clover term.

When analyzing smooth configurations on larger lattices obtained using the improved cooling method in [18], we even find improvement of the spectral properties when adding the clover term, i.e. the eigenvalues at the physical edge of the spectrum align along an ellipse and the pseudoscalar matrix elements are close to $±1$.

For the thermalized configurations $(12^4, \beta = 2.4)$ a naive attempt to interpret the real spectrum in terms of a probabilistic manifestation of the index theorem by simply counting the real eigenvalues in the physical branch is problematic. We observe, that there is no reasonable separation of physical modes and the doubler branches. The real eigenvalues in the physical branch which have to be taken into account for the lattice version of the index theorem cannot be identified reliably for this setting. We remark however, that summing over large samples seems to average out the error in the number of real eigenvalues in the physical branch and the distribution of the topological charge agrees with the result from improved cooling [12]. It would be interesting to understand this mechanism in more detail.

Adding the clover term makes the separation of physical eigenmodes and doublers even more difficult by creating new real eigenvalues. Based on an argument using zero crossings of the spectral flow of the auxiliary operator $H(\rho)$ we showed that the additional real eigenvalues come in pairs
and the corresponding eigenvectors have opposite chirality. A perturbative argument indicates that existing real eigenvalues are not destroyed by the clover term.

Certainly there is hope, that this situation improves as one goes over to larger lattices and higher $\beta$. Such an improvement of the spectral properties, i.e. a clearer separation of physical modes and doublers, leading to a simple probabilistic realization of the index theorem as one gets closer to the continuum limit was observed for QED$_2$. Only further analysis can settle the question if a similar scenario holds for SU(N) in 4 dimensions. Also new approaches such as the interpolation idea [10] or perfect actions [23] or other actions [31, 32] which obey the Ginsparg-Wilson relation [33] and are known to obey the index theorem [34] would be interesting to study numerically in 4 dimensions.

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