Improving the Dirac Operator in Lattice QCD

Christof Gattringer\textsuperscript{a,1}, C. B. Lang\textsuperscript{b}

\textsuperscript{a}Inst. f. Theoret. Physik, Univ. Regensburg, Universitätstr. 31, D-93053 Regensburg, Germany
\textsuperscript{b}Inst. f. Theoret. Physik, Universität Graz, A-8010 Graz, AUSTRIA

Abstract

Recently various new concepts for the construction of Dirac operators in lattice Quantum Chromodynamics (QCD) have been introduced. These operators satisfy the so-called Ginsparg-Wilson condition (GWC), thus obeying the Atiyah-Singer index theorem and violating chiral symmetry only in a modest and local form. Here we present studies in 4-d for SU(3) gauge configurations with non-trivial topological content. We study the flow of eigenvalues and we compare the numerical stability and efficiency of a recently suggested chirally improved operator with that of others in this respect.

Key words: Lattice quantum field theory, Dirac operator spectrum, Ginsparg-Wilson operators

PACS: 11.15.Ha, 11.10.Kk

1. Motivation and technicalities

A priori continuum Dirac operators have chiral symmetry, which then is broken spontaneously in the full QCD dynamics. Lattice discretizations of the Dirac operator are bound to violate the chiral symmetry. However, if they obey the GWC this violation is in its mildest form. Currently three types of exact realizations of so-called Ginsparg-Wilson (GW) operators are known: The overlap operator, perfect actions and domain wall fermions; for reviews on recent developments cf. [1]. In [2] we suggested a method to systematically expand the lattice Dirac operator in terms of a series of simple lattice operators and to turn the GWC into a large algebraic system of coupled equations for the expansion coefficients. The solution for a finite parametrization leads to an approximate GW-operator. Such a chirally improved Dirac operator has been constructed in 2-d for the Schwinger model [3] and also for 4-d QCD [4], where an analysis of its spectrum revealed intriguing properties.

The spectral properties of QCD Dirac operators provide an efficient means to study properties of the QCD vacuum related to chiral symmetry breaking. The spectral density in the limit of vanishing eigenvalues is proportional to the order parameter of chiral symmetry breaking via the Banks-Casher relation [5]. The microscopic distribution density exhibits features in a universality class discussed in random matrix theory [6]. The eigenmodes for exactly vanishing eigenvalues appear to represent instantons (classical solutions of the QCD field equations). In the quantization of
a lattice-regularized field theory it may come as a surprise that instanton-like objects (originally defined on differentiable manifolds) may play a role. Indeed, they are a miniscule contribution to the total action of a gauge configuration. However, as will be seen, they are observed in realistic gauge field configurations and they characterize the sector of small eigenmodes.

The overlap operator has the form

\[ D_{ov} = 1 - Z \quad \text{with} \quad Z \equiv \gamma_5 \, \text{sign}(H), \]

where \( H \) is related to the hermitian Dirac operator. This is constructed from an arbitrary Dirac operator \( D_0 \) (like e.g. the Wilson operator), \( H = \gamma_5 (s - D_0) \), and \( s \) is a parameter which may be adjusted in order to minimize the probability for zero modes of \( H \). In case \( D_0 \) is already an overlap operator one reproduces \( D_{ov} = D_0 \) for \( s = 1 \) due to \( \text{sign}(H) = \text{sign}(H) \).

The sign-function may be defined through the spectral representation, but this is technically impossible for realistic QCD Dirac operators, which for \( L^4 \) lattices have dimension \( O(10^5 - 10^6) \) (~ \( n_{\text{color}} \cdot n_{\text{Dirac}} \cdot L^4 \)). Note, that in the subsequent applications the operator has to be determined many times, since it may be entering a diagonalization or a conjugate gradient inversion tool. One therefore relies on the relation \( \text{sign}(H) = H/\sqrt{H^2} \) and approximates the inverse square by some method. In our computations we follow the methods discussed by \cite{11, 12, 13}. One approximates the inverse square root by a Chebychev polynomial, which has exponential convergence in \([\epsilon, 1]\), where \( \epsilon \) (and thus the order of the polynomial) depends on the ratio of smallest to largest eigenvalue of \( H^2 \). Clenshaw’s recurrence formula provides further numerical stability.

Depending on the input Dirac operator \( D_0 \) the rate of convergence may be quite unfavorable due to small eigenvalues of \( H^2 \). Therefore one computes the inverse square separately for the subspace of the smallest 20 eigenvalues (using the spectral representation) and the reduced operator (with polynomial approximation). The subspace has to be determined with high accuracy. All diagonalizations have been done with the Arnoldi method \cite{14}.

Fig. 1. We display the flow of eigenvalues of a matrix \( Z \) derived from a randomly constructed matrix \( H \) with all eigenvalues \( \pm 1 \) except for one, which is slowly changed between \(+1\) and \(-1\) (begin and end positions: full circles, value 0: square, intermediate values: dots).

2. Flow of eigenvalues

Lattice Dirac operators are necessarily non-hermitian, but “\( \gamma_5 \)-hermitian”, i.e. one may always define a “hermitian Dirac operator” \( \gamma_5 D \). The eigenvalues of a realistic “hermitian (e.g. Wilson-) Dirac operator” are distributed broadly on the real axis and have also values close to the origin. The sign-operator in (1) projects all \( +1 \) except for one, which is slowly changed to \(-1\). The difference \( n_+ - n_- \) is twice the number of zero modes of \( D_{ov} \).

We are interested in the case when \((1 - D_0)\) is close to, but not quite an overlap operator. In particular we want to study here the emergence or vanishing of zero modes. As a test case we construct a random, hermitian matrix operator like \( H \) with eigenvalues \( \pm 1 \). For \( \gamma_5 \) we choose an arbitrary realization like \( \Gamma_{ij} = (-1)^{i} \delta_{ij} \). The eigenvalues of the corresponding \( Z \) are then distributed randomly on a unit circle around the origin. Due to “\( \gamma_5 \)-hermiticity” of \( Z \) its eigenvalues occur in complex conjugate pairs. Real eigenvalues are at positions \( \pm 1 \) giving rise to vanishing eigenvalues of \( D_{ov} \), hence we call them zero modes.

Starting with a matrix where \( n_+ = n_- \) we will find no such “zero modes”. Let us change contin-
3. “Artificial” and realistic instantons

We construct gauge configurations with artificial instantons as discussed in [13, 10] and study for given lattice size 16^4 such configurations for instantons of varying size R (Fig. 2). Real eigenvalues may be associated with instanton modes.

We recover the typical features of our test example: The Wilson operator reacts quite slowly on the change of size and “looses” the instanton at size O(2), the overlap operator looses the instanton around R ≃ 1.5. The chirally improved operator is for R ≥ 3 similar to the overlap operator, but identifies also smaller instantons.

The chirally improved operator may be used either for its own sake, as a Dirac operator, or in order to improve performance by using it as a starting point for the determination of the overlap Dirac operator. From Fig. 2 one finds, that the improved operator is clearly superior to the Wilson operator, since it spends less time (fewer configurations) in the central region due to its steeper slope.

In Fig. 3 we show the distribution of eigenvalues of the chirally improved operator. The gauge configurations have been obtained with the Lüscher-Weisz action [16] as detailed in [8]. Compared to the Wilson action the eigenvalues are much more localized around 0 and therefore H will have much fewer zero modes. This ought to improve the convergence properties significantly. However, in our computations we found an improvement factor of only 2 in the necessary order of the Chebychev polynomials. This is likely due to the explicit treatment of the sector of small eigenvalues of H. Due to the numerical complexity of the improved operator (it has more coupling terms and is typically a factor of 20 more expensive than Wilson’s action), we find that using it as input for the overlap operator is not economically warranted. However, to use it as an approximate Ginsparg-Wilson-type operator may be quite successful, as we discuss below.

The (normalized) gauge-invariant densities
Fig. 4. Comparing the inverse participation ratio for the overlap operator with the chirally improved operator. For both values of the gauge coupling we plot the results of 200 gauge configurations with a single zero mode.

\[ p_\alpha(x) = \langle \psi_0(x) \mid \gamma_\alpha \mid \psi_0(x) \rangle \]  

(2)

(Implied summation over color and Dirac indices) are determined from the zero mode eigenvector \( |\psi_0\rangle \); \( \gamma_\alpha \) is one of the 16 \( \gamma \)-matrices of the 4D-Clifford algebra with \( \gamma_0 = 1 \). Comparing \( p_0 \) and \( p_5 \) as determined for a realistic gauge configuration with one zero mode for the three Dirac operators considered we find clear instanton bumps at the same position in all cases. However, Fig. 2 pointed at a varying sensitivity of different Dirac operators with regard to identifying instantons. The space-time integral \( I_0 = \int d^4x \ p_\alpha^2(x) \) defines the so-called inverse participation ratio and constitutes a measure of localization. For instantons with radius \( R \) one expects \( I_0 \propto 1/R^4 \).

In Fig. 4 we compare \( I_0 \) for realistic gauge configurations. We find that the overlap operator typically underestimates the localization of the zero mode, confirming earlier findings for artificial instantons [4]. A possible interpretation lies in the “size” of the different lattice Dirac operators. The matrix elements of the overlap operator fall off like roughly \( \sim 1/2|x-y| \) whereas the chirally improved operator is ultra-local (i.e. with non-vanishing coupling only for \( |x-y| \leq \sqrt{5} \)). At typical lattice spacings \( O(0.1 \text{ fm}) \) of today’s simulations the chirally improved operator appears to keep better track of structures smaller than \( O(0.3 \text{ fm}) \). Closer to the continuum limit, at smaller lattice spacings, this feature of the overlap operator may be no problem, though.

Acknowledgment: We wish to thank our collaborators (M. Gökêlêr, R. Rakow, S. Schaefer and A. Schäfer) for their support and many discussion and the Leibniz Rechenzentrum in Munich for computer time on the Hitachi SR8000 and their team for training and support. C.B.L. wants to thank K. Jansen for instructive discussions.

References

[1] F. Niedermayer, Nucl. Phys. B (Proc.Suppl.) 73 (1999) 105. H. Neuberger, Nucl. Phys. B (Proc. Suppl.) 83-84 (2000) 67. M. Lüscher, Nucl. Phys. B (Proc. Suppl.) 83-84 (2000) 34.
[2] C. Gattringer, Phys. Rev. D 63 (2001) 114501.
[3] C. Gattringer and I. Hip, Phys. Lett. B 480 (2000) 112.
[4] C. Gattringer, I. Hip, and C. B. Lang, Nucl. Phys. B 597 (2001) 451.
[5] T. Banks and A. Casher, Nucl. Phys. B 169 (1980) 103.
[6] J. J. M. Verbaarschot and T. Wettig, Ann.Rev.Nucl.Part.Sci. 50 (2000) 343.
[7] T. DeGrand and A. Hasenfratz, Phys. Rev. D 64 (2001) 034512; hep-lat/0103003. R. G. Edwards and U. M. Heller, hep-lat/0105004, 2001. T. Blum et al., hep-lat/0105004, 2001. I. Horvath et al., hep-lat/0102003, 2001.
[8] C. Gattringer et al., hep-lat/0105023, 2001; hep-lat/0107010, 2001.
[9] R. Narayanan and H. Neuberger, Phys. Lett. B 302 (1993) 62; Nucl. Phys. B 443 (1995) 305.
[10] C. Gattringer et al., hep-lat/0108001, 2001.
[11] P. Hernández, K. Jansen, and M. Lüscher, Nucl. Phys. B 552 (1999) 363.
[12] P. Hernandez, K. Jansen, and L. Lellouch, hep-lat/0001008, 2000.
[13] B. Bunk, Nucl. Phys. B (Proc. Suppl.) 63 (1998) 952.
[14] D. C. Sorensen, SIAM J. Matrix Anal. Appl. 13 (1992) 357. R. B. Lehoucq, D. C. Sorensen, and C. Yang, ARPACK User’s Guide, SIAM, New York, 1998.
[15] I. A. Fox et al., Phys. Lett. B 158 (1985) 332.
[16] M. Lüscher and P. Weisz, Commun. Math. Phys. 97 (1985) 59.