Resolving Exceptional Configurations in Quenched Lattice QCD\textsuperscript{*}

M. Göckeler\textsuperscript{a}, A. Hoferichter\textsuperscript{b}, R. Horsley\textsuperscript{c}, D. Pleiter\textsuperscript{b,d}, P. Rakow\textsuperscript{a}, G. Schierholz\textsuperscript{b,e}, and P. Stephenson\textsuperscript{f}

\textsuperscript{a} Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg
\textsuperscript{b} Deutsches Elektronen-Synchrotron DESY and NIC, D-15735 Zeuthen
\textsuperscript{c} Institut für Physik, Humboldt-Universität zu Berlin, D-10115 Berlin
\textsuperscript{d} Institut für Theoretische Physik, Freie Universität Berlin, D-14195 Berlin
\textsuperscript{e} Deutsches Elektronen-Synchrotron DESY, D-22603 Hamburg
\textsuperscript{f} Dipartimento di Fisica, Università di Pisa, I-56126 Pisa

Quenched lattice QCD calculations with Wilson-type fermions at small quark masses are impeded by exceptional configurations. We show how this problem can be resolved in a practicable way without changing the physics in the chiral limit.

1. INTRODUCTION

We consider Wilson fermions with or without \(O(a)\) improvement. The fermionic action reads

\[ S_F = \sum \bar{\psi} \mathcal{K} \psi, \quad \mathcal{K} = W + M, \tag{1} \]

where \(W\) is the Wilson-Dirac operator:

\[ W = \mathcal{D} + X \tag{2} \]

with

\[ D_{\mu} = \frac{1}{2} (D_{\mu}^+ + D_{\mu}^-), \tag{3} \]

\[ X = -\frac{1}{2} D_{\mu}^+ D_{\mu}^- + \frac{i}{4} c_{SW} \sigma_{\mu\nu} F_{\mu\nu}, \tag{4} \]

\(D_{\mu}^+ (D_{\mu}^-)\) being the forward (backward) lattice derivative, and where \(M\) is the Wilson mass term:

\[ M = \frac{1}{2\kappa} - 4. \tag{5} \]

The critical value of the hopping parameter, \(\kappa_c\), is taken to be the limiting value at which the ensemble averaged pion mass vanishes. We call this limit the chiral limit.

\textsuperscript{*}Poster presented by G. Schierholz at Lattice 1998.

Figure 1. The pion correlator on the \(32^3 \times 64\) lattice at \(\beta = 6.2\) and \(\kappa = 0.1354\) for improved fermions with \(c_{SW} = 1.614\). At these parameters \(m_\pi/m_\rho \approx 0.5\) which corresponds to a quark mass of \(\approx 40\,\text{MeV}\). The solid symbols (and line) represent the ensemble average with the exceptional configurations omitted. The dashed line is the result of a single, particularly exceptional configuration.
Figure 2. A sketch of the eigenvalue spectrum of $W_c$ (before the rotation) and $W_c^{\phi=\pi/4}$ (after the rotation).

In quenched lattice calculations with Wilson fermions one encounters exceptional configurations [1] which give rise to poles in fermionic observables, such as hadron correlators, at small quark masses. The origin of these poles are real eigenvalues $\lambda_i$ of the Wilson-Dirac operator $W$ at

$$\lambda_i < 4 - \frac{1}{2\kappa_c}. \quad (6)$$

Exceptional configurations are particularly aggravating for improved fermions, and they have limited calculations to larger quark masses and larger values of $\beta$. We expect to find such poles also in the full theory, i.e. with dynamical fermions, at hopping parameters $\kappa \neq \kappa_{sea}$, where $\kappa_{sea}$ refers to the sea quark mass.

In Fig. 1 we give an example of an exceptional configuration which we encountered in a recent simulation with improved fermions [2]. We see a dramatic deflection from the anticipated ensemble average. Similar peaks are observed in the $\rho$ and nucleon correlators. It is quite clear from this figure that the problem of exceptional configurations cannot be solved by accumulating larger statistical samples.

Bardeen et al. [3] identify the eigenvalues (6) with the zero modes of the continuum theory, and they propose to shift each such $\lambda_i$ to $\lambda_i = 4 - 1/2\kappa_c$. There are doubts, however, that this identification is correct in general [4]. An elegant solution would be to employ Neuberger’s action [5]. But whether this is numerically feasible has still to be seen.

2. PROPOSAL

The solution we propose makes use of a freedom in regularizing lattice fermions. It has the advantage that it is easy to implement numerically, and that it does not change the physics in the chiral limit so that the improvement program à la Sheikholeslami and Wohlert [6] remains unaltered.

We rewrite $K$ in (1) as

$$K = W_c + m, \quad (7)$$

where $W_c$ and $m$ are the critical Wilson-Dirac operator and the physical bare mass, respectively:

$$W_c = \slashed{D} + X_c, \quad X_c = X + \frac{1}{2\kappa_c} - 4, \quad (8)$$

$$m = \frac{1}{2\kappa} - \frac{1}{2\kappa_c}. \quad (9)$$

We then apply a chiral rotation to $W_c$,

$$W_c \rightarrow W_c^{\phi} = e^{i\gamma_5 \phi} W_c e^{i\gamma_5 \phi},$$

$$= \slashed{D} + X_c (\cos 2\phi + i\gamma_5 \sin 2\phi), \quad (10)$$

and take $K^{\phi} = W_c^{\phi} + m$ to be the new fermion matrix. The resulting action is equally well founded as (1) and (7), though, in general, it breaks parity invariance. In Fig. 2 we show the effect of the transformation on the eigenvalue spectrum of the Wilson-Dirac operator for $\phi = \pi/4$. In this
Figure 3. The pion correlator for a single exceptional configuration on the $16^3 \times 32$ lattice at $\beta = 5.7$ and $c_{SW} = 2.25, \kappa = 0.1295$ before ($\circ$) and after the rotation by $\phi = \pi/4$ ($\bullet$), with $\kappa_c = 0.13074$ [8]. The data for improved fermions are compared with the result for Wilson fermions ($\bigcirc$) at an equivalent quark mass.

The rotation (10) is mathematically equivalent to the transformation of the mass:

$$m \rightarrow m^\phi = m (\cos 2\phi - i\gamma_5 \sin 2\phi).$$

In the following we shall use this transformation. Furthermore we take $\phi = \pi/4$. But we found that the method works equally well for angles as small as $|\phi| = 0.05$.

To test the idea, we have looked at exceptional configurations which we encountered in our runs with improved fermions [8] on the $16^3 \times 32$ lattice at $\beta = 5.7$. If the method works at this coupling, we expect that it will work also at larger values of $\beta$. In Fig. 3 we show the pion correlator for a single exceptional configuration before and after the rotation. Before the rotation we find a similar peak in the pion correlator as seen in Fig. 1. After the rotation we find a correlator which is perfectly well behaved. It turns out to be in good agreement with the ensemble average [8]. Note that in first approximation the physical quark mass is left unchanged by the rotation. For comparison we have computed the pion correlator also for Wilson fermions. The hopping parameter was chosen so as to give roughly the same pion mass. We find good agreement with the rotated action.

4. DISCUSSION

From both, Figs. 1 and 3 it follows that the (suspected) near-zero eigenmode of $K$ acts as a source term, and that the excitation it induces decays exponentially with roughly the mass of the pion. We would not expect to find such a behavior for an instanton configuration. There is also no sign of an abnormal fluctuation found in the case of Wilson fermions.

We conclude that the problem of exceptional configurations may be resolved by a chiral rotation of the critical Wilson-Dirac operator. The method allows calculations at any quark mass. On top of that, the results of the improvement program remain valid.

REFERENCES

1. For a first mention see: K.-H. Mütter et al., Proceedings International Symposium on Lattice Gauge Theory, Brookhaven, 1986, p. 257 (Plenum, New York, 1987).
2. D. Pleiter, these proceedings.
3. W. Bardeen et al., Nucl. Phys. B (Proc. Suppl.) 63 (1998) 141.
4. C. Gattringer and I. Hip, UNIGRAZ-UTP28-06-98 (1998) [hep-lat/9806032].
5. H. Neuberger, Phys. Lett. B417 (1998) 141; ibid. B427 (1998) 353.
6. K. Jansen et al., Phys. Lett. B372 (1996) 275.
7. G. Immirzi and K. Yoshida, Nucl. Phys. B210 (1982) 499; K. Osterwalder and E. Seiler, Ann. Phys. 110 (1978) 440; W. Kerler, Phys. Rev. D24 (1981) 1595; E. Seiler and I. O. Stamatescu, Phys. Rev. D25 (1982) 2177.
8. M. Gökeler et al., Phys. Rev. D57 (1998) 5562.