Cutoff–effects in the spectrum of dynamical Wilson fermions

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We investigate the low–lying eigenvalues of the improved Wilson–Dirac operator in the Schrödinger functional with two dynamical quark flavors. At a lattice spacing of approximately 0.1 fm we find more very small eigenvalues than in the quenched case. These cause problems with HMC–type algorithms and in the evaluation of fermionic correlation functions. Through a simulation at a finer lattice spacing we are able to establish their nature as cutoff–effects.

1. Motivation

Recently more and more evidence has been accumulated that for dynamical improved Wilson fermions at a lattice spacing of $a \approx 0.1$ fm the cutoff–effects are much larger than expected from quenched experience (for a summary of large scaling violations in the two–flavor–theory see ref. [1]). As an extreme example, for three flavors the existence of a phase transition in the $\beta$–$\kappa$–plane has been numerically conjectured and is interpreted as a lattice artifact [2].

In addition several collaborations have reported algorithmic difficulties with (improved) Wilson fermions on relatively coarse lattices (see e.g. [3]), which seem to be related to small eigenvalues of the Dirac operator. Through the inversion of the Dirac operator these small eigenvalues can result in large driving force during the molecular dynamics evolution of Hybrid Monte Carlo (HMC) algorithms. In turn, the large forces are likely to trigger instabilities of the numeric integrator employed, which produces large Hamiltonian violations and can result in long periods of rejection [4]. In this way small eigenvalues affect algorithmic performance.

The occurrence of very small eigenvalues generates not only algorithmic problems. On the configurations in question the quark propagator becomes large and one observes ”spikes” in fermionic correlation functions. This affects not only their mean value but also their autocorrelation function, making the statistical analysis difficult. This is discussed in more detail in ref. [4].

For dynamical simulations this is an unexpected problem since naïvely it is assumed that the determinant should suppress small eigenvalues compared to the quenched situation. In our setup we have two infrared cutoffs (finite quark mass and Schrödinger functional boundary conditions) that should prevent the Dirac operator from developing very small eigenvalues. Nevertheless we observe them in simulations with a lattice spacing of about 0.1 fm. Here we show that these small eigenvalues disappear if one goes to smaller lattice spacings and can thus be interpreted as a lattice artifact.

2. Setup and error analysis

We simulate the Schrödinger functional (SF) with two dynamical flavors of non–perturbatively improved Wilson fermions. The algorithms used are HMC with two pseudo–fermion fields [5] and PHMC [6]. In the following the term ’eigenvalue’ always refers to the eigenvalue (in lattice units) of the square of the Hermitian even–odd–preconditioned Wilson–Dirac operator in the normalization of [7]. For PHMC the parameters of the polynomial are chosen such that more configurations with small eigenvalues are produced compared to the QCD Boltzmann weight. After reweighting this gives a very good estimate of the path–integral weight of such configurations. Another benefit of using PHMC is that the polynomial provides a regularized inversion, thus also addressing the algorithmic problems due to large forces mentioned above. With this algorithm the
correct ensemble average of an estimator $O$ is given by
\[
\langle O \rangle = \frac{\langle OW \rangle_P}{\langle W \rangle_P},
\]
where $W$ is the reweighting factor and the subscript $P$ indicates an average over the PHMC-generated ensemble. HMC-type algorithms are expensive and generate strongly autocorrelated data, which makes a careful data analysis indispensable. We use an explicit integration of the autocorrelation function as described in ref. [8].

To obtain a histogram for a quantity $f = \langle \phi \rangle$ we analyze
\[
P_n = \langle \chi_n(\phi) \rangle = \frac{\langle \chi_n(\phi)W \rangle_P}{\langle W \rangle_P},
\]

3. Comparison to the quenched case

In order to test the na"ive expectation that the fermionic determinant suppresses small eigenvalues we compare quenched and dynamical ensembles of $8^3 \times 18$ lattices at roughly matched physical parameters. Using the quenched data from ref. [9] and the dynamical data from refs. [10] and [11] we choose the parameters such that the lattice spacing and the (large volume) pseudo–scalar mass are matched.

The distribution of the smallest eigenvalue $\lambda_{\text{min}}$ is shown in Figure 1. The quite small error bars we obtain from eq. 2 at the lower end of the spectrum are due to the enhanced occurrence of small eigenvalues by PHMC. While $\langle \lambda_{\text{min}} \rangle$ is increased from $1.44(1) \cdot 10^{-4}$ to $1.72(5) \cdot 10^{-4}$ with two dynamical flavors we see that in the infrared tail the dynamical data show more events. More precisely, the probability of finding a smallest eigenvalue below $4 \cdot 10^{-5}$ increases from $0.81(16)\%$ to $1.88(26)\%$. To show that this long tail towards zero is a cutoff–effect we now compare dynamical data from different lattice spacings at matched parameters.

4. Finer lattices

Through measurements of the SF coupling $g^2$ [12,13] we found that increasing $\beta$ from 5.2 to 5.5 changes the lattice spacing by roughly a factor of $2/3$. Anticipating that the algorithmic problems due to very small eigenvalues would no longer be present at this finer lattice spacings we used HMC with two pseudo–fermions to generate an ensemble of $12^3 \times 27$ lattices. Ignoring small changes in the renormalization factor we compare this to an $8^3 \times 18$ PHMC ensemble at $\beta = 5.2$, which is matched using $L_{\text{PTAC}}$, the box size times the bare PCAC mass. To plot both lattice spacings simultaneously we divide by $\langle \lambda_{\text{min}} \rangle$ in Figure 2.

Going from $\beta = 5.2$ to 5.5 reduces the variance (normalized by the mean value) of the small-
Figure 3. Comparison of the smallest eigenvalue distribution at a lattice spacing of approximately 0.07 fm.

The smallest eigenvalue from 0.178(10) to 0.127(19). The long tail at the infrared has disappeared at the finer lattice spacing and we thus interpret it as a cutoff–effect.

In a final step we compare the dynamical data at $\beta = 5.5$ to another quenched run at approximately the same lattice spacing ($\beta = 6.26$), volume and bare quark mass.

In Figure 3 both the quenched and the dynamical data show very similar behavior at the infrared end of the spectrum. A comparison to Figure 1 shows that the excess of very small eigenvalues we found at the coarser lattice spacing has disappeared entirely. As at $a = 0.1$ fm the average smallest eigenvalue is still shifted upwards by the fermionic determinant.

5. Conclusions

The problems in simulating dynamical Wilson fermions at a lattice spacing of approximately 0.1 fm are due to the occurrence of very small eigenvalues in the spectrum of the Wilson–Dirac operator. We use PHMC to better sample this part of the spectrum in a comparison of two–flavor and quenched simulations at matched physical parameters.

As expected we find the average smallest eigenvalue to be larger in the dynamical case. However, due to its increased variance the dynamical data shows more very small eigenvalues despite the finite quark mass and the cutoff provided by the Dirichlet boundary conditions.

At a lattice spacing of approximately 0.07 fm both the dynamical and a matched quenched run show a spectrum that is well separated from zero. As before $\langle \lambda_{\text{min}} \rangle$ is larger for two flavors.

We conclude that at $\beta = 5.2$, corresponding to a lattice spacing of 0.1 fm, the spectrum of the Wilson–Dirac operator is strongly distorted. Our simulations show that this is a cutoff–effect that disappears rapidly with increasing $\beta$.

We do not expect that these findings are specific to the Schrödinger functional. Without the additional infrared cutoff due to the boundary conditions one should see these problems already at larger quark masses.

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