Konrad-Zuse-Zentrum
für Informationstechnik Berlin

Takustraße 7
D-14195 Berlin-Dahlem
Germany

HINNERK STÜBEN

Decorrelation of the Topological Charge in Tempered Simulations of Full QCD

Contribution to the NATO Advanced Research Workshop "Lattice Fermions and Structure of the Vacuum", October 5–9, 1999, Dubna, Russia.

Preprint SC 99–47 (December 1999)

DECORRELATION OF THE TOPOLOGICAL CHARGE IN TEMPERED SIMULATIONS OF FULL QCD

H. STÜBEN

Konrad-Zuse-Zentrum für Informationstechnik Berlin
Takustrasse 7, 14195 Berlin, Germany

Abstract. The improvement of simulations of QCD with dynamical Wilson fermions by combining the Hybrid Monte Carlo algorithm with parallel tempering is studied. As an indicator for decorrelation the topological charge is used.

1. Introduction

Decorrelation of the topological charge in Hybrid Monte Carlo (HMC) simulations of QCD with dynamical fermions is a long standing problem. For staggered fermions an insufficient tunneling rate of the topological charge Q_t has been observed [1, 2]. For Wilson fermions the tunneling rate is adequate in many cases [3, 4]. However on large lattices and for large values of κ near the chiral limit the distribution of Q_t is not symmetric even after more than 3000 trajectories (see Figure 1 of [3] and similar observations by CP-PACS [5]).

It has also been observed that sensitive observables like the η' correlator are Q_t dependent [10]. Thus it appears to be important to look for simulation methods that give good distributions of Q_t.

The idea of parallel tempering is to improve transitions in parameter regions where tunneling is suppressed by opening ways through parameter regions with little suppression. In QCD the method has been applied successfully for staggered fermions [6]. In [7] parallel tempering has been used to simulate QCD with O(a)-improved Wilson fermions without finding any gain, however, with only two ensembles which does not take advantage of the main idea of the method.

Here parallel tempering is used in conjunction with HMC to simulate QCD with (standard) Wilson fermions. The gain achieved is demonstrated by studying time series and histograms of the topological charge and by comparing statistical errors of the topological susceptibility $\langle Q_t^2 \rangle$.

2. Parallel Tempering

In standard Monte Carlo simulations one deals with one parameter set λ and generates a sequence of configurations C. The set λ here includes β, κ, the leapfrog time step and the number of time steps. C comprises the gauge field and the pseudo fermion field.

In the parallel tempering approach [8, 9] one simulates N ensembles $(\lambda_i; C_i)$, $i = 1, \ldots, N$ in a single combined run. Two steps alternate: (a) update of N configurations in the standard way, (b) exchange of configurations by swapping pairs. Swapping of a pair of configurations means

$$((\lambda_i; C_i), (\lambda_j; C_j)) \to \begin{cases} ((\lambda_i; C_j), (\lambda_j; C_i)), & \text{if accepted} \\ ((\lambda_i; C_i), (\lambda_j; C_j)), & \text{else} \end{cases} \tag{1}$$

with the Metropolis acceptance condition

$$P_{\text{swap}}(i, j) = \min\left(1, e^{-\Delta H}\right) , \tag{2}$$

$$\Delta H = H_{\lambda_i}(C_i) + H_{\lambda_j}(C_j) - H_{\lambda_i}(C_j) - H_{\lambda_j}(C_i). \tag{3}$$

Since after swapping both ensembles remain in equilibrium, the swapping sequence can be freely chosen. In order to achieve a high swap acceptance rate one will only try to swap (β, κ)-pairs that are close together. If the chosen (β, κ)-values lie on a curve in the (β, κ)-plane there are three obvious choices for the swapping sequence of neighboring (β, κ)-pairs. One can step through the curve in either direction or swap randomly. It has turned out that it is advantageous to step along such a curve in the direction from high to low tunneling rates of Q_t.

3. Simulation Details

The standard Wilson action for the gauge and the fermion fields was used. The lattice size was 8^4. The HMC program applied the standard conjugate gradient inverter with even/odd preconditioning. The trajectory length was always 1. The time steps were adjusted to get acceptance rates of about 70%. In all cases 1000 trajectories were generated (plus 50–100 trajectories for thermalization).

Q_t was measured by the field-theoretic method after 50 cooling steps of Cabibbo-Marinari type. This method gives close to integer values which were rounded to the nearest integers. (Note that the results presented in [11] were obtained without rounding.)

Statistical errors were obtained by binning, i.e., the values given are the maximal errors calculated after blocking the data into bins of sizes $10, 20, 50$ and 100.

4. Results

Several tempered HMC simulations were run in the quenched approximation (tempering in β) and with dynamical fermions (tempering in κ, at fixed $\beta = 5.5$ and $\beta = 5.6$). For comparison also standard HMC simulations have been performed.

Figures 1 and 2 show typical comparisons of time series and histograms of Q_t. One sees that with tempering considerably more topologically non-trivial configurations occur and that the histograms of Q_t become in general more symmetrical and broader.

In standard runs Q_t frequently stayed for quite some time near 1 or near -1, while with tempering this never occurred. The standard run at $\kappa = 0.156$ shown in Figure 2, where Q_t gets trapped in this way for about 200 trajectories, provides an example of this. Such observations have also been made on large lattices [3, 5].

While a correlation analysis cannot be carried out with the given size of samples, some quantitative account of the improvement by tempering is possible using the mean of the absolute change of Q_t, called mobility in [3],

$$D_1 = \frac{1}{N_{\rm traj}} \sum_{i=1}^{N_{\rm traj}} |Q_t(i) - Q_t(i-1)| \ . \tag{4}$$

Results for D_1 are given in Tables 1 and 2. If $|Q_t(i) - Q_t(i-1)| \leq 1$ for all trajectories then $1/D_1$ is the HMC time between topological events. Since that condition holds in most of the cases presented here one gets an idea of the quantitative improvement by tempering.

Another quantitative estimate of improvement comes from the statistical errors of $\langle Q_t^2 \rangle$. The fact that statistical errors decrease with the square of HMC time provides a second quantitative criterion for the speed-up of a simulation.

Quantitative results at $\beta = 5.5$ are summarized in Table 1. From the ratios of mobilities and squared ratios of errors of susceptibilities one obtains speed-ups between 2 (ratio of D_1 at $\kappa = 0.158$) and 16 (squared ratio of the errors of $\langle Q_t^2 \rangle$ at $\kappa = 0.160$). This is a considerable gain, especially if runs at several values of κ need to be done, what is usually the case.

At $\beta = 5.6$ tempering looks even better in the sense that the standard HMC runs do not really resolve the topological properties for $\kappa \geq 0.156$ (see Table 2 and Figures 2 and 3).

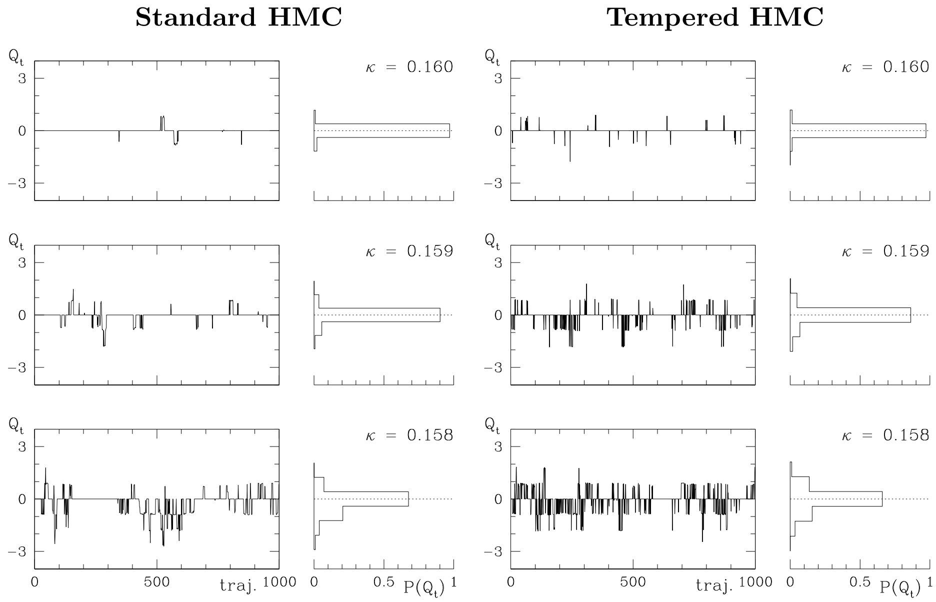

Figure 1. Comparison of time series and histograms of Q_t obtained from standard and tempered HMC on the 8^4 lattice at $\beta = 5.5$. In the tempered run 5 ensembles were used, $0.158 \leq \kappa \leq 0.160$ and $\Delta\kappa = 0.0005$. The swap acceptance rate was about 56%.

TABLE 1. Mobilities D_1 and topological susceptibilities $\langle Q_t^2 \rangle$ for the plots shown in Figure 1.

	Standard HMC		Tempered HMC	
κ	D_1	$\langle Q_t^2 \rangle$	D_1	$\langle Q_t^2 \rangle$
0.158	0.171(35)	0.51(19)	0.398(53)	0.49(8)
0.159	0.058(20)	0.12(5)	0.248(40)	0.20(5)
0.160	0.012(8)	0.030(27)	0.056(13)	0.031(7)

In the following the choice of κ-values at $\beta = 5.6$ is motivated. The run with 21 ensembles can be considered as a reference run. In a large scale simulation one would want to use less ensembles. The run with 6 ensembles demonstrates that comparable speed-up can be achieved with a smaller number of ensembles. The run with 7 ensembles covers exactly the parameter range investigated by SESAM [3]. It was mainly done to get estimates for the swap acceptance rate on larger lattices for $\Delta\kappa = 0.00025$ (see section 5).

It is interesting to compare the runs with 6 and 7 ensembles. In the run with 6 ensembles the mobility is higher. This reflects the main idea of the tempering method which is to connect areas of low tunneling rates with areas of high tunneling rates.

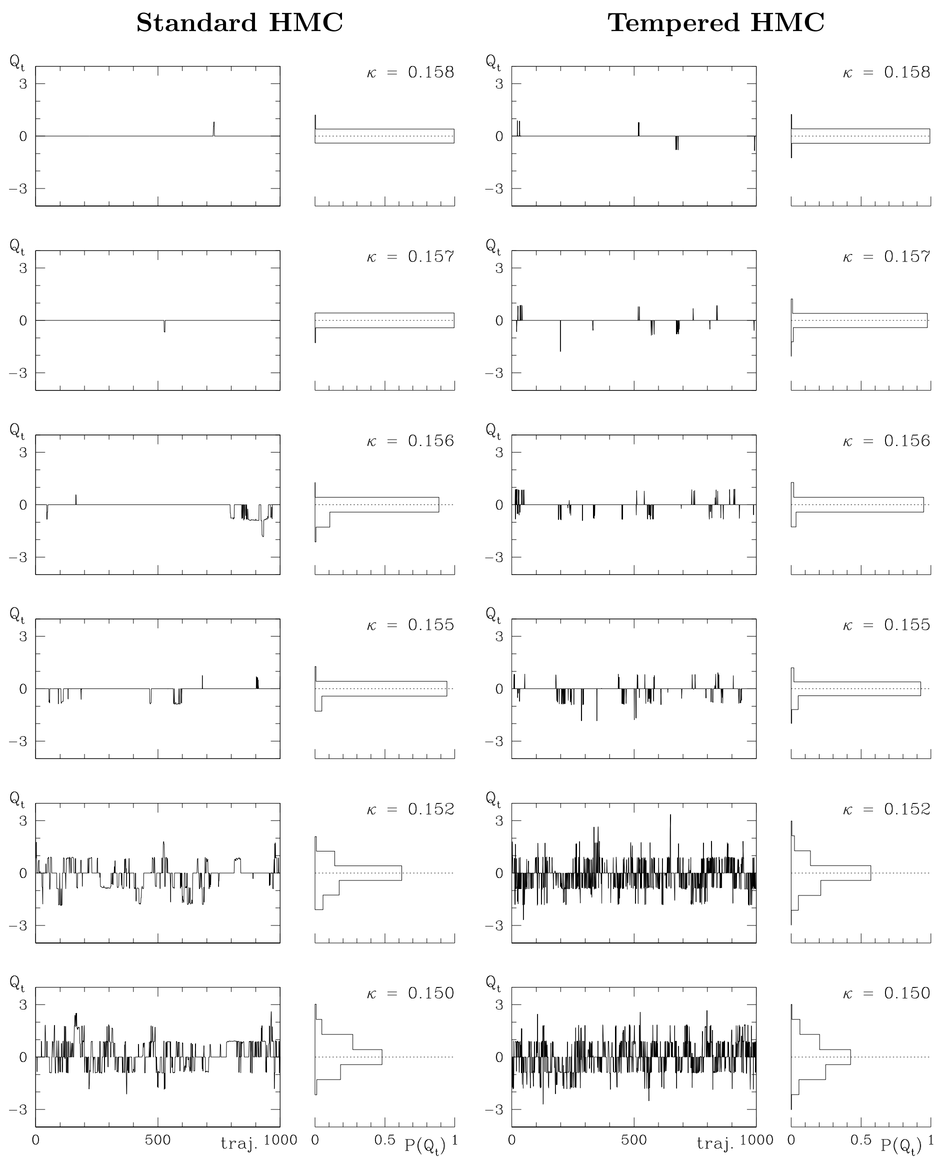

Figure 2. Comparison of time series and histograms of Q_t obtained from standard and tempered HMC on the 8^4 lattice at $\beta = 5.6$. The corresponding quantitative results can be found in Table 2.

TABLE 2. Mobilities D_1 and topological susceptibilities $\langle Q_t^2 \rangle$ on the 8^4 lattice at $\beta = 5.6$. The swap acceptance rates achieved were about 82% for $\Delta\kappa = 0.00025$ and about 63% for $\Delta\kappa = 0.0005$.

	Standard HMC		Tempered HMC	
		7 ensembles $0.156 \le \kappa \le 0.1575$ $\Delta\kappa = 0.00025$	6 ensembles $0.155 \le \kappa \le 0.1575$ $\Delta\kappa = 0.0005$	21 ensembles $0.15 \le \kappa \le 0.16$ $\Delta\kappa = 0.0005$
κ			D_1	
0.1500	0.325(39)			0.764(46)
0.1520	0.174(29)			0.735(50)
0.1550	0.031(11)		0.167(42)	0.132(32)
0.1555			0.176(43)	0.118(30)
0.1560	0.030(17)	0.064(27)	0.108(36)	0.096(26)
0.1565		0.040(15)	0.102(28)	0.074(22)
0.1570	0.002(2)	0.022(8)	0.068(19)	0.046(15)
0.1575		0.004(3)	0.044(14)	0.034(12)
0.1580	0.002(2)			0.016(8)
0.1600	0			0
κ			$\langle Q_t^2 \rangle$	
0.1500	0.77(14)			0.993(92)
0.1520	0.58(13)			0.707(57)
0.1550	0.056(29)		0.144(40)	0.085(21)
0.1555			0.100(25)	0.071(18)
0.1560	0.134(83)	0.044(20)	0.062(23)	0.052(14)
0.1565		0.020(8)	0.055(17)	0.040(14)
0.1570	0.004(4)	0.011(4)	0.037(11)	0.028(9)
0.1575		0.002(1)	0.030(11)	0.017(6)
0.1580	0.004(4)			0.008(4)
0.1600	0			0

5. Going to larger Lattices

With regard to large scale simulations of QCD performance predictions are needed. One potential problem of the tempering method has been stressed in [7], namely the decrease of the swap acceptance rate $\langle A \rangle$ with the lattice volume. In [7] it has been checked that the relation [12]

$$\langle A \rangle = \mathrm{erfc}\left(\frac{1}{2}\sqrt{\langle \Delta H \rangle}\right) \tag{5}$$

is valid for a large range of $\langle \Delta H \rangle$. Relation (5) also holds in all simulation done in this work.

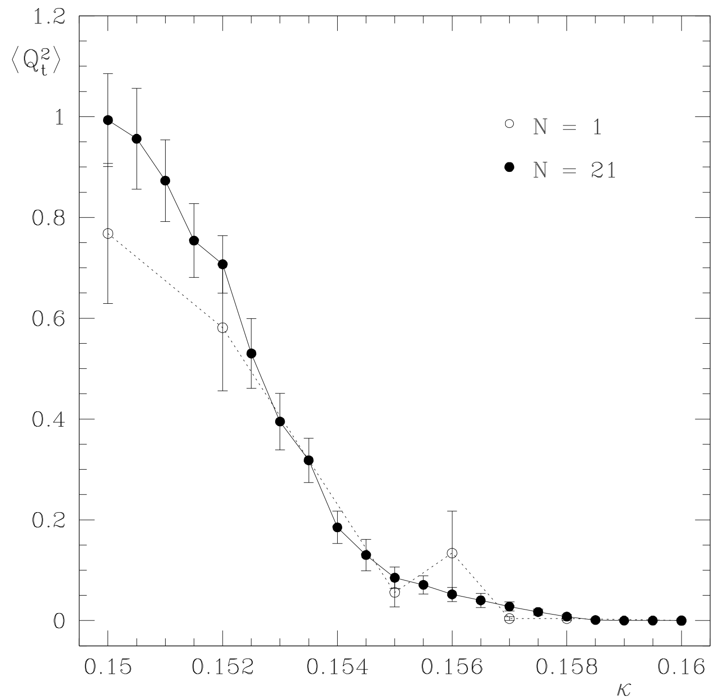

Figure 3. Comparison of topological susceptibilities on the 8^4 lattice at $\beta = 5.6$. The plot shows results from standard HMC ($N = 1$) and the tempered HMC run with $N = 21$ ensembles.

Because $\langle \Delta H \rangle$ scales linearly with the lattice volume V, relation (5) allows one to predict $\langle A \rangle$ by inserting values measured on the 8^4 lattice. Table 3 lists predictions using values of $\langle A \rangle$ from the runs shown in Table 2. Some caution is necessary with these predictions because on the 8^4 lattice at $\beta = 5.6$ and $0.15 \leq \kappa \leq 0.16$ the finite temperature phase transition [13] is crossed.

TABLE 3.

$\Delta\kappa$	V	$\langle A \rangle$
0.0005	8^4	63%
	$16^3 \times 32$	0.6%
0.00025	8^4	82%
	$16^3 \times 32$	20%
	$24^3 \times 48$	0.4%

Indeed more and more ensembles will be needed on larger lattices if one wants to keep $\langle A \rangle$ and the parameter range constant. However it is an open question which effect is stronger, the decrease of $\langle A \rangle$ or the slowing down of tunneling between topological sectors. The hope is that the need to take more ensembles more than compensates the slowing down of tunneling.

6. Conclusions

On the 8^4 lattice parallel tempering considerably enhances tunneling between different sectors of topological charge and generates samples with more symmetrical charge distributions than can be obtained by standard HMC. The histograms also get slightly broader or even become nontrivial thanks to this technique.

The enhancement of tunneling indicates an improvement of decorrelation also for other observables. More satisfactory histograms are important for topologically sensitive quantities. Both of these features make parallel tempering an attractive method for large-scale QCD simulations. The method is particularly economical when several parameter values have to be studied anyway.

A potential problem is that for a given parameter set the swap acceptance rate (2) decreases for increasing lattice volume [7]. To settle the question whether on larger lattices the need for increasing the number of ensembles is compensated by improved tunneling between topological sectors this study will be continued on larger lattices.

Acknowledgements

This work was done in collaboration with E.-M. Ilgenfritz and W. Kerler. I would like to thank M. Müller-Preussker for supporting the project. The simulations were done on the CRAY T3E at Konrad-Zuse-Zentrum für Informationstechnik Berlin.

References

1. M. Müller-Preussker, Proc. of the XXVI Int. Conf. on High Energy Physics, Dallas, Texas (1992), 1545.
2. B. Allés et al., Phys. Lett. B 359 (1996) 107.
3. B. Allés et al., Phys. Rev. D 58 (1998) 071503.
4. CP-PACS Collaboration, contribution to Lattice '99, `hep-lat/9909045`.
5. R. Burkhalter, private communication.
6. G. Boyd, Nucl. Phys. B (Proc. Suppl.) 60A (1998) 341.
7. B. Joó et al., Phys. Rev. D 59 (1999) 114501.
8. K. Hukushima et al., `cond-mat/9512035`.
9. E. Marinari, `cond-mat/9612010`.
10. K. Schilling, this workshop.
11. E.-M. Ilgenfritz et al., contribution to Lattice '99, `hep-lat/9908022`.
12. S. Gupta et al., Phys. Lett. B 242 (1990) 437.
13. Y. Iwasaki et al., Phys. Rev. D 54 (1996) 7010.