Thermodynamics with 2 + 1 + 1 Dynamical Quark Flavors

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Abstract We report on our calculation of the equation of state of Quantum Chromodynamics (QCD) from first principles, through simulations of Lattice QCD. We use an improved lattice action and $N_f = 2 + 1 + 1$ dynamical quark flavors and physical quark mass parameters.

1 Introduction

The aim of our project is to compute the charmed equation of state for Quantum Chromodynamics (for details, see [1]). We are using the lattice discretized version of Quantum Chromodynamics, called lattice QCD, which allows simulations of the theory through importance sampling methods. Our results are important input quantities for phenomenological calculations and are required to understand experiments aiming to generate a new state of matter, called Quark-Gluon-Plasma, such as the upcoming FAIR at GSI, Darmstadt.

The present status of the field is marked by our papers on the $N_f = 2 + 1$[1] equation of state [2, 3]. In the time since the publication of the aforementioned works, the hotQCD collaboration have improved the precision of their results. It was found that some discrepancies between our and their results still remain (see e.g. [4]). It is the aim of this work to provide a high precision calculation of the equation of state of QCD including the (dynamical) effects of the charm quark, in order to remedy the above situation.

[1]This refers to dynamical up/down and strange quarks – including a dynamical charm quark is what was proposed here.

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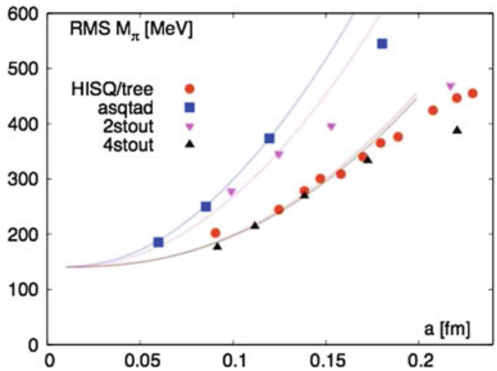

Fig. 1 RMS pion mass for different staggered fermion actions, in the continuum limit

Our simulations are performed using so-called staggered fermions. In the continuum limit, i.e. at vanishing lattice spacing a, one staggered Dirac operator implements four flavors of mass degenerate fermions. At finite lattice spacing, however, discretization effects induce an interaction between these would be flavors lifting the degeneracy. The "flavors" are, consequentially, renamed to "tastes", and the interactions are referred to as "taste-breaking" effects. Even though the tastes are not degenerate, in simulations one takes the fourth root of the staggered fermion determinant to implement a single flavor. This procedure is not proven to be correct – however, practical evidence suggests that is does not induce errors visible with present day statistics.

Taste-breaking is most severely felt at low pion masses and large lattice spacing, as the pion sector is distorted through the taste-breaking artifacts: there is one would-be Goldstone boson, and 15 additional heavier "pions", which results in an RMS pion mass larger than the mass of the would-be Goldstone boson. This effect is depicted in Fig. 1 for different staggered type fermion actions. As can be seen for this figure, the previously used twice stout smeared action ("2stout") has a larger RMS pion mass and thus taste-breaking effects than the HISQ/tree action. If, however, the number of smearing steps is increased to four, with slightly smaller smearing strength ("4stout"), the RMS pion mass measured agrees with that of the HISQ/tree action. In order to have an improved pion sector, we, therefore, opted to switch to this new action and to restart our production runs.

2 Status

The status of our production is summarized in Table 1 and Fig. 2. We generated most finite temperature ensembles on less scalable architectures, such as GPU clusters, available to the collaboration at Wuppertal and Budapest universities. Our (zero temperature) renormalization runs require a scalable architecture, and we, as

Table 1 Production status with the new "4stout" action

Data set	Status
$N_t = 6$	Ready
$N_t = 8$	Ready
$N_t = 10$	Ready
$N_t = 12$	Production

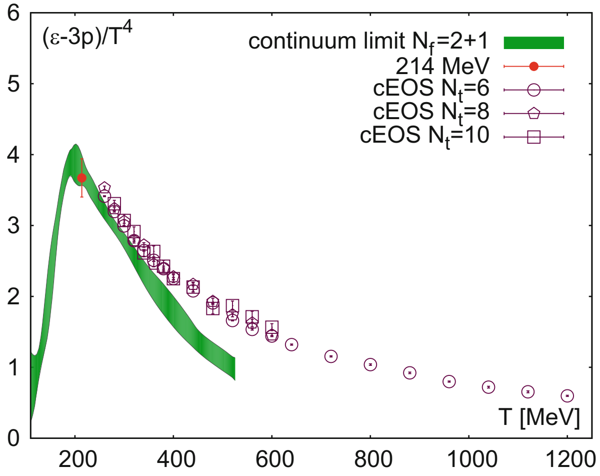

Fig. 2 Production status with the new "4stout" action. Presently available statistics with $N_t = 6, 8, 10$ is shown and compared to our result of [3]. Clearly, the curves start to deviate in a temperature range of $T = 300 \ldots 400$ MeV, as suggested by perturbative calculations [5]

proposed, used HERMIT to generate these essential ensembles. Our present and upcoming finite temperature simulations on finer, thus, larger lattices also benefit from scalability.

2.1 Results

In order to be able to reach very fine lattice spacings, or, equivalently, large temperatures at $N_t = 12$, we had to extend our line-of-constant-physics (LCP) beyond the range of lattice spacings available to us. Our previous strategy was the following ($m_c = 11.85\, m_s$):

1. Simulate a "reasonable" rectangle of up/down and strange quark mass values and to measure M_π / f_π and M_K / f_π.
2. Interpolate to the quark mass values where above ratios take their physical values. This gives m_{ud} and m_s.
3. Extract the lattice spacing by interpolating $a f_\pi$ to the above quark mass point.

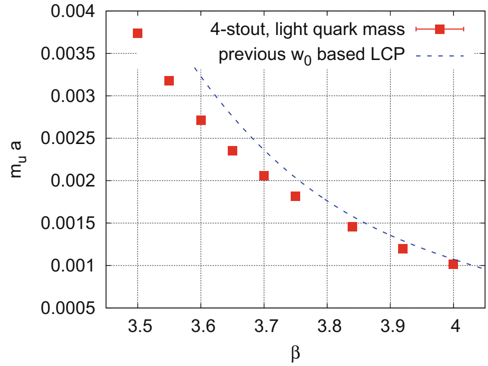

Fig. 3 LCP for our new 4stout action. Shown are the new data points for the light quark mass parameter. The *dashed line* indicates a first iteration using w_0 [6]. We prefer to use the ratio M_π/f_π as it is directly related to the pion sector

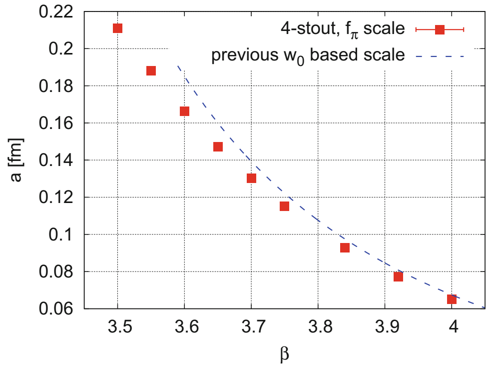

Fig. 4 LCP for our new 4stout action. Shown are the new data points for the lattice spacing. The *dashed line* indicates a first iteration using w_0 [6]. We prefer to use the pion decay constant as it is directly related to the pion sector

The results of this procedure are shown in Figs. 3 and 4, for the data points with $\beta < 3.9$. The remaining points have been generated with the procedure described in the following. At very fine lattice spacing, the zero temperature runs at physical mass parameters would require enormous lattices and would also likely face issues related to the freezing of the topological charge at $a \approx 0.5$ fm. We, therefore, adapted our strategy:

1. For every $\beta < 3.9$: Simulate $N_f = 3+1$ flavors in the flavor-symmetric point [7] $(\bar{m} = (2m_{ud,phys} + m_{s,phys})/3)$, using the quark mass parameters found above.
2. Measure f_{PS} and M_{PS}/f_{PS}.
3. Perform a continuum extrapolation.

We now can estimate the expected values for f_{PS} and M_{PS}/f_{PS} at the target $\beta > 3.9$, see Figs. 5 and 6. Simulating several $\bar{m}$ values at these β we can find the value where the expected M_{PS}/f_{PS} is reproduced. This gives $\bar{m}(\beta)$, while the lattice spacing will be set through f_{PS}. The procedure is shown for one β in Figs. 7 and 8. It gives the LCP entries at $\beta > 3.9$ as shown above in Figs. 3 and 4.

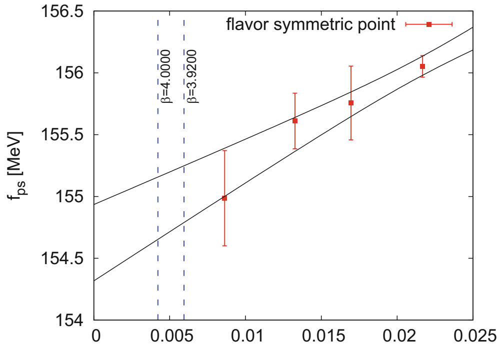

Fig. 5 Continuum extrapolation of the pion decay constant in the flavor-symmetric point (see text) using our new 4stout action. The target beta values are indicated by *dashed lines*. This extrapolation provides expected values for the pion decay constant at these β values

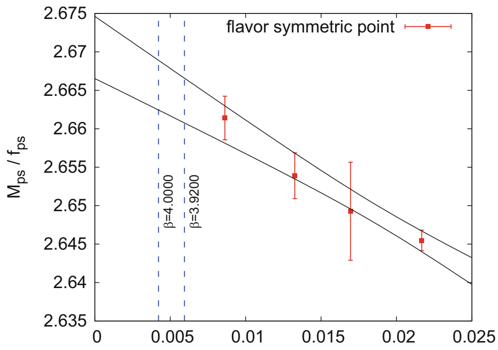

Fig. 6 Continuum extrapolation of the ration M_{PS}/f_{PS} in the flavor-symmetric point (see text) using our new 4stout action. The target beta values are indicated by *dashed lines*. This extrapolation provides expected values for the ratio at these β values

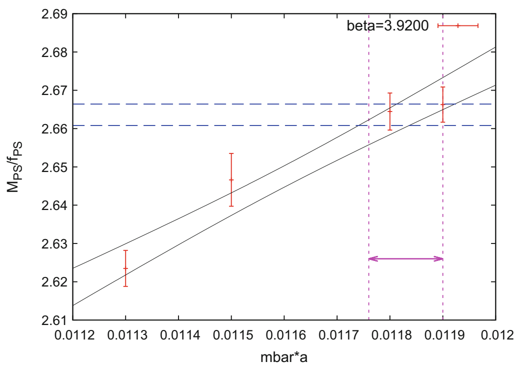

Fig. 7 Calculation of the (1σ region of) bare mass parameter for our new 4stout action. The *blue band marks* the expected value for the ration M_{PS}/f_{PS} at this β value, taken from the continuum extrapolation as shown in Fig. 6

2.2 *Additional Results*

The reduced taste breaking allowed us to determine a further observable, which is of particular interest of the heavy ion community. While the equation of state is an input to the relativistic hydrodynamic calculations that reproduce the observed

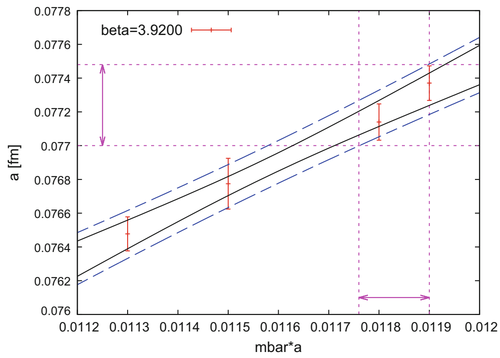

Fig. 8 Calculation of the lattice spacing at $\beta = 3.92$ for our new 4stout action. The correct value for $a\bar{m}$ has been extracted as shown in Fig. 7. The *blue band marks* the region defined by the measured f_π divided by the expected value from the continuum extrapolation (including errors)

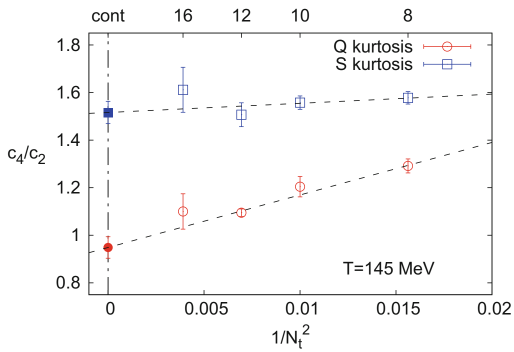

Fig. 9 Continuum limit of the c_4/c_2 (kurtosis × variance) at $T = 145$ MeV temperature for the net charge and strangeness. These data were taken using our new 4stout action

flow characteristics, there is an observable that can and is being directly measured at LHC: the non-gaussianity of the net charge and strangeness fluctuations at freeze-out temperature. We concentrated all our efforts on a single temperature, so far, and show a continuum extrapolation in Fig. 9. This of course will need to be extended to a couple of more temperatures. The temperature dependence could be then used to measure the freeze-out temperature in heavy-ion collisions.

3 Production Specifics and Performance

Most of our production is done using modest partition sizes, as we found these to be most efficient for our implementation.

3.1 Performance

Our code shows nice scaling properties on HERMIT. For our scaling analysis below, we used two lattices ($N_s = 32$ and 48) and several partition sizes up to 256 nodes. We timed the most time consuming part of the code: the fermion matrix multiplication. The results are summarized in the following table:

No of nodes	Gflop/node $N_s = 32$	Gflop/node $N_s = 48$
1	16.3	15.4
2	16.8	16.0
4	16.5	16.2
8	16.3	16.3
16	16.3	16.3
32	16.8	16.0
64	17.1	16.5
128	19.2	16.5
256	16.3	16.0

3.2 Production

Given the nice scaling properties of our code, we were able to run at the sweet spot for queue throughput, which we found to be located at a job size of 64 nodes. Larger job sizes proved to have a scheduling probability sufficiently low that benefits in the runtime due to the larger number of cores were compensated and the overall production throughput decreased. We, therefore, opted to stay at jobs sizes with 64 nodes.

4 Outlook

At the present level of ensemble generation, we believe we will be able to publish within 2014. Since we, unfortunately, ran out of quota very quickly, we were not able keep up our earlier estimates. Still, HERMIT has proved to be an essential tool to be able to achieve this goal.

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