QCD Thermodynamics with Domain-Wall Fermions

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HotQCD Collaboration

Introduction

A key challenge in QCD thermodynamics is to clarify the nature of the chiral transition and its influence on the thermodynamics of QCD matter. Here, the computation of thermodynamic observables sensitive to the light-quark sector relies heavily on an accurate realization of chiral symmetry in the discretized/regularized theory (lattice QCD). This has, for instance, important implications on the pion spectrum. Chiral symmetry can be generalized for finite lattice spacing, by replacing the continuum expression, $\{D, \gamma_5\} = 0$, with the *Ginsparg-Wilson equation* (GWE),

$$\{D, \gamma_5\} \; = \; aD\gamma_5 D \quad , \tag{1}$$

where D is a lattice Dirac operator and γ_5 is the chirality operator and the relation reduces to the continuum expression at vanishing lattice space a. However, the most commonly used lattice actions, Wilson- and staggered fermions, do not preserve chiral symmetry in a proper way. While, in the case of staggered fermions, chiral symmetry is only broken partially, the action suffers from taste violations at finite lattice spacing.

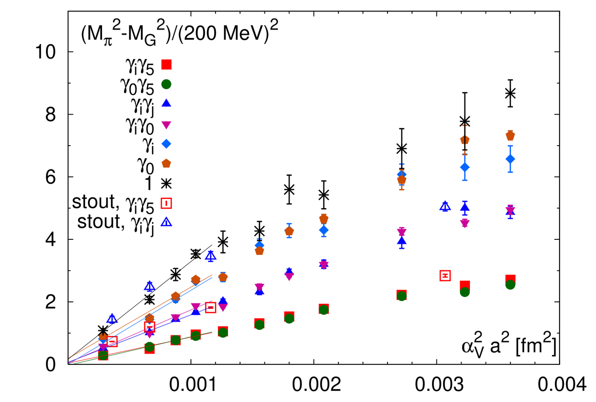

Fig. 1: Difference of the squared mass of the non-Goldstone- and Goldstone states, for HISQ/tree-and stout actions, as a function of $\alpha_V^2 a^2$, serving as a measure for taste violations. [7]

Apart from the direct taste violation effects in the light pion sector, as a result of the large effective pion masses also certain Δ-resonance decay channels are prohibited, influencing the spectrum of heavier hadron resonances. Taste violations are reduced in improved actions, such as the highly improved staggered-quarks (HISQ) action [7]. Two doubler-free solutions of the GWE are overlap- and domain-wall fermions (DWF). The latter separates chiral modes by means of a 5$^{\text{th}}$ dimension and only has exact chiral symmetry if the extent L_s of the 5$^{\text{th}}$ dimension is infinite. On the lattice, the finite extent L_s breaks chiral symmetry in a controlled manner and the degree to which chiral symmetry is broken can be monitored with the *residual mass*,

$$m_{\text{res}} \;=\; \lim_{t\to\infty} \frac{\sum_{\mathbf{x},\mathbf{y}} \left\langle J^a_{5q}(\mathbf{x},t)\, J^a_5(\mathbf{y},0)\right\rangle}{\sum_{\mathbf{x},\mathbf{y}} \left\langle J^a_5(\mathbf{x},t)\, J^a_5(\mathbf{y},0)\right\rangle} \quad , \tag{2}$$

where $J^a_5(x)$ and $J^a_{5q}(x)$ are 4-dimensional pseudoscalar densities, defined on the boundaries and on the central hyperplanes. Since fully dynamical calculations with DWF are still computationally demanding, a mixed-action (MA) approach has been developed, in which the Möbius DWF (MDWF) matrix is used for the calculation of observables on gauge field configurations generated with the HISQ action. MDWF introduce two additional, so-called Möbius parameters, b_5 and c_5, which can be tuned to reduce the residual mass. This approach comes with mixed-action effects, which can be reduced using the gradient flow, where we evolve gauge fields in an introduced flow time τ_F. A proper tuning of the MDWF action at zero temperature is necessary, which comes with costly calculations on large lattices. To reduce the costs, we also investigate whether the tuning is possible with screening masses on finite temperature lattices.

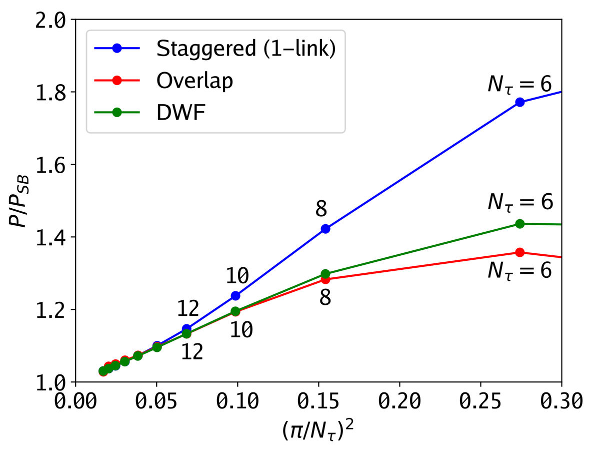

Fig. 2: Pressure of overlap- and DW fermions, for Wilson kernel and $M_5 = 1$. In both cases the large-N_τ expansion coincides with that of the 1-link staggered action. [8]

Computer Ressources & Benchmarks

We use code developed by us, using the publically-available `Grid`- [1] and `Hadrons` [2] libraries, as well as the `Grid Python Toolkit` (GPT) [3]. GPT benchmarks where computed on the JUWELS Booster machine using 1 Node with 4 GPUs, with double precision [3]. DSlash was applied 1000 times on a $64 \cdot 32^3$ lattice with $L_s = 12$ and color- and spin-color matrix multiplication was done 10 times each on a $48^3 \cdot 128$ lattice.

Operation	Performance	Bandwidth
$\not{D}$	5.75 TFlops/s	7.9 TB/s
Color Matrix		5.3 TB/s
Spin-Color Matrix		4.4 TB/s

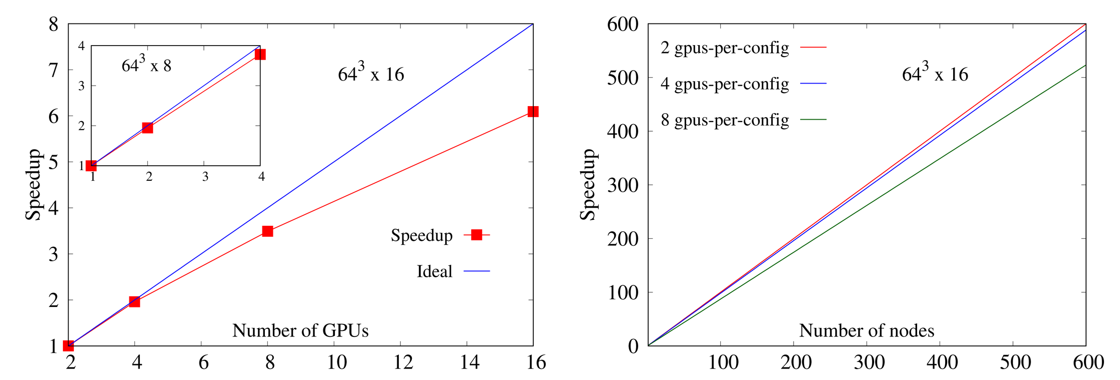

Fig. 3: Left: Scaling behavior of the CG inverter using the Grid library on the JUWELS Booster of problem size $64^3 \times 16 \times 12$. The inset shows the scaling behavior on the 4 GPUs of a single node for lattice size of $64^3 \times 8$. Right: Weak-scaling behavior of problem size $64^3 \times 16 \times 12$ for the analysis of (number of nodes)/X configurations with each configuration being distributed over X=2,4,8 GPUs.

A. Parameter and Mass Tuning

We tuned the MDWF action at zero temperature using $64^3 \times 64$ HISQ lattices with $(2+1)$-flavors. First we varied the MDWF parameters L_s, M_5, b_5 and set $c_5 = 1 - b_5$ to reduce m_{res}. After we fixed one set of parameters for different flow times, we extract the ground state of the temporal light- (ll) and strange- (ss) correlator and vary the quark masses until the ground states match with the corresponding particle masses (see Fig. 4).

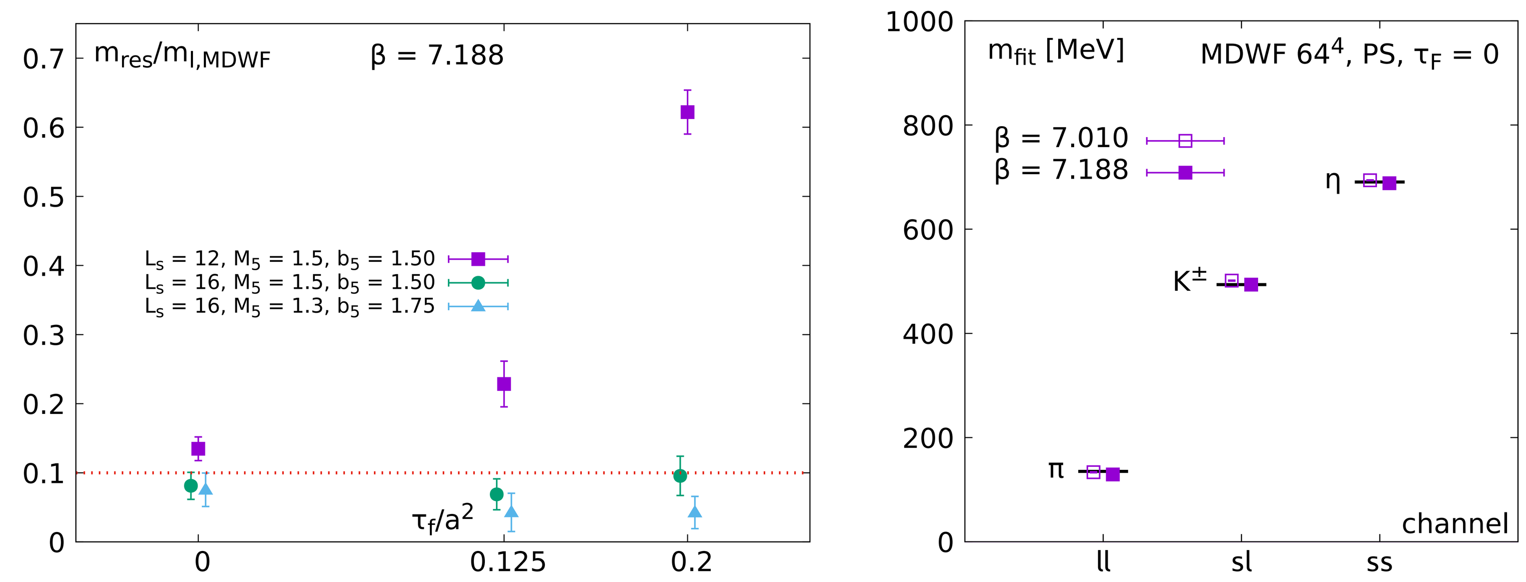

Fig. 4: Parameter Tuning of MDWF parameters (left) and tuned masses for zero flow time (right).

B. Screening Masses

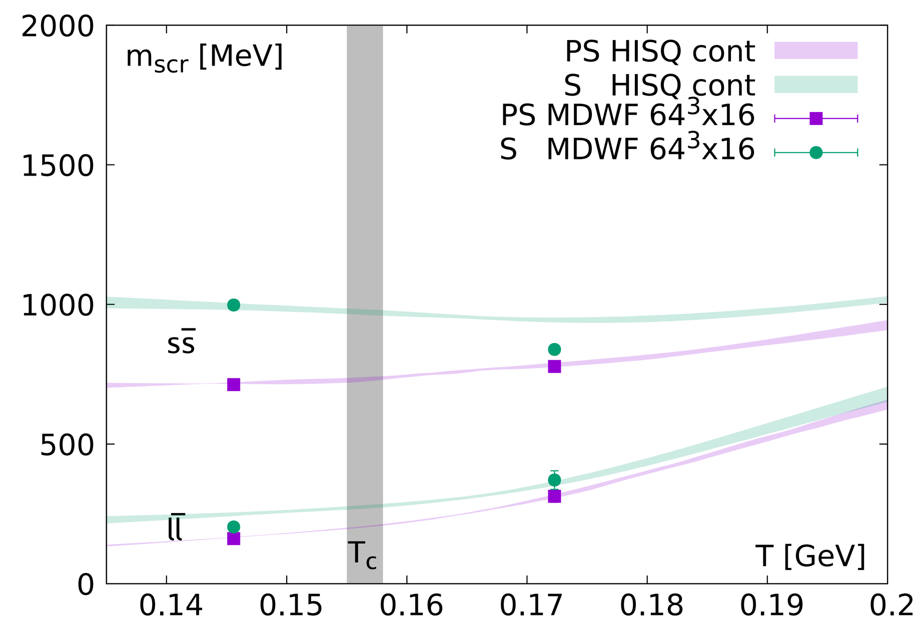

Fig. 5: Comparison between screening masses obtained from the MDWF on HISQ action and the continuum values, extrapolated from HISQ screening masses calculated in [4].

C. Cumulants of Electric-Charge Fluctuations

Conserved-charge fluctuations are crucial thermodynamic observables, containing information about the temperature and chemical potentials at the time of hadronization and are also measured in heavy-ion experiments, providing good approximations for the pseudo-critical parameters of the QCD phase transition. Fluctuations of the electric charge are highly sensitive to chiral-symmetry- and taste violations. The higher-order moments also receive sizable contributions from the decay of the Δ^{++} resonances. We want to show that, with the mixed-action MDWF approach, cut-off effects can be strongly reduced already on $N_\tau = 8$ lattices. To do so we calculate the 4th-order cumulant of Baryon-number- and electric-charge correlations,

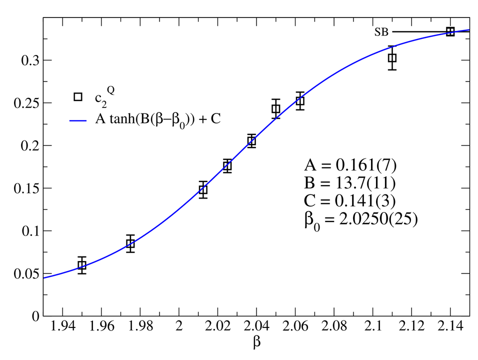

Fig. 6: Electric-charge susceptibility as a function of β and resulting fit parameters, including the inflection point β_0. Calculations were done using 2+1 flavors of domain-wall fermions on $16^3 \times 8$ lattices with $L_s = 32$. [5]

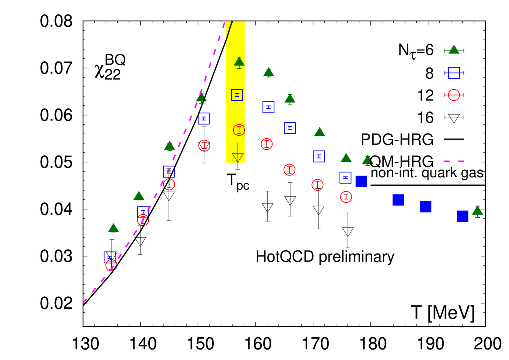

Fig. 7: 4th-order cumulant of baryon-number- and electric-charge correlations, calculated with the HISQ action on different-size lattices [6] with physical light- and strange-quark masses. The unusually large cut-off dependence may be related to threshold effects in the Δ-resonance decay channels.

$$\chi_{22}^{BQ} \;=\; \frac{\partial^4}{\partial \mu_B^2\, \partial \mu_Q^2} \ln \mathcal{Z}(T, \mu_B, \mu_Q, \mu_S)\,\Big|_{(\mu_B,\mu_Q,\mu_S)=\mathbf{0}} \quad , \tag{3}$$

at the pseudocritical temperature, giving the leading correction to quadratic electric-charge fluctuations at non-vanishing baryon chemical potential,

$$\chi_2^Q(T,\mu_B) \;=\; \chi_2^Q(T,0) \,+\, \tfrac{1}{2}\,\chi_{22}^{BQ} \cdot \left(\tfrac{\mu_B}{T}\right)^2 + \ldots \quad , \tag{4}$$

on the pseudocritical line of the QCD phase transition. We plan to analyze 2000 gauge-field configurations at this temperature, using 1000 random sources for the inversion of the Dirac matrix on each configuration – **this work is in progress**.

References

[1] Grid public code repository, https://github.com/paboyle/Grid.

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