# TOWARDS 2+1 FLAVOR LATTICE QCD RESULTS FOR THE HEAVY QUARK DIFFUSION COEFFICIENT\*

## LUIS ALTENKORT, OLAF KACZMAREK

Physics Department, Bielefeld University, 33615 Bielefeld, Germany

## RASMUS LARSEN

Department of Mathematics and Physics, University of Stavanger 4036 Stavanger, P.O. Box 8600, Norway

Peter Petreczky, Swagato Mukherjee

Department of Physics, Brookhaven National Laboratory Upton, New York 11973, USA

Hai-Tao Shu

#### Institut für Theoretische Physik, Universität Regensburg 93040 Regensburg, Germany

Received 31 July 2022, accepted 2 October 2022, published online 14 December 2022

We apply and extend a novel approach to non-perturbatively estimate the heavy-quark momentum diffusion coefficient  $\kappa$ , which is a key input for the theoretical description of heavy quarkonium production in heavyion collisions, and is important for the understanding of the elliptic flow and nuclear suppression factor of heavy flavor hadrons. In the heavy-quark limit, this coefficient is encoded in the spectral functions of color-electric and color-magnetic correlators that we calculate on the lattice to high precision by applying gradient flow. In a recent study we have considered quenched QCD at  $1.5 T_c$ , where we performed a detailed study of the lattice spacing and flow time dependence of the color-electric correlator, and, using theoretically well-established model fits for the spectral reconstruction, we estimated the heavy-quark diffusion coefficient. Equipped with the experience obtained in quenched QCD, we estimate  $\kappa$  from 2+1 flavor QCD ensembles at small but finite lattice spacing and flow time without increasing systematic errors significantly.

DOI:10.5506/APhysPolBSupp.16.1-A77

<sup>\*</sup> Presented at the 29<sup>th</sup> International Conference on Ultrarelativistic Nucleus–Nucleus Collisions: Quark Matter 2022, Kraków, Poland, 4–10 April, 2022.

#### 1. Introduction

A remarkable observation made in heavy-ion collision experiments is the considerable participation of heavy quarks in the collective motion of the produced medium. Evidence for this comes from the detection of decay products of heavy flavor hadrons, which reveals a strong suppression of the yields at high transverse momentum  $p_{\rm T}$  as well as a large azimuthal asymmetry inferred from the elliptic flow parameter  $v_2$  [1, 2]. On hydrodynamical grounds, these findings imply that heavy hadrons should equilibrate on time scales of the medium's formation,  $\sim 1/T$ , which is unexpected as heavy quarks should take a factor of M/T longer to thermalize compared to the mostly light degrees of freedom in the bulk of the medium. From the theoretical side the kinetic equilibration time  $\tau_{kin}$  can be accessed by describing the behavior of heavy quarks with mass M in a hot medium with temperature T through a Langevin approach, given that  $M \gg \pi T$  [3]. The Langevin dynamics depend on a transport coefficient,  $\kappa$ , the heavy-quark diffusion coefficient. For a first-principles calculation of this transport coefficient, it is necessary to facilitate a non-perturbative approach, as weak-coupling calculations not only disagree with a small equilibration time, but also turn out to converge poorly [4]. In a recent lattice QCD study [5],  $\kappa$  was calculated in the quenched approximation at  $T = 1.5 T_{\rm c}$  using a novel approach that utilizes gradient flow. In this contribution, we want to take the first step towards 2+1 flavor QCD by showing how little systematic error is introduced when estimating  $\kappa$  from finite lattice spacing and flow time data.

#### 2. Diffusion physics from color-electric correlations

On the lattice, it is not possible to calculate transport coefficients directly; instead, one calculates two-point functions  $G(\tau)$  of conserved currents whose spectral functions  $\rho(\omega)$  encode them in their infrared limits [8–10]. By utilizing Heavy Quark Effective Theory, one can access  $\kappa$  through the spectral function of a purely gluonic correlator of color-electric fields [11]

$$\kappa = \lim_{\omega \to 0} 2T \frac{\rho(\omega)}{\omega}, \qquad G(\tau) = \int_{0}^{\infty} \frac{\mathrm{d}\omega}{\pi} \frac{\cosh(\omega(\tau - \beta/2))}{\sinh(\omega\beta/2)} \rho(\omega), \quad (1)$$

$$G(\tau) = -\frac{1}{3} \sum_{i=1}^{3} \frac{\langle \operatorname{Re}\left[\operatorname{tr}\left[U(\beta,\tau) \ gE_{i}(\mathbf{0},\tau) \ U(\tau,0) \ gE_{i}(\mathbf{0},0)\right]\right] \rangle}{\langle \operatorname{Re}\left[\operatorname{tr}\left[U(\beta,0) \ \right]\right] \rangle}, \quad (2)$$

with  $\beta = 1/T$ , the temporal Wilson line U(b, a), the color-electric field operator  $E_i$ , and the coupling g. The discretization of  $gE_i$  in terms of link variables can be found in Eq. (7) of Ref. [5]. In the following figures, the correlator data will always be shown normalized to  $G^{\text{norm}}(\tau) \equiv G_{\text{cont}}^{\text{LO}}(\tau)/(g^2 C_{\text{F}})$ , which captures the structure of the weak-coupling leading-order continuum result for the color-electric correlator (see Eq. (3.1) of Ref. [11]).

In practice, a noise reduction method is needed to compute Eq. (2) with sufficient precision as the long-distance correlation is overshadowed by highfrequency gauge-field fluctuations. The solution to this problem is gradient flow [5, 12], which, unlike other noise reduction techniques, does not depend on the locality of the action, making it applicable also to 2+1 flavor ensembles. The original idea of the flow method is to measure the correlator at many successive and not too large flow times  $\tau_{\rm F}$ , and then, after a continuum extrapolation at fixed flow time, to extrapolate back to the physical boundary ( $\tau_{\rm F} = 0$ ). The details of this procedure are explained and demonstrated in reference [5].

## 3. Spectral reconstruction from correlators at finite lattice spacing and flow time

The technique to invert Eq. (2) and obtain  $\rho(\omega)$  that is used in our recent study [5] makes use of theoretically motivated models that constrain the form of the spectral function in the low- and high-frequency regimes, which enables the extraction of the heavy-quark momentum diffusion coefficient  $\kappa$ through a least-squares fit of the discrete correlator data.

On paper, the connection between the correlator and spectral function is valid in the continuum on the physical boundary (zero flow time) [5]. Our current ensemble of 2+1 flavor gauge configurations (see below) does not vet allow for a continuum extrapolation; this will happen in the near future in a separate publication. In the meantime, however, we notice that the color-electric correlator  $G(\tau)$  does not appear to be very sensitive to finite lattice spacing and flow time effects, especially for larger distances. One reason for this is the tree-level improvement (see appendix A.1 of [5]) obtained from calculating the perturbative lattice correlator. In a recent work [6], this calculation was extended to various combinations of discretization schemes for the flow action (here: Zeuthen flow) and gluon propagator (here: Wilson action for quenched QCD, Fig. 1, Symanzik-improved for 2+1 flavor, Fig. 2). This prompts us to try constraining  $\kappa$  from the data we already have. However, for a given nonzero flow time, one always encounters one of two problems: either the small distances are too distorted, or the large distances are too noisy, making a fit unreasonable in both cases. The solution is to consider each distance individually by fixing the smoothing radius in terms of distance according to  $\sqrt{8\tau_{\rm F}} = \tau/{\rm const.} \lesssim \tau/3$  (see also [13])<sup>1</sup>. In this

<sup>&</sup>lt;sup>1</sup> In practice, we find  $\sqrt{8\tau_{\rm F}}/\tau \in [0.20\text{-}0.25]$  to exhibit a particularly good balance between noise reduction and flow distortion. Systematic errors for  $\kappa/T^3$  from the choice of this value turn out to be negligible if the signal is good enough.



Fig. 1. This figure shows data from quenched QCD at  $T = 1.5 T_c$  from the same gauge configurations used in [5]. Left: comparison of tree-level improved colorelectric correlators G divided by  $G^{\text{norm}}$  at different lattice spacings a and flow times  $\tau_{\text{F}}$ . Dashed lines depict fits to the model given at the top of the figure. The fit ranges can be inferred from the figure on the right. Right: fit results for  $\kappa/T^3$ for the corresponding data and model from the left figure. Results are set into the context of the total systematic uncertainty for  $\kappa/T^3$  (grey band) from the model choice, obtained from the  $a \to 0, \tau_{\text{F}} \to 0$  data. Note: the correlator data and total uncertainty for  $\kappa/T^3$  slightly differ compared to [5], as we make use of tree-level improvement at nonzero flow time [6] and improved the model choices (more details will be given in an upcoming publication).

way, finite flow time effects can be thought of as small corrections to the zero-flow-time correlator. In fact, fitting the long-distance data ( $\tau T \ge 0.35$ ) using this approach, even at nonzero lattice spacing a, we find the additional systematic error for  $\kappa/T^3$  to be well below the total systematic error coming from different spectral function models, as can be seen in Fig. 1.

Equipped with this knowledge, we fit correlators calculated on 2+1 flavor configurations using the Highly Improved Staggered Quarks (HISQ) action with physical strange quark masses  $m_s$  and light quark masses  $m_l = m_s/5$ (pion mass  $m_{\pi} \approx 320 \text{ MeV}$ ). We consider temperatures of 196, 220, 251, 296, and 352 MeV with temporal lattice extents of  $N_{\tau} = 36, 32, 28, 24$ , and 20, respectively; the spatial lattice volumes are fixed to 96<sup>3</sup> and the lattice spacing is a = 0.028 fm (the scale is set via  $r_1$  using data from Ref. [14]).



Fig. 2. This figure shows data from 2+1 flavor QCD (see Section 3). Left: comparison of tree-level improved color-electric correlator G divided by  $G^{\text{norm}}$  at small but nonzero lattice spacing a = 0.028 fm and flow time  $\tau_{\text{F}}$ . Dashed lines depict fits to the model given at the top of the figure. Right: fit results for  $\kappa/T^3$  for the corresponding data and model from the left figure. Note that only a single model is shown here, meaning that the errors depict just the statistical uncertainty from this specific model. A systematic analysis will follow in an upcoming publication. AdS/CFT estimate is taken from [7].

The results are shown in Fig. 2. Due to the change in the coupling the correlators are now an overall factor ~ 2 larger than the quenched results when normalizing to  $G^{\text{norm}}$  (cf. Fig. 1). The most striking observation is that  $\kappa/T^3$  is also increased by roughly 2× compared to results of quenched QCD. In the near future, we will provide a detailed systematic analysis of the spectral function model choice, and move to continuum- and flow-time-to-zero extrapolated correlators.

The authors acknowledge support from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through the CRC-TR 211 'Strong-interaction matter under extreme conditions' — project number 31-5477589 — TRR 211. The computations in this work were performed in part on the GPU cluster at the Bielefeld University. This material is based upon work supported by the U.S. Department of Energy, Office of Science, through contract No. DE-SC0012704. This research used resources of the National Energy Research Scientific Computing Center (NERSC), the U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under contract No. DE-AC02-05CH11231.

#### REFERENCES

- ALICE Collaboration (S. Acharya *et al.*), *Phys. Rev. Lett.* **120**, 102301 (2018).
- [2] ALICE Collaboration (S. Acharya et al.), J. High Energy Phys. 2018, 174 (2018).
- [3] G.D. Moore, D. Teaney, *Phys. Rev. C* **71**, 064904 (2005).
- [4] S. Caron-Huot, G.D. Moore, *Phys. Rev. Lett.* 100, 052301 (2008).
- [5] L. Altenkort *et al.*, *Phys. Rev. D* **103**, 014511 (2021).
- [6] S. Stendebach, «Perturbative analysis of operators under improved gradient flow in lattice QCD», Master Thesis, Tech. Hochsch. Darmstadt, 2022.
- [7] J. Casalderrey-Solana, D. Teaney, Phys. Rev. D 74, 085012 (2006).
- [8] R. Kubo, M. Toda, N. Hashitsume, «Statistical Physics II, Springer Series in Solid-State Sciences», Springer, 1978.
- [9] D. Forster, «Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions», Advanced Book Classics, Perseus Books, 1990.
- [10] H.B. Meyer, Eur. Phys. J. A 47, 86 (2011).
- [11] S. Caron-Huot, M. Laine, G.D. Moore, J. High Energy Phys. 2009, 053 (2009).
- [12] M. Lüscher, J. High Energy Phys. 1008, 071 (2010); Erratum ibid. 1403, 092 (2014).
- [13] A.M. Eller, G.D. Moore, *Phys. Rev. D* 97, 114507 (2018).
- [14] A. Bazavov, P. Petreczky, J.H. Weber, *Phys. Rev. D* 97, 014510 (2018).

1 - A77.6