Lattice QCD results for the heavy quark diffusion coefficient from gradient-flowed color-electric correlators

1. Precise calculation in quenched QCD at $1.5 T_c$
   Bielefeld U.: Altenkort, Kaczmarek, Mazur, Shu
   TU Darmstadt: Eller, Moore

2. First preliminary results from $2 + 1$ flavor QCD
   Bielefeld U.: Altenkort, Kaczmarek, Shu
   Brookhaven NL: Petreczky, Mukherjee
   U. of Stavanger: Larsen
How fast do heavy quarks thermalize in a hot medium?

- Hydrodynamics $\Rightarrow$ kinetic equilibration time $\tau_{\text{kin}}^{\text{heavy}} \simeq \frac{M}{T} \tau_{\text{kin}}^{\text{light}}$, where $\tau_{\text{kin}}^{\text{light}} \approx \frac{1}{T}$
- But: significant collective motion ($v_2$)!

Can we calculate $\tau_{\text{kin}}^{\text{heavy}}$ from first principles?

- Consider non-relativistic limit ($M \gg \pi T$):
  $$\tau_{\text{kin}}^{\text{heavy}} = \eta_D^{-1}$$
  $$\eta_D = \frac{\kappa}{2M_{\text{kin}}T} \left(1 + \mathcal{O}\left(\frac{\alpha_s^3}{2} \frac{T}{M_{\text{kin}}}\right)\right)$$
  $$D = 2T^2/\kappa$$

- Problem: perturbative series for $D$ or $\kappa$ ill-behaved!
  $\Rightarrow$ need for non-perturbative ab-initio calculation
  $\Rightarrow$ lattice QCD

Figure: Steffen Bass, mod. by O. Kaczmarek
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- But: significant collective motion ($v_2$)!
  \[ \tau_{\text{kin}}^{\text{heavy}} \approx \frac{1}{T} \Rightarrow \tau_{\text{kin}}^{\text{light}} \ll \frac{1}{T} \]

Can we calculate $\tau_{\text{kin}}^{\text{heavy}}$ from first principles?

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How to calculate diffusion coefficients from the lattice?

- Linear response theory: diffusion physics ⇔ low-energy in-equilibrium spectral functions (SPF)

- SPF of HQ vector current

  \[ \rho^{ii}(\omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} \int d^3 x \left\langle \frac{1}{2} [ \hat{J}^i(x,t), \hat{J}^i(0,0) ] \right\rangle \]

- reconstruct from Euclidean correlation functions:

  \[ G(\tau) = \int_0^\infty d\omega \, \rho(\omega) \frac{\cosh(\omega(\tau - \frac{\beta}{2}))}{\sinh(\omega \frac{\beta}{2})} \]

- utilize HQET: \( M \to \infty \) (expansion in \( 1/M \))
  \[ \Rightarrow \text{replace } \hat{J}^i \text{ with leading-order versions} \]

- obtain Euclidean color-electric two-point function \( G(\tau) \) whose SPF encodes momentum diffusion coeff.

  \[ \kappa = \lim_{\omega \to 0} 2T \frac{\rho(\omega)}{\omega} \]

  \[ \Rightarrow \text{smooth } \omega \to 0 \text{ limit expected: no transport peak} \]
  (much easier to reconstruct)
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The Euclidean correlator that encodes $\kappa$

- **Gluonic color-electric correlator:** Caron-Huot et al. 2009

\[
G(\tau) \equiv \frac{1}{3} \sum_{i=1}^{3} - \frac{\langle \text{Re tr} \ U(\beta, \tau) \ gE_i(\tau) \ U(\tau,0) \ gE_i(0) \rangle}{\langle \text{Re tr} \ U(\beta,0) \rangle}
\]

\[
= \int_{0}^{\infty} d\omega \ \rho(\omega) \ \frac{\cosh(\omega(\frac{\tau}{2} - \frac{\tau}{T}))}{\sinh(\omega \frac{\tau}{T})}, \quad \kappa = \lim_{\omega \to 0} 2T \frac{\rho(\omega)}{\omega} \ K(\omega, \tau)
\]

- **Leading order, small $\tau$:** $G(\tau) \propto \tau^{-4}$

The drawback of the $M \to 0$ limit

- $G(\tau)$ is purely gluonic $\Rightarrow$ UV gauge fluctuations dominate for large $\tau$
- ... but those are most sensitive to small $\omega$ due to $K(\omega, \tau)$!
  $\Rightarrow$ need noise reduction (gauge smoothing) method

\[
\begin{align*}
\rho(\omega) K(\omega, \tau) / T^2
\end{align*}
\]
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Solution to gauge noise problem: gradient flow Lüscher 2010

- applicable to nonlocal actions (e.g. 2+1 flavor QCD)
- introduces “flow time” $\tau_F \equiv ta^2$ ($t$ dimensionless)
- evolves gauge fields $A_\mu(x)$ towards minimum of action $S_G$

LO: Gaussian smearing with width $\sim \sqrt{8\tau_F}$ “flow radius”

$A_\mu(x, \tau_F = 0) = A_\mu(x)$

$\frac{dA_\mu(x, \tau_F)}{d\tau_F} \sim -\frac{\delta S_G[A_\mu]}{\delta A_\mu(x, \tau_F)}$

$A_\mu^{LO}(x, \tau_F) = \int dy \left(\frac{\sqrt{2\pi}}{\sqrt{8\tau_F}}\right)^{-4} \exp \left(-\frac{(x - y)^2}{\sqrt{8\tau_F^2}}\right) A_\mu(y)$

- suppresses high-energy modes (noise reduction) & lattice renormalization artifacts...
- ...but contaminates $EE$ correlator $G(\tau)$ for $\sqrt{8\tau_F} \gtrsim \tau/3$ according to LO pert. theory Eller, Moore 2018

$\Rightarrow$ idea: flow no more than $\sqrt{8\tau_F} \approx \tau/3$ (“flow limit”), extrapolate back to $\tau_F = 0$
Gradient flow for $EE$ correlator

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  \(\Rightarrow\) lattice: each link is replaced by well-defined local “average”

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Leading-order perturbative $EE$ correlator under Wilson flow

**flow limit:**
cont. correlator deviates $<1\%$ for

$$\tau T \gtrsim 3\sqrt{8\tau_F T} \Rightarrow \text{vertical lines}$$

**Use to enhance nonpert. lattice results:**
- filter out $\tau^{-4}$ behavior via $G_{\text{nonpert}}/G_{\text{norm}}$
  $\Rightarrow$ increases visibility of details
- comparison of LO cont. and LO latt. correlators
  $\Rightarrow$ approx. remove tree-level discretization errors

continuum corr. from Eller, Moore 2018,
lattice corr. from Eller, Moore, LA et al. 2021
**Quenched, \(1.5T_c\): renormalized continuum \(EE\) correlator**

**Lattice setup**

<table>
<thead>
<tr>
<th>(N^3 \times N_\tau)</th>
<th>(a) [fm]</th>
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<tbody>
<tr>
<td>(80^3 \times 20)</td>
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- 10000 quenched conf. each
- well-separated: 500 sweeps of (1 HB, 4 OR)
- \(O(a^2)\)-improved "Zeuthen flow"
- 3rd-order RK with adaptive stepsize

- measure correlator, apply flow, repeat...
- \(a \to 0\) extrapolation at each \(\tau_F\), then \(\tau_F \to 0\) at each \(\tau\)
- for details see LA et al. 2021

![Graph](image)

- double-extrapolated EE correlator
- shape consistent with previous (only pert. renorm.) results
  - Francis et al. 2015, Christensen, Laine 2016

- overall shift due to
  - nonperturbative renormalization
  - difference in statistical power of gauge conf.
  - systematic uncertainty introduced by flow extr.
- only large-\(\tau\) of correlator can be obtained
  - not a problem for diffusion physics!
Quenched, $1.5T_c$: renormalized continuum $EE$ correlator

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**Gradient flow method**

\[
\begin{array}{c}
\frac{G_{\text{cont}}(\tau)}{G_{\text{norm cont}}(\tau)}\\
\end{array}
\]

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- only large-$\tau$ of correlator can be obtained
  ⇒ not a problem for diffusion physics!
Spectral reconstruction through pert. model fits

\[ G(\tau) = \int_0^\infty d\omega \, \rho(\omega) \, K(\omega, \tau), \quad \kappa = \lim_{\omega \to 0} 2T \frac{\rho(\omega)}{\omega} \]

⇒ integral inversion problem; on paper valid only at \( \tau_F = 0 \) Eller 2021

Strategy: constrain allowed form of \( \rho(\omega) \) using IR and UV asymptotics:

\[ \phi_{\text{IR}}(\omega) \equiv \frac{\kappa}{2T} \omega, \quad \phi_{\text{UV}}(\omega) \equiv \frac{g^2(\bar{\mu}_\omega) C_F}{6\pi} \omega^3, \ldots \]

and various interpolations \( I(\omega) \):

⇒ \( \rho_{\text{model}}(\omega) \equiv I(\omega) \sqrt{[\phi_{\text{IR}}(\omega)]^2 + [\phi_{\text{UV}}(\omega)]^2} \)

⇒ well-defined fit with parameters \( \kappa/T^3 \) and \( c_n \) via

\[ \chi^2 \equiv \sum_{\tau} \left[ \frac{G(\tau) - G_{\text{model}}(\tau)}{\delta G(\tau)} \right]^2 \]
Quenched, $1.5T_c$: HQ momentum diffusion coefficient $\kappa$

We find:

\[ \frac{\kappa}{T^3} = 2.31 \ldots 3.70 \]

convert via $2\pi TD = \frac{4\pi}{\kappa/T^3}$:

\[ 2\pi TD = 3.40 \ldots 5.44 \]

kinetic equilibration time:

\[ \tau_{\text{kin}} = \eta_D^{-1} = (1.63 \ldots 2.61) \left( \frac{T_c}{T} \right)^2 \left( \frac{M}{1.5 \text{ GeV}} \right) \text{ fm/c} \]

$\kappa/T^3$-value in agreement with previous studies, e.g. Francis et al. 2015 (multi-level method + pert. renorm.)

Comparison to previous studies:

- pQCD (NLO, $\alpha \approx 0.2$)
- AdS/CFT
  - $M \to \infty$, quenched
  - Francis et al. '15
  - Brambilla et al. '20
  - Altenkort et al. '21

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Lattice setup
- 2 + 1 flavor HISQ fermions
- $m_l = m_s / 5$ (pion mass $\approx 320$ MeV)

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- $O(a^2)$-improved “Zeuthen flow”
- 3rd-order RK with adaptive stepsize

Current situation
- need $N_\tau \gtrsim 20$ to extract diffusion physics
- no continuum extr. with current ensemble
  - no well-def. flow-time-to-zero extrapolation

However:
- long-distance correlation insensitive to finite $a$ and $\tau_F$
  - may still carry enough information to constrain $\kappa$!
- shape of correlator largely preserved for $\sqrt{8\tau_F}/\tau = \text{const.}$
  (flow radius proportional to separation)

Strategy
- treat finite $(a, \tau_F)$ as systematic uncertainties
- use quenched data to estimate additional systematic error
**Quenched, $1.5T_c$: systematics of simple model fits**

Fit: \[ \rho(\omega) = \sqrt{\left[\frac{\kappa \omega}{2T}\right]^2 + [c \phi_{UV}(\mu)]^2}, \quad \mu = \sqrt{[\pi T]^2 + \omega^2} \]

\[ \frac{G}{G_{\text{norm}}} = \left( N_{\tau}, \sqrt{8\tau_F/\tau} \right) \]

- (cont, $\tau_F \rightarrow 0$)
- (cont, 0.20)

**Conclusions**

- shape of correlator preserved at fixed small $\sqrt{8\tau_F/\tau}$
- for large $\tau$ also preserved at finite $a$!

⇒ sufficient to still constrain $\kappa/T^3$ using a simple model fit
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2 + 1 flavor: simple model fits at finite $\alpha$ and $\tau_F$

Fit: $\rho(\omega) = \sqrt{[\kappa\omega/2T]^2 + [c\phi_{UV}(\mu)]^2}$, $\mu = \sqrt{[2\pi T]^2 + \omega^2}$

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First impressions

- much larger $\kappa/T^3$ compared to quenched ($\sim 2 \times$)
- $\kappa/T^3$ seems to decrease with increasing $T$
Comparison of first impressions from 2+1 flavor QCD

\[2\pi TD\] -- pQCD (NLO, \(\alpha \approx 0.2\))

\[\cdots\] AdS/CFT

\(M \to \infty\), quenched
Francis et al. '15
Brambilla et al. '20
Altenkort et al. '21

\(M \to \infty\), 2+1 flavor
PRELIMINARY
(systematic errors missing)

\(2\pi TD\) = \(4\pi \kappa^{-3} T^3 \propto \tau_{\text{kin}} \frac{T^2}{M}\)

\[\begin{array}{l}
\text{very preliminary: systematic error analysis missing!} \\
\text{(first impressions from fits of one simple model)}
\end{array}\]

\[\begin{array}{l}
\text{Reminder: } 2\pi TD = \frac{4\pi}{\kappa/T^3} \propto \tau_{\text{kin}} \frac{T^2}{M}
\end{array}\]
### Recap

<table>
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<tr>
<th>What do we want?</th>
<th>a first-principles nonpert. estimate from full QCD for the HQ momentum diffusion coefficient $\kappa$ (or in turn $D$, $\tau_{\text{kin}}$)</th>
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<tr>
<td>Why?</td>
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<td>crucial input for transport simulations</td>
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<th>What did we achieve so far?</th>
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|                             | proof-of-concept for gradient flow method  
|                             | consistent results for $\kappa$ compared to previous studies |
|                             | $(a, \tau_F) \to 0$ data serves as benchmark for systematics of finite $(a, \tau_F)$ data |
|                             | $2+1$ flavor QCD |
|                             | preliminary explorations to constrain $\kappa$ using finite $(a, \tau_F)$ data |

<table>
<thead>
<tr>
<th>What to do next?</th>
<th>$2+1$ flavor QCD: increase statistics, add more lattices (cont. extr.)</th>
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|                  | determine finite mass correction (color-magnetic correlator)  
|                  | Bouttefeux, Laine 2021 |
|                  | LA et al. 2021 |