Heavy quark momentum diffusion from the lattice
using gradient flow

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10.1103/PhysRevD.103.014511 (2021)
How fast do heavy quarks thermalize in a hot medium?

- Hydrodynamics $\Rightarrow$ kinetic equilibration time $\tau_{\text{kin}}^{\text{heavy}} \approx \frac{M}{T} \tau_{\text{kin}}^{\text{light}}$

- But: significant collective motion ($v_2$)!

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

- Consider non-relativistic limit ($M \gg \pi T$):

  $$\tau_{\text{kin}} = \eta_D^{-1}$$

  $$\eta_D = \frac{\kappa}{2M_{\text{kin}}T} \left(1 + O\left(\frac{\alpha_s^{3/2} T}{M_{\text{kin}}}\right)\right)$$

  $$D = \frac{2T^2}{\kappa}$$

- 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
How to calculate diffusion coefficients from the lattice?

- Linear response theory $\Rightarrow$ diffusion physics $\Leftrightarrow$ in-equilibrium spectral functions (SPF)

$\Rightarrow$ SPF of HQ vector current

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

- Lattice: reconstruct SPF from Euclidean correlation functions

A. Spatial diffusion, hadronic correlators

- reconstruct $\rho^{ii}(\omega)$ from hadron corr.

$\Rightarrow$ $\rho^{ii}(\omega)$ encodes spatial diffusion coeff. $D$ through Kubo-formula:

$$D = \frac{1}{3\chi^{00}} \lim_{\omega \to 0} \sum_{i=1}^{3} \frac{\rho^{ii}(\omega)}{\omega}$$

- difficult to resolve transport peak at $\omega \to 0$

$\Rightarrow$ see recent talk by H.-T. Shu at SQM ’21

B. Momentum diffusion, gluonic correlators

- start from $\rho^{ii}(\omega)$ but utilize HQET (nonrelativistic limit $M \gg \pi T$)

$\Rightarrow$ construct “color-electric correlator” whose SPF encodes momentum diff. coeff. $\kappa$:

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

- smooth $\omega \to 0$ limit expected: no transport peak!

$\Rightarrow$ this talk
From HQET to $EE$ correlator to $\kappa$

- HQET: do Foldy-Wouthuysen trans. of $S_{\text{QCD}} \Rightarrow$ decouple quarks and anti-quarks (up to $O(1/M^2)$)
- insert leading-order $(1/M)$ currents in SPF, ..., translate to Euclidean
  - find gluonic "$EE$ correlator" $\rho$ Caron-Huot et al. 2009

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

$$= \int_{0}^{\infty} d\omega \frac{\cosh(\omega(\tau - \beta/2))}{\sinh(\omega\beta/2)} \rho(\omega)$$

- encodes transport physics of static heavy quark in thermalized medium

$$\Rightarrow \kappa = \lim_{\omega \to 0} 2T \frac{\rho(\omega)}{\omega}$$
  - no transport peak, smooth limit expected

Lattice discretization

- Problem: IR part of $\rho(\omega)$ encoded in large-$\tau$ part of $G(\tau)$
  - underlying signal overshadowed by UV fluctuations
  - large statistical errors!
  - need noise reduction (= gauge smoothing) method
Solution to noise problem: gradient flow  

- applicable to dynamical QCD (nonlocal action)
- introduces flow time \( \tau_F \equiv t a^2 \) with dimensionless parameter \( t \)
  \[
  \frac{dA_\mu(x, \tau_F)}{d\tau_F} \sim -\frac{\delta S_G[A_\mu(x, \tau_F)]}{\delta A_\mu(x, \tau_F)} , \quad A_\mu(x, \tau_F=0) = A_\mu(x)
  \]
- evolves gauge fields \( A_\mu(x) \) towards minimum of the action \( S_G \)
- smears them over Gaussian envelope (LO); width: flow radius \( \simeq \sqrt{8\tau_F} \)
  \[
  A_{\mu,LO}(x, \tau_F) = \int dy \left( \sqrt{\frac{2}{\pi}} \sqrt{\frac{8\tau_F}{2}} \right)^{-4} \exp \left( -\frac{(x - y)^2}{\sqrt{8\tau_F^2}/2} \right) A_\mu(y)
  \]

- improves signal & produces renormalized fields...
  ...but contaminates \( EE \) correlator \( G(\tau) \) for \( \sqrt{8\tau_F} \gtrsim \tau/3 \) according to LO pert. theory  
  
  \[
  \Rightarrow \text{flow up to flow limit } \sqrt{8\tau_F} \approx \tau/3, \text{ extrapolate back to } \tau_F = 0
  \]
Leading-order perturbative $EE$ correlator under Wilson flow

- **flow limit:**
  - cont. correlator deviates $< 1\%$ for $\tau T \gtrsim 3\sqrt{8\tau_F T}$ ⇒ vertical lines

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

continuum corr. from Eller, Moore 2018, lattice corr. from Eller, Moore, LA et al. 2021
Nonpert. *EE* correlator (quenched approximation, Wilson action, $T \approx 1.5 T_c$)

- Data normalized to pert. lattice correlator
  - Dominant $\tau^{-4}$ behavior filtered out, tree-level improvement
- Dashed line: flow limit as lower bound for separation $\tau T \gtrsim 3\sqrt{8\tau_F T}$
  - More flow = higher precision, but smaller window of noncontaminated data
- Interpolation through cubic splines (no smoothing)

<table>
<thead>
<tr>
<th>$N^3 \times N_T$</th>
<th>$a$ [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$80^3 \times 20$</td>
<td>0.0213</td>
</tr>
<tr>
<td>$96^3 \times 24$</td>
<td>0.0176</td>
</tr>
<tr>
<td>$120^3 \times 30$</td>
<td>0.0139</td>
</tr>
<tr>
<td>$144^3 \times 36$</td>
<td>0.0116</td>
</tr>
</tbody>
</table>
EE correlator as a function of flow time

- flow limit \( \sqrt{8\tau_F T} \lesssim \tau T / 3 \) ⇒ markers
- for large \( \tau T \): modest flow dependence
  ⇒ extrapolation to \( \tau_F = 0 \)
- need some flow to get signal, but too much contaminates the physics
- initial rising behavior (visible for \( \tau T = 0.056 \)): discretization-induced tadpole renormalization effect also found in pert. NLO lattice QED

\[ \tau T = \begin{array}{cccc}
0.500 & 0.250 \\
0.472 & 0.222 \\
0.444 & 0.194 \\
0.417 & 0.167 \\
0.389 & 0.139 \\
0.361 & 0.111 \\
0.333 & 0.083 \\
0.306 & 0.056 \\
0.278 & 0.028 \\
\end{array} \]
1. Continuum extrapolation (linear in $N^{-2}_\tau$)

- ansatz motivated by gauge action discretization
- taken separately for each flow time
- removes $a^2/\tau^2$-type discretization errors
- $a^2/\tau_F$-type errors only vanish if **continuum limit** is taken first!

2. Flow-time-to-zero extrapolation (linear in $\tau_F$)

- ansatz motivated by NLO pert. theory Eller 2021
- removes $\tau_F/\tau^2$-type effects
- flow time window depends on:
  - signal-to-noise ratio
  - $\sqrt{8\tau_F} \gtrsim a$ (renormalization, suppression of latt. artifacts)
  - $\sqrt{8\tau_F} \lesssim \tau/3$ (flow limit)
Renormalized continuum $EE$ correlator

Gradient flow method
Multi-level method

- Nonpert.-renormalized continuum $EE$ correlator after $a \to 0$ and $\tau_F \to 0$ extrapolations
  - 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!
Spectral reconstruction through pert. model fits

- for details see LA et al. 2021

- Reminder:
  \[ G(\tau) = \int_0^\infty d\omega \frac{\cosh(\omega(\tau - \beta/2))}{\sinh(\omega\beta/2)} \rho(\omega), \]
  \[ \kappa = \lim_{\omega \to 0} 2T \frac{\rho(\omega)}{\omega} \]

  \( \Rightarrow \) integral inversion problem; valid only at \( \tau_F = 0 \) Eller 2021

- Strategy: constrain allowed form of \( \rho(\omega) \) to
  \[ \rho^{(\mu,i)}_{\text{model}}(\omega) = \left[ 1 + \sum_{n=1}^{n_{\text{max}}} c_n e_n^{(\mu)}(y) \right] \sqrt{[\phi_{\text{IR}}(\omega)]^2 + [\phi_{\text{UV}}^{(a)}(\omega)]^2} \]

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

  \( \Rightarrow \) well-defined fit with parameters \( \kappa/T^3 \) and \( c_n \) via
  \[ \chi^2 \equiv \sum_\tau \left[ \frac{G^{\text{cont}}(\tau) - G^{\text{model}}(\tau)}{\delta G^{\text{cont}}(\tau)} \right]^2 \]
HQ momentum diffusion coefficient $\kappa$ at $T = 1.5 \, T_c$

We find

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

and (for $M \gg \pi T$ using $D = 2T^2/\kappa$):

$$2\pi TD = 3.40 \ldots 5.44$$

kinetic equilibration time:

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

$k/T^3$-value similar / slightly larger compared to previous study \cite{Francis2015} (using quenched-only multi-level method + pert. renorm.)
Recap

What do we want?
- a first-principles nonpert. estimate from dynamical QCD for the HQ momentum diffusion coefficient $\kappa$ (or in turn $D$, $\tau_{\text{kin}}$)

Why?
- phenomenology: explain experimental data for HQ
- crucial input for transport simulations

What did we achieve so far?
- proof-of-concept for gradient flow method in quenched QCD
  - no restrictions for application to dynamical QCD!
  - high-prec. data for IR part of $EE$ correlator (nonpert. renorm.)
  - consistent results for $\kappa$ from reconstructed spectral function (pert. model fits)

What to do next?
- measure dynamical QCD lattices (HISQ) [in progress]
- determine finite mass correction (color-magnetic correlator) [Bouttefeux, Laine 2021] [in progress]