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Heavy quark momentum diffusion from the lattice using gradient flow

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What happens to heavy quarkonia in HICs?

- Heavy quarkonia mainly produced in early hard collisions ($M \gg T$)
 - some remain as bound states $(J/\Psi,\Upsilon)$
 - some melt into constituents
 - travel through medium, thermalize to some extent via diffusion
 - form $D\bar{D}$ or $B\bar{B}$ meson pairs, decay into dileptons
- Evidence of in-medium interactions from strong modification of heavy hadron p_T distributions
 - probes for transport properties of QGP

J/Ψ	Υ
$c\bar{c}$	$b\overline{b}$
$3.1{ m GeV}$	$9.5{ m GeV}$
cf. $T \sim \mathcal{O}(100) \mathrm{MeV}$	

How much do heavy quarks thermalize in the hot medium formed in HICs?

- Naive picture: full thermalization needs many collisions, not possible within $5 10 \, {\rm fm}/c$
 - \Rightarrow kinetic equilibration time (hydrodynamics): $\tau_{\rm kin}^{\rm heavy} \simeq \frac{M}{T} \tau_{\rm kin}^{\rm light} \gg \tau_{\rm kin}^{\rm light}$
- But: significant collective motion $(v_2)! \Rightarrow \tau_{kin}^{heavy} \approx \tau_{kin}^{light}$

Can we calculate τ_{kin} from first principles?

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

$$\begin{aligned} \tau_{\rm kin} &= \eta_D^{-1} \\ \eta_D &= \frac{\kappa}{2M_{\rm kin}T} \left(1 + \mathcal{O}\left(\frac{\alpha_s^{3/2}T}{M_{\rm kin}}\right) \right) \\ D &= 2T^2/\kappa \end{aligned}$$

- Problem: perturbative series for D or κ ill-behaved!
 ⇒ need for non-perturbative ab-initio calculation
 - Iattice QCD

How to calculate diffusion coefficients from the lattice?

- Linear response theory: diffusion physics encoded in in-equilibrium spectral function (SPF)
 - ⇒ on the lattice: reconstruct SPF from Euclidean correlation functions

Two approaches on the lattice:

A. Spatial diffusion from hadronic correlators

Starting point: SPF of HQ vector current

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

encodes spatial diffusion coeff. *D* through Kubo-formula:

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

 $\hfill \hfill \hfill$

⇒ see *≥* yesterday's talk by H.-T. Shu

B. Momentum diffusion from gluonic correlators

- Same starting point, but: utilize nonrelativistic limit $M \gg \pi T$
 - can construct "color-electric correlator" whose SPF encodes momentum diff. coeff.

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

- smooth $\omega \to 0$ limit expected: no transport peak!
- needs sophisticated noise reduction method

⇒ this talk

κ and the color-electric (*EE*) correlator

Where does κ hide on the lattice for $M \gg \pi T$?

nonrel. limit enables Foldy-Wouthuysen transformation of S_{QCD} (Heavy Quark Effective Theory)

- \Rightarrow decouples quarks and anti-quarks (up to $\mathcal{O}(1/M^2)$)
- starting from spectral function of HQ current, derive/construct Euclidean correlator / Caron-Huot et al. 2009

 \Rightarrow $G(\tau)$: purely gluonic "color-electric correlator" or "EE correlator"

$$G(\tau) \equiv -\frac{1}{3} \sum_{i=1}^{3} \frac{\langle \operatorname{Re}\left[\operatorname{tr}\left[U_{(\beta,\tau)} \ gE_{i}(\mathbf{0},\tau) \ U_{(\tau,0)} \ gE_{i}(\mathbf{0},0) \ \right] \right] \rangle}{\langle \operatorname{Re}\left[\operatorname{tr}\left[U_{(\beta,0)} \ \right] \right] \rangle}$$
$$= \int_{0}^{\infty} \mathrm{d}\omega \ \frac{\cosh(\omega(\tau - \beta/2))}{\sinh(\omega\beta/2)} \ \boldsymbol{\rho}(\omega)$$

encodes transport physics of static heavy quark in thermalized medium

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

■ lattice discretization:

needs sophisticated noise reduction method!

Gradient flow for *EE* correlator

- Problem: transport physics encoded in long-distance (low frequency) correlation
 - ⇒ high freq. gauge field fluctuations overshadow low freq. ones ⇒ poor signal-to-noise ratio!
 - need noise reduction method that's valid in full dynamical QCD
- Solution: gradient flow & Lüscher 2010
 - \blacksquare introduces "flow time" $\tau_{\rm F}:=ta^2$ with dimensionless parameter t

$$\frac{\mathrm{d}A_{\mu}(\boldsymbol{x},\tau_{\mathrm{F}})}{\mathrm{d}\tau_{\mathrm{F}}} \sim \frac{-\delta S_{G}[A_{\mu}(\boldsymbol{x},\tau_{\mathrm{F}})]}{\delta A_{\mu}(\boldsymbol{x},\tau_{\mathrm{F}})}, \quad A_{\mu}(\boldsymbol{x},\tau_{\mathrm{F}}=\mathbf{0}) = A_{\mu}(\boldsymbol{x})$$

- evolves gauge fields $A_{\mu(x)}$ towards minimum of the action
- \blacksquare smears them over spherical extent with "flow radius" $\simeq \sqrt{8\tau_{\rm F}}$

$$A^{\rm LO}_{\mu}(x,\tau_{\rm F}) = \int \mathrm{d}y \, \left(\sqrt{2\pi}\sqrt{8\tau_{\rm F}}/2\right)^{-4} \exp\left(\frac{-(x-y)^2}{\sqrt{8\tau_{\rm F}}^2/2}\right) A_{\mu}(y)$$

- improves signal & produces renormalized fields...
 - ...but destroys EE correlator $G(\tau)$ for $\sqrt{8\tau_{\rm F}}T \gtrsim \tau T/3$ according to LO pert. theory \mathscr{P} Eller, Moore 2018
 - \Rightarrow flow "a little", extrapolate back to $\tau_{\rm F}=0$ after continuum extrapolation



- continuum from *d* Eller, Moore 2018 , lattice from *d* Eller, Moore, LA et al. 2021
- "flow limit:" cont. correlator deviates <1% for $\sqrt{8\tau_{\rm F}}T\lesssim \tau T/3$ \Rightarrow vertical lines $\,\mathscr{P}\,{\rm Eller},$ Moore 2018

Use this to enhance non-pert. lattice results:

- filter out dominant τ^{-4} behavior of $G_{\text{non-pert.}}^{\text{latt}}$ using $G_{\text{non-pert.}}^{\text{latt}}/G^{\text{norm}}$
 - increases visibility of details
- approx. remove tree-level discretization errors from comparison of LO cont. and LO latt. correlators

EE correlator, non-pert. lattice, $T \approx 1.5 \, T_c$

$N_{\sigma}^3 \times N_{\tau}$	$a \; [\mathrm{fm}]$
$80^3 \times 20$	0.0213
$96^3 \times 24$	0.0176
$120^3 \times 30$	0.0139
$144^3 \times 36$	0.0116

- 10000 quenched conf. each
- well-separated: 500 sweeps of (1 HB, 4 OR)
- $\mathcal{O}(a^2)$ -improved "Zeuthen flow"
- 3rd-order RK with adaptive stepsize



- divided by pert. correlator: dominant τ^{-4} behavior filtered out, tree-level improvement
- interpolation through cubic splines (no smoothing)
- flow limit $\sqrt{8\tau_{\rm F}}T\approx \tau T/3$ \Rightarrow dashed line
 - > more flow = smaller window of noncontaminated data



- flow limit $\sqrt{8\tau_{\rm F}}T \approx \tau T/3 \Rightarrow$ vertical lines
- for large τT : modest flow dependence
 - \Rightarrow extrapolation to $\tau_{\rm F} = 0$
- 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

Continuum and flow-time-to-zero extrapolation

• 1. Continuum extrapolation (linear in N_{τ}^{-2})



- taken separately for each flow time
- removes a^2/τ^2 -type discretization errors
- ansatz motivated by gauge action discretization

2. Flow-time-to-zero extrapolation (linear in $\tau_{\rm F}$)



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

 $a^2/\tau_{
m F}$ -type errors only vanish if **continuum limit** is taken **first!**

Renormalized continuum *EE* correlator



- Nonpert.-renormalized continuum EE correlator after $a \rightarrow 0$ and $\tau_{\rm F} \rightarrow 0$ extrapolations
- shape consistent with previous (only pert. renorm.) results

 P Francis et al. 2015,
 P Christensen, Laine 2016
- overall shift due to
 - nonperturbative renormalization
 - difference in statistical power of gauge conf.
 - systematic uncertainty introduced by flow extrapolation
- only infrared part of correlator can be obtained
 - > not a problem for transport physics!

Spectral reconstruction through pert. model fits

• valid only at $\tau_{\rm F}=0$: 2 Eller 2021

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

- ill-posed integral inversion problem
- \blacksquare strategy: constrain allowed form of $\rho(\omega)$ to

$$\rho_{\text{model}}^{(\mu,i)}(\omega) \equiv \left[1 + \sum_{n=1}^{n_{\text{max}}} c_n e_n^{(\mu)}(y)\right] \sqrt{\left[\phi_{\text{IR}}(\omega)\right]^2 + \left[\phi_{\text{UV}}^{(i)}(\omega)\right]^2}$$

using IR and UV asymptotics:

$$\phi_{\rm IR}(\omega) \equiv \frac{\kappa\omega}{2T}, \quad \phi_{\rm UV}^{(a)}(\omega) \equiv \frac{g^2(\bar{\mu}_\omega)C_F\omega^3}{6\pi}, \quad \dots$$

 \Rightarrow well-defined fit with parameters κ/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 κ at $T=1.5\,T_{ m c}$



We find

$$\kappa/T^3 = 2.31 \dots 3.70$$

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

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

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

Recap

What do we want?

 a first-principles nonperturbative estimate from dynamical QCD for the heavy quark momentum diffusion coefficient κ (or in turn D, τ_{kin})

Why?

- phenomenologically interesting: explain experimental data for heavy quarks
- crucial input for transport simulations

What did we achieve so far?

- proof-of-concept for gradient flow method using quenched QCD
 - no restrictions for application to dynamical QCD!
 - high-precision data (nonperturbatively renormalized) for relevant infrared part of *EE* correlator
 - consistent results for κ from reconstructed spectral function (pert. model fits)

What to do next?

- perform analysis on a set of dynamical QCD lattices (HISQ) [in progress]
- determine finite mass correction from color-magnetic (*BB*) correlator *P* Bouttefeux, Laine 2021 [in progress]