Funded by DFG Deutsche Forschungsgemeinschaft German Research Foundation

How fast do heavy quarks thermalize?

The heavy quark diffusion coefficient from lattice QCD

1. Review of quenched lattice QCD at $1.5\,T_c$ 10.1103/PhysRevD.103.014511 (2021)

Bielefeld U.:	Altenkort, Kaczmarek, Mazur, Shu
TU Darmstadt:	Eller, Moore

2. First results from $2+1$ flavor lattice QCD (in preparation)

Bielefeld U.:	Altenkort, Kaczmarek, Shu
Brookhaven NL:	Petreczky, Mukherjee
U. of Stavanger:	Larsen
	(HotQCD collaboration)

Luis Altenkort
Bielefeld University

Zimányi School 2022
Budapest, December 05

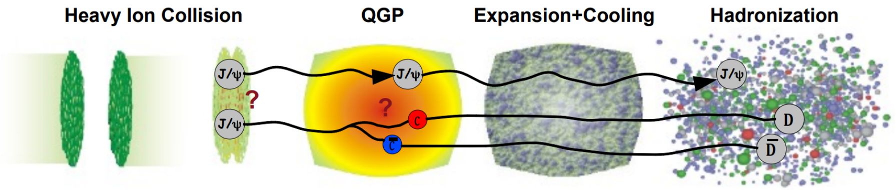


Figure: Steffen Bass

Why heavy quark diffusion?

- direct window into strong in-medium QCD force:
  - Exp. data (v_2, R_{AA}) $\to$ considerable collective motion! $\to$ eq. time: $\tau_{\text{heavy}} \overset{?}{\approx} \frac{1}{T}$
    ALICE (2019) , ALICE (2018)
  - Naive hydro: $\tau_{\text{heavy}} \simeq \frac{M}{T} \tau_{\text{light}}$ $\to$ $\tau_{\text{light}} \overset{?}{\ll} \frac{1}{T}$
- input or crosscheck for quarkonium production/evolution models
  Brambilla et al. (2021) Capellino et al. (2022) Torres-Rincon et al. (2022)
- varying results for T-dep. between models Dong, Lee, Rapp (2019)

Calculate τ_{heavy} from first principles?

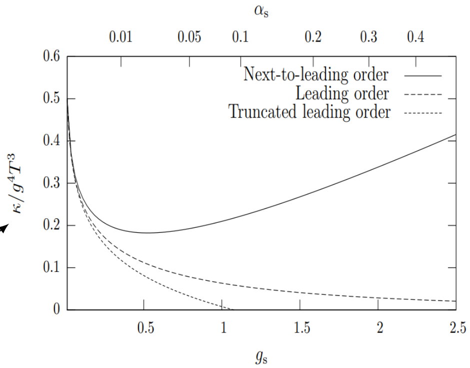
- nonrel. limit $M \gg \pi T$ → Langevin dynamics
  Moore, Teaney (2005) Casalderrey-Solana, Teaney (2006)

  → **(momentum) diffusion coefficient**

$$\tau_{\text{heavy}} = \frac{M}{T} D = \frac{2MT}{\kappa}$$

- Perturbation theory unreliable! Caron-Huot, Moore (2008)

  → **nonpert. lattice QCD**



Diffusion coefficients from the lattice?!

Caron-Huot, Laine, Moore (2009)
Petreczky, Teaney (2005)

- Linear response theory
  ⇒ **in-eq. spectral functions** (SPF)

$$D \sim \lim_{\omega \to 0} \frac{\rho^{ii}(\omega)}{\omega}$$

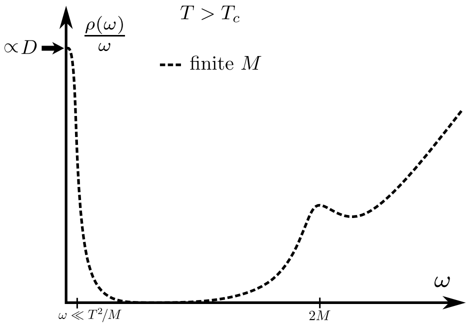
with

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

↳ HQ vector current

- reconstruct from **Euclidean time correlators**:

$$G(\tau) = \int_0^\infty \mathrm{d}\omega \, \rho(\omega) \frac{\cosh\left(\omega(\tau - \frac{\beta}{2})\right)}{\sinh\left(\omega \frac{\beta}{2}\right)}$$



1. instead of D, consider κ (encoded in the tail)

2. use HQET:
   expand in $1/M$,
   replace $\hat{\mathcal{J}}^i$ with LO version,
   ...

⇒ $G(\tau)$ = **color-electric two-point function** (force-force correlator)

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

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($\hat{\mathcal{J}}^i$ → HQ vector current)

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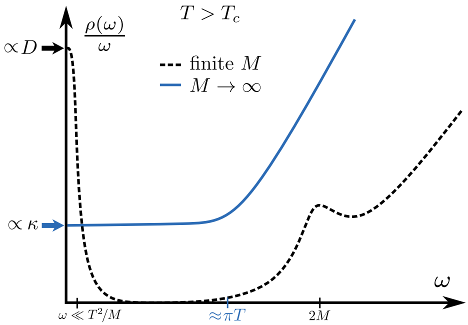

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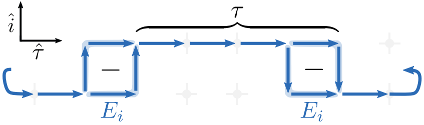
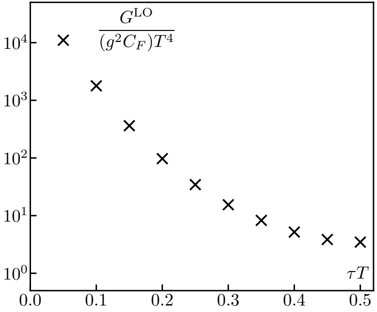
Gluonic color-electric correlator
Caron-Huot, Laine, Moore (2009)

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

$\downarrow$



Weak-coupling structure (LO)



Laine et al. (2011)

Drawback of $M \to \infty$

- UV gauge fluctuations dominate for large τ
- large τ most sensitive to $\omega \to 0$
  - ⇒ need noise reduction!

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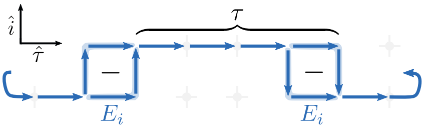

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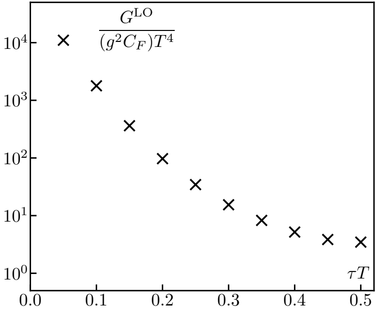

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Noise reduction via gradient flow Lüscher (2010)

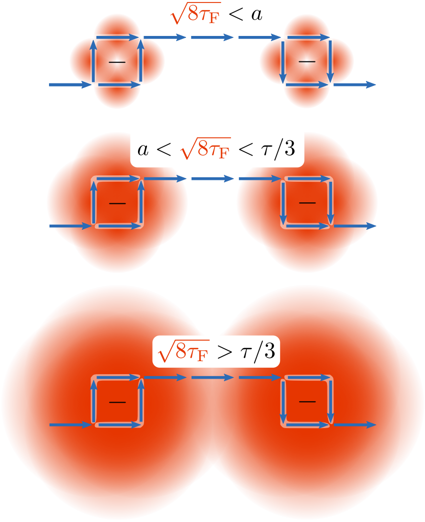
- supports nonlocal actions! (e.g. 2+1 flavor HISQ)
- new gaugefield parameter: “flow time” τ_F

Flow = smooth regulator:

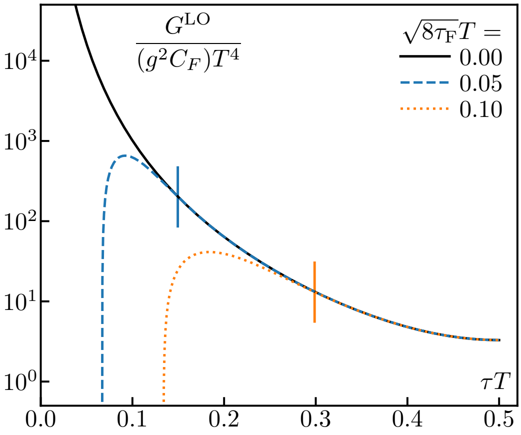
- links continuously smeared, width $\simeq \sqrt{8\tau_\mathrm{F}}$, “flow radius”
- lattice renorm. artifacts suppressed if $\sqrt{8\tau_\mathrm{F}} \gtrsim a$
- $G(\tau)$ free of distortion if $\sqrt{8\tau_\mathrm{F}} \lesssim \tau/3$ (next slide)

Idea:

1. step-wise smearing + $G(\tau)$ measurement
2. at each τ_F step, extrapolate $a \to 0$
3. extrapolate $\tau_\mathrm{F} \to 0$, only consider $a < \sqrt{8\tau_\mathrm{F}} < \tau/3$



Weak coupling + Wilson flow



Eller, Moore (2018)

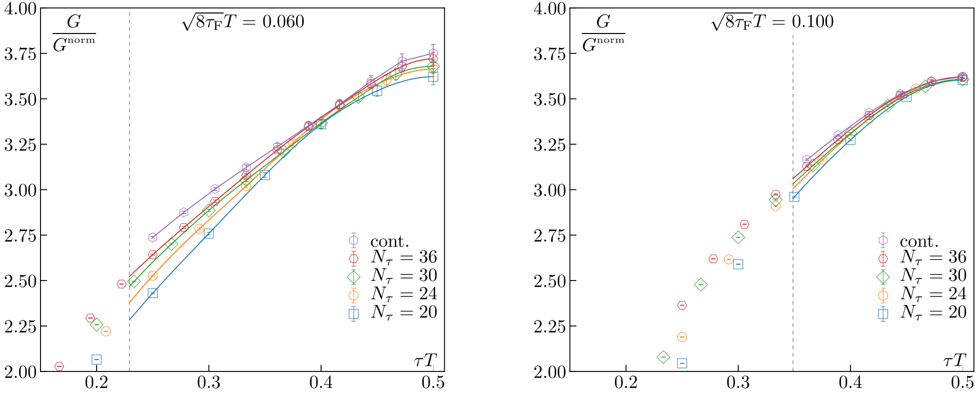
Flow limit = lower bound for τ

- correlator deviates $< 1\%$ for $\tau \gtrsim 3\sqrt{8\tau_\mathrm{F}}$ (vertical lines)

Enhance nonpert. lattice data:

- normalize to weak-coupling structure $\equiv$ G^{norm}
- remove tree-level discretization errors

Pure gauge, $1.5\,T_c$, Wilson action



Lattice & flow setup

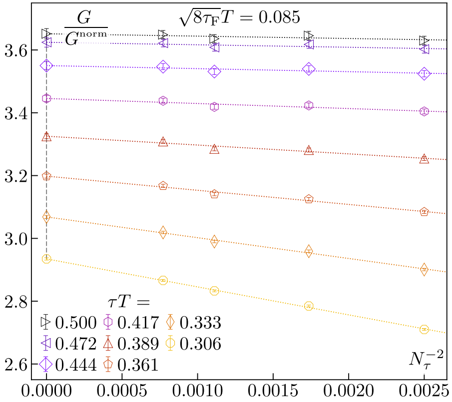
$N_\sigma^3 \times N_\tau$	a [fm]
$80^3 \times 20$	0.0213
$96^3 \times 24$	0.0176
$120^3 \times 30$	0.0139
$144^3 \times 36$	0.0116

- 10000 conf. each
- separation:
  500 sweeps of (1 HB + 4 OR)
- $\mathcal{O}(a^2)$-improved “Zeuthen flow”
- 3rd-order RK with adaptive stepsize

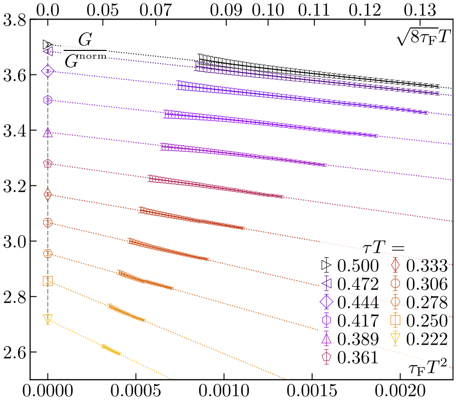
LA et al. 2021

Pure gauge, $1.5\,T_c$, Wilson action

- **1. Continuum extrapolation** (linear in a^2)



- **2. Flow-time-to-zero extrapolation** (linear in τ_F)

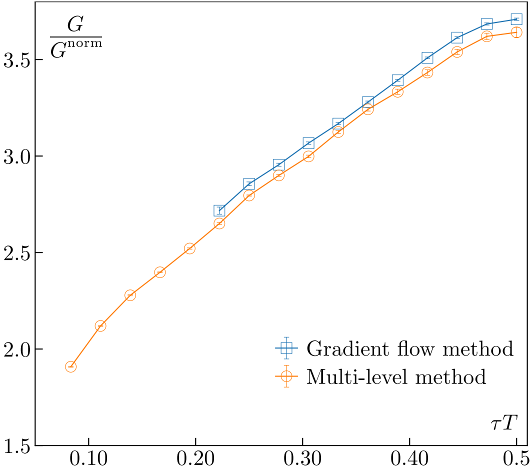


- ansatz from weak-coupling NLO Eller 2021

LA et al. 2021

Pure gauge, $1.5\,T_c$

$a \to 0, \tau_F \to 0$



(continuum + renormalized,
normalized to weak-coupling structure)

Comparison to previous method

- shape consistent with Multi-level results (only pert. renormalized)

  Francis et al. (2015) Christensen, Laine (2016)

- overall shift?
  - nonperturbative renormalization
  - better statistics

LA et al. 2021

Spectral reconstruction = integral inversion problem

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

Strategy: use spectral function models

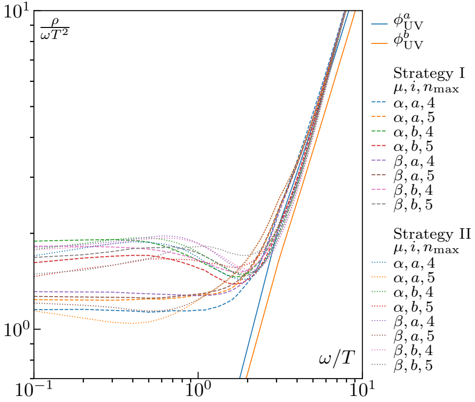
- $\rho_{\mathrm{model}}(\omega) \equiv I(\omega)\sqrt{[\phi_{\mathrm{IR}}(\omega)]^2 + [\phi_{\mathrm{UV}}(\omega)]^2}$

with known $\phi_{\mathrm{IR}}(\omega) \equiv \frac{\boldsymbol{\kappa}}{2T}\omega$, $\phi_{\mathrm{UV}}(\omega) \sim \omega^3$, ...

and various **interpolations** $I(w)$

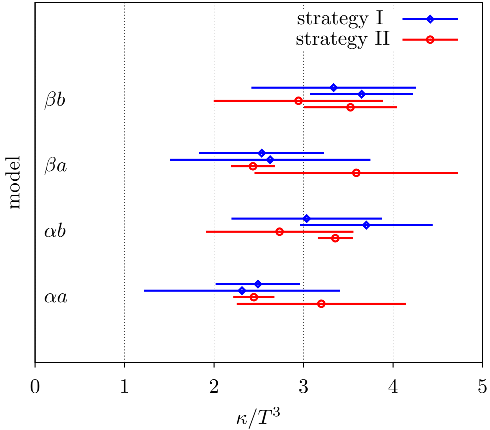
⇒ obtain $\boldsymbol{\kappa}/T^3$ by fitting

$$\chi^2 \equiv \sum_\tau \left[\frac{G(\tau) - G_{\mathrm{model}}(\tau)}{\delta G(\tau)}\right]^2$$



LA et al. 2021

Pure gauge, $1.5T_c$



Final estimate:

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

$$\Leftrightarrow \quad 2\pi T D = 3.40 \ldots 5.44$$

$$\Leftrightarrow \quad \tau_{\text{heavy}} = (1.63 \ldots 2.61) \left(\frac{T_c}{T}\right)^2 \left(\frac{M}{1.5\text{GeV}}\right) \text{fm/c}$$

LA et al. 2021

2+1 flavor QCD, HISQ action

- $T \approx 200 \dots 350\,\mathrm{MeV}$, $m_\pi \approx 310\,\mathrm{MeV}$
- no $a \to 0$ and $\tau_\mathrm{F} \to 0$ yet

Intermediate strategy

1. use "relative flow time" $\frac{\sqrt{8\tau_\mathrm{F}}}{\tau} \equiv \mathrm{const.} < \frac{1}{3}$

   ⇒ nonzero τ_F = small correction

2. use flow-dep. tree-level improvement

   Stendebach, Moore (2022, unpublished)

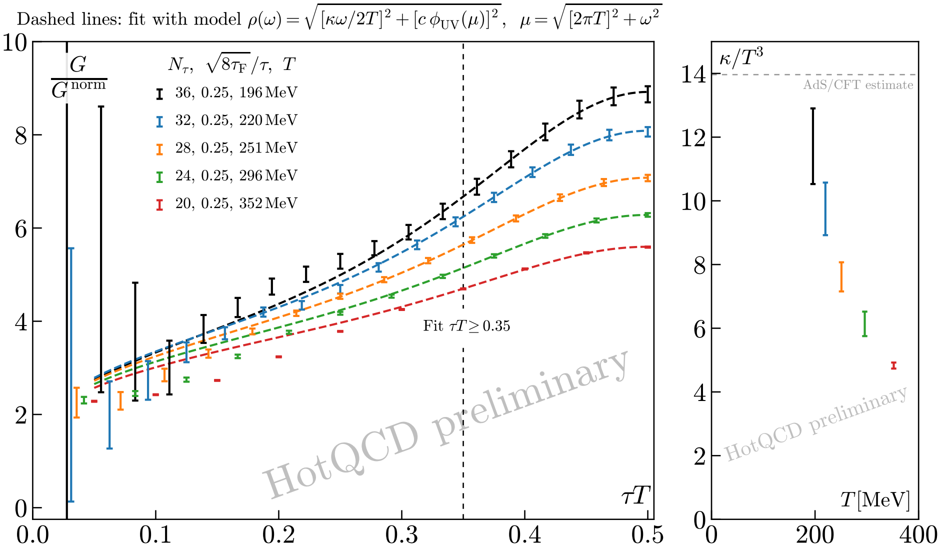
3. fit simple models to $\tau T \geq 0.35$

⇒ **tiny add. systematic error for** κ/T^3 compared to SPF model systematics

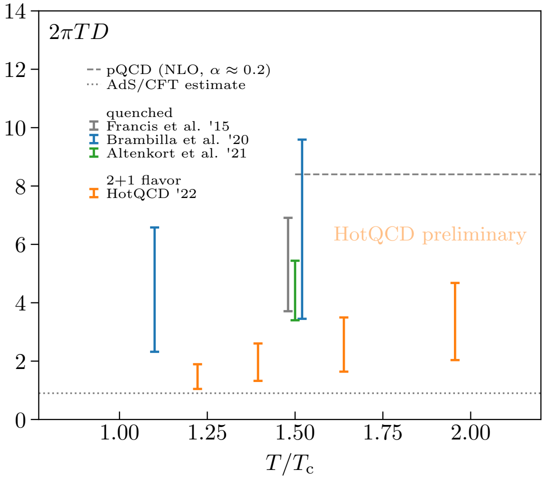
Lattice setup (planned)

m_l	T [MeV]	$N_\sigma^3 \times N_\tau$	a [fm]
$m_s/5$	195	$96^3 \times 36$	0.028
		$64^3 \times 24$	0.042
		$64^3 \times 20$	0.051
	220	$96^3 \times 32$	0.028
		$64^3 \times 24$	0.037
		$64^3 \times 20$	0.045
	251	$96^3 \times 28$	0.028
		$64^3 \times 24$	0.033
		$64^3 \times 20$	0.039
	296	$96^3 \times 24$	0.028
		$64^3 \times 22$	0.031
		$64^3 \times 20$	0.034
$m_s/27$	≤ 195	$64^3 \times 24$	
	...		

2 + 1 flavor QCD



Comparison to other results



- Reminder:

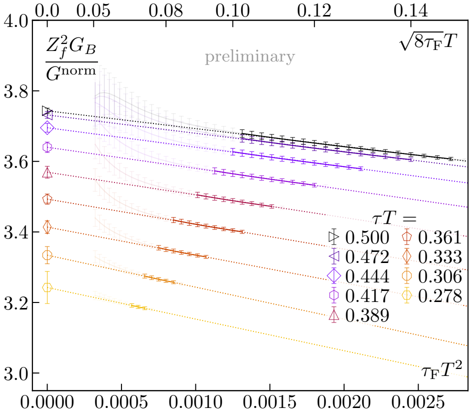
$$\frac{4\pi}{\kappa/T^3} = 2\pi TD \sim \frac{T^2}{M}\tau_{\text{heavy}}$$

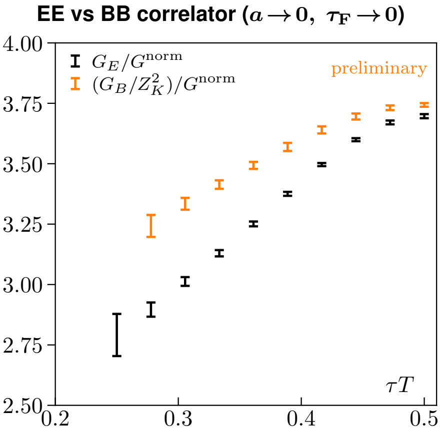
pQCD: Caron-Huot, Moore (2008)
AdS/CFT: Casalderrey-Solana, Teaney (2006)

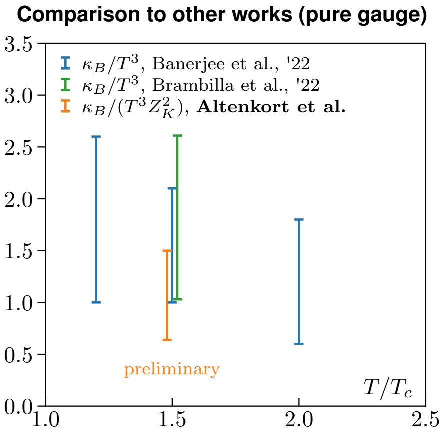
$\mathcal{O}(T/M)$ correction

- $\kappa \simeq \kappa_E + \frac{2}{3}\langle \mathbf{v}^2\rangle \kappa_B$ Bouttefeux, Laine (2020) Laine (2021)
  - ⇛ color-**magnetic** correlator G_B
- Problem: anomalous dimension
  $\to$ logarithm in $G_B(\tau_F)$
- Solution: consider $Z_B^2(Z_K^2 Z_f^2 G_B)_{\tau_F \to 0}$
  - Z_f^2 → cancel scale-dependence
  - Z_K^2 → match flow to $\overline{MS}$ scheme
  - Z_B^2 → $\overline{MS}$ renorm. factor
  - ⇛ $Z_f^2(\tau_F, g^2_{\tau_F})$ obtained by integrating RG equation, ($g^2_{\tau_F}$ measured at $T=0$)
- expect $Z_K^2 \sim 1$, pert. calculation in progress

Pure gauge, $1.5\,T_c$: $\tau_F \to 0$ for $Z_f^2 G_B$




EE vs BB correlator ($a \to 0,\ \tau_F \to 0$)
G_E/G^{norm}
$(G_B/Z_K^2)/G^{\text{norm}}$
preliminary
4.00
3.75
3.50
3.25
3.00
2.75
2.50
0.2
0.3
0.4
0.5
τT


Comparison to other works (pure gauge)
κ_B/T^3, Banerjee et al., '22
κ_B/T^3, Brambilla et al., '22
$\kappa_B/(T^3 Z_K^2)$, **Altenkort et al.**
preliminary
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.0
1.5
2.0
2.5
T/T_c

Quenched QCD

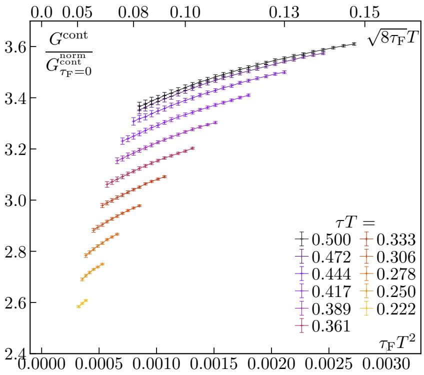
- proof-of-concept for gradient flow method LA et al. 2021
- results serve as crosscheck for systematics of 2+1 flavor data
- **Next:**
  determine finite-mass correction (color-magnetic correlator) Bouttefeux, Laine 2021

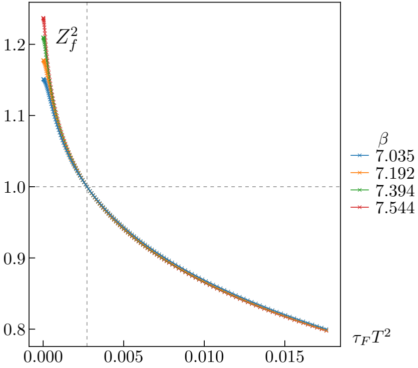
2+1 flavor QCD

- preliminary results to constrain κ
- **Next:**
  continuum extrapolation,
  investigate light quark mass effects,
  finite mass correction

Backup

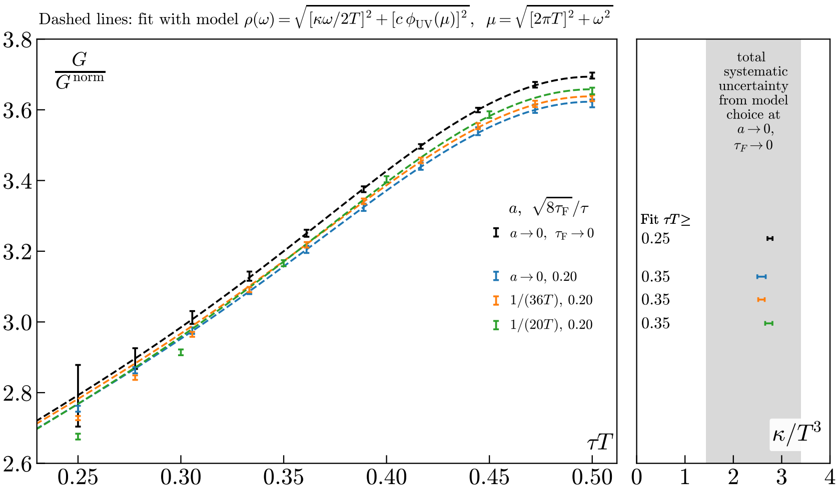
“bare” BB correlator





$\tau_F \to 0$ impossible

Quenched, $1.5T_c$: systematics of simple model fits

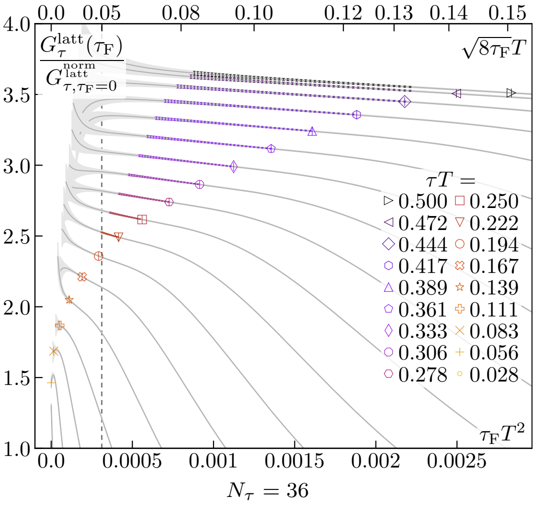


Conclusions

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

→ sufficient to still constrain κ/T^3 (using simple models)

EE correlator as a function of flow time (quenched, $1.5T_c$)



- inside extrapolation window: single colorful data points. outside: data points connected via grey lines.
- markers at $\sqrt{8\tau_F} \approx \tau/3$
- dashed line: minimum flow such that $\sqrt{8\tau_F} \gtrsim a$ for our coarsest lattice
- small τ_F: strong flow dependence (suppress noise and renorm. artifacts)
- intermediate τ_F: minor dependence (for large τ)

LA et al. 2021

Heavy Quark Effective Theory

- for $M \gg T$ and $\omega < \omega_{\mathrm{UV}}$: spectral function is a Lorentzian[1]

$$D \overset{\omega \lesssim \omega_{\mathrm{UV}}}{\approx} \sum_i \frac{\rho^{ii}(\omega)}{\omega} \frac{1}{3\chi^{00}} \frac{\eta^2 + \omega^2}{\eta^2}, \qquad D \simeq 2T^2/\kappa, \quad \eta \simeq \kappa/(2M_{\mathrm{kin}}T)$$

$$\kappa_{(M)} \equiv \frac{M_{\mathrm{kin}}^2 \omega^2}{3T\chi^{00}} \sum_i \frac{2}{\beta\omega} \rho^{ii}(\omega) \bigg|^{\eta \ll |\omega| \lesssim \omega_{\mathrm{UV}}}$$

- κ is defined as the coefficient of the powerlaw fall-off of the Lorentzian
- perform Foldy-Wouthuysen transformation of default lattice qcd action:

$$\Rightarrow \mathcal{L}_{\mathrm{QCD}} = \hat{\theta}^\dagger \left(iD_0 - M + \frac{D_i D^i + \sigma_i g B^i}{2M} \right) \hat{\theta} + \hat{\phi}^\dagger \left(iD_0 + M - \frac{D_i D^i + \sigma_i g B^i}{2M} \right) \hat{\phi}$$
$$+ \frac{i}{2M} \left(\hat{\theta}^\dagger \sigma_i g E^i \hat{\phi} - \hat{\phi}^\dagger \sigma_i g E^i \hat{\theta} \right) + \mathcal{O}\left(1/M^2\right) + \mathcal{L}_{\mathrm{light}} + \mathcal{L}_{\mathrm{gauge}}$$

- obtain the LO currents from EOM and insert into SPF, do some algebra and take limits[2]:

$$\kappa = \frac{\beta}{3} \sum_{i=1}^{3} \lim_{M \to \infty} \frac{1}{\chi^{00}} \int \mathrm{d}t \int \mathrm{d}^3\mathbf{x} \left\langle \frac{1}{2} \left\{ \left[\hat{\phi}^\dagger g E^i \hat{\phi} - \hat{\theta}^\dagger g E^i \hat{\theta} \right]_{(\mathbf{x},t)}, \left[\hat{\phi}^\dagger g E^i \hat{\phi} - \hat{\theta}^\dagger g E^i \hat{\theta} \right]_{(\mathbf{0},0)} \right\} \right\rangle$$

- Carry out contractions and Wick-rotate to obtain Euclidean correlator

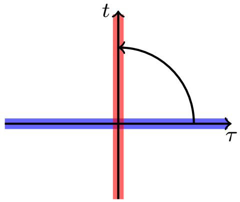
Spectral reconstruction at finite flow time?!

LO spectral function:

$$\rho_{\mathsf{E}}^{(2)}(\omega, {\color{red}\tau_{\mathrm{F}}}) = \frac{g^2 C_{\mathcal{R}}}{6\pi}\omega^3$$

Relation between Euclidean correlator and spectral function is **broken by Grad. flow**

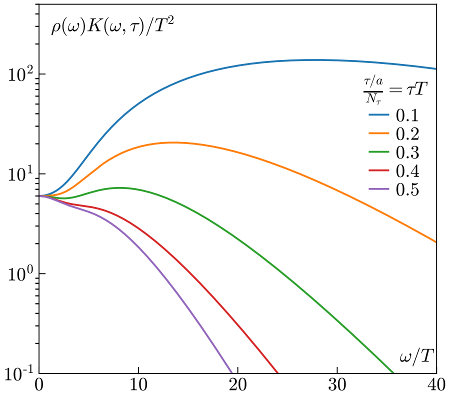
$$G_{\mathsf{E}}(\tau, {\color{red}\tau_{\mathrm{F}}}) {\color{red}\neq} \int_0^\infty \frac{d\omega}{\pi}\rho(\omega, {\color{red}\tau_{\mathrm{F}}})\frac{\cosh\left[\omega(\frac{\beta}{2} - \tau)\right]}{\sinh\left[\frac{\beta\omega}{2}\right]}$$



Physical: Contact terms **break causality** of theory

Mathematical: Exponential suppression becomes exponential enhancement after Wick rotation $\Rightarrow$ Kramers-Kronig relation is broken

Integration kernel effect



Gradient flow equations

- introduces extra dimension: “flow time” τ_F
- evolves gauge fields $A_\mu(x)$ towards minimum of action S_G

$$A_\mu(x,\boldsymbol{\tau_\mathrm{F}=0}) = A_\mu(x)$$

$$\frac{\mathrm{d}A_\mu(x,\tau_\mathrm{F})}{\mathrm{d}\tau_\mathrm{F}} \sim \frac{-\,\delta S_G[A_\mu]}{\delta A_\mu(x,\tau_\mathrm{F})}$$

Flow = smooth regulator:

- suppression of high-momentum modes in gluon prop.
- A_μ^LO: average over Gaussian, width $\simeq \sqrt{8\tau_\mathrm{F}}$ “flow radius”

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

Kubo-formula for D

- Approach I, phenomenological
  Diffusion equation: $\partial_t \langle A(\mathbf{x},t)\rangle = D\nabla^2 \langle A(\mathbf{x},t)\rangle$
  ⇒ Formal solution: $\langle A(\mathbf{k},\omega)\rangle = \frac{i}{\omega + iD\mathbf{k}^2}\langle A(\mathbf{k},t{=}0)\rangle$
- Approach II, Linear response th.
  Hamiltonian: $H(t) = H_0 - \int \mathrm{d}\mathbf{x} A(\mathbf{x}) h(\mathbf{x})\, \mathrm{e}^{\epsilon t}\,\Theta(-t)$
  ⇒ Formal solution ($\mathcal{O}(h)$): $\delta\langle A(\mathbf{k},\omega)\rangle = \frac{1}{i\omega}\left[\frac{G_R(\mathbf{k},\omega)}{\chi(\mathbf{k})} - 1\right]\delta\langle A(\mathbf{k},t{=}0)\rangle$
- Comparison (for small ω, $|\mathbf{k}|$): $\Rightarrow G_R(\mathbf{k},\omega) = \frac{iD\mathbf{k}^2}{\omega + iD\mathbf{k}^2}\chi(\mathbf{k})$

⇒ **Kubo**-type **formula** $\Leftrightarrow D = \frac{1}{\chi_s}\lim_{\omega\to 0}\left[\lim_{k\to 0}\frac{\omega}{k^2}\boldsymbol{\rho}(k,\omega)\right]$

- diffusion physics encoded in **spectral function** $\boldsymbol{\rho}(k,\omega) \sim \int_{\boldsymbol{x},t} \mathrm{e}^{i(\omega t - \mathbf{k}\mathbf{x})}\,\langle[A(\mathbf{x},t), A(\mathbf{0},0)]\rangle_{\mathrm{eq.}}$
- directly relates **macroscopic** <u>**non**</u>**-eq. evolution** and **microscopic** <u>**in**</u>**-eq. fluctuations**!

external pert. h, retarded correlator G_R, susceptibility χ, static suscept. χ_s

Thermalization through diffusive motion

Phenomenological diffusion

- consider classical fluid of particles
  - some local quantity $A(\mathbf{x})$, $\langle A(\mathbf{x})\rangle_{\text{eq}} = 0$
  - after perturbation in A: $\partial_t \langle A(\mathbf{x},t)\rangle \neq 0 \;\rightarrow\;$ relax back to eq.
  - if A **varies slowly** in space & time:

  ⇛ $\partial_t \langle A(\mathbf{x},t)\rangle = D\nabla^2 \langle A(\mathbf{x},t)\rangle$

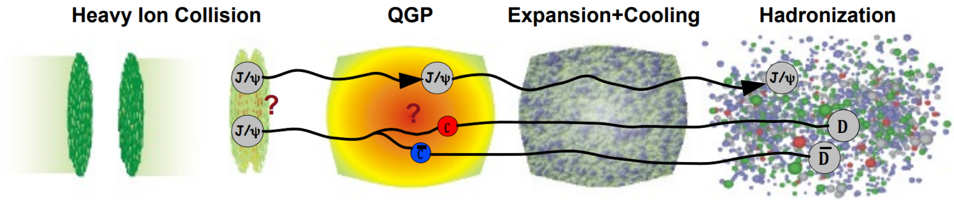
⇛ thermalization of A characterized by **diffusion coefficient D**

Heavy quark diffusion in a hot medium

- $A \rightarrow$ heavy quark current $\hat{\mathcal{J}}^\mu$
- perturbation in heavy quark chemical potential
- rigorous approach:
  - finite temperature field theory + **linear response theory**

  ⇛ $H(t) = H_0 - \int \mathrm{d}\mathbf{x}\, A(\mathbf{x}) h(\mathbf{x})\, \mathrm{e}^{\epsilon t}\, \Theta(-t)$

- How to identify D here?



- 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
$c\bar{c}$	$b\bar{b}$
$3.1\,\mathrm{GeV}$	$9.5\,\mathrm{GeV}$

cf. $T \sim \mathcal{O}(100)\,\mathrm{MeV}$

What is transport?

Transport phenomena are spontaneous **statistical processes** that cause a quantity of a system that is **out of equilibrium** to evolve towards its **equilibrium** distribution.

Basic examples

Process	Quantity	Transport coefficient	Unit
Heat conduction	Energy	Thermal conductivity	$\mathrm{Wm^{-1}K^{-1}}$
Particle diffusion	Mass	Diffusion coefficient	$\mathrm{m^2s^{-1}}$
Fluid flow	Momentum	Shear/bulk viscosity	$\mathrm{kg\,m^{-1}s^{-1}}$

- Transport phenomena are quanitified through **transport coeffcients**
- For near-equilibrium strong-interaction matter:
  - fluid flow $\rightarrow$ shear/bulk viscosity
  - chemical composition $\rightarrow$ flavor diffusion coefficients