Lattice QCD results for the heavy quark diffusion coefficient

How fast do heavy quarks thermalize in the QGP?

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**

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

Luis Altenkort
Bielefeld University

INT-22-3
Seattle, October 19, 2022

Heavy Ion Collision　　**QGP**　　**Expansion+Cooling**　　**Hadronization**

Figure: Steffen Bass
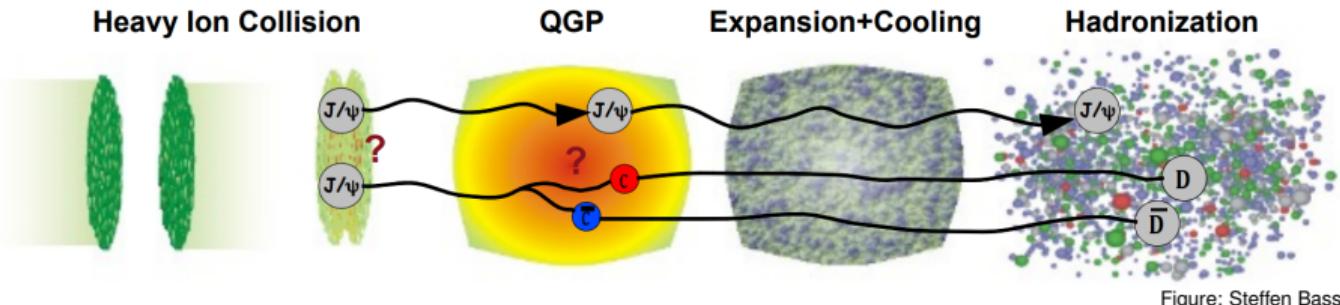
Why heavy quark diffusion?

- direct window into strong in-medium QCD force:

  - Exp. data (v_2, R_{AA}) → considerable collective motion! → $\boxed{\tau_{\text{heavy}} \overset{?}{\approx} \dfrac{1}{T}}$

    ⊘ ALICE (2019) , ⊘ ALICE (2018)

    - Naive hydro: $\boxed{\tau_{\text{heavy}} \simeq \dfrac{M}{T} \tau_{\text{light}}}$ → $\boxed{\tau_{\text{light}} \overset{?}{\ll} \dfrac{1}{T}}$

- input for quarkonium production models　⊘ Brambilla et al. (2021)

- varying results for T-dep. across theoretical models　⊘ Dong, Lee, Rapp (2019)

Calculate τ_{heavy} from first principles?

■ nonrel. limit $\boxed{M \gg \pi T}$ ⇨ 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**
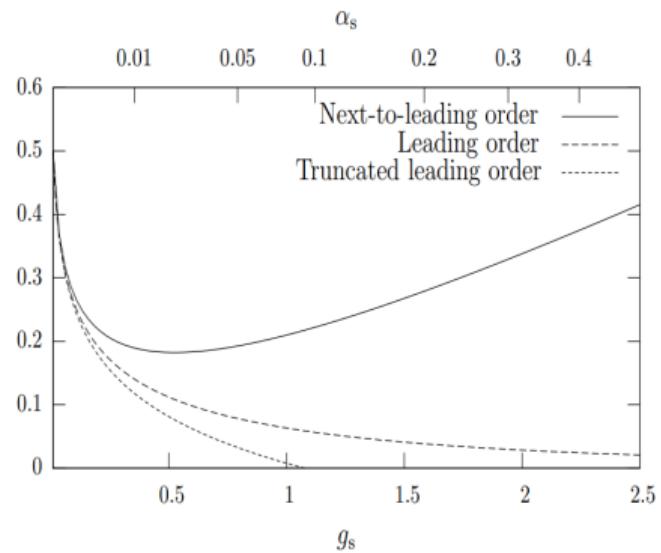
Diffusion coefficients from the lattice?! 🖉 Caron-Huot, Laine, Moore (2009)
🖉 Petreczky, Teaney (2005)

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

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

└─▶ HQ vector current

■ reconstruct from **Euclidean time correlators**:

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

$T > T_c$

$\propto D$

$\frac{\rho(\omega)}{\omega}$

--- finite M

$\omega \ll T^2/M$ $2M$ ω
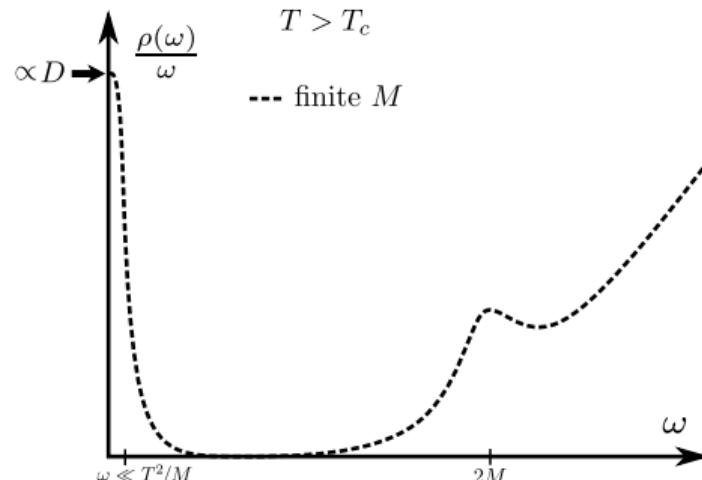
1. instead of D, consider κ
   (encoded in the tail)

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)

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

Diffusion coefficients from the lattice?! [Caron-Huot, Laine, Moore (2009)] [Petreczky, Teaney (2005)]

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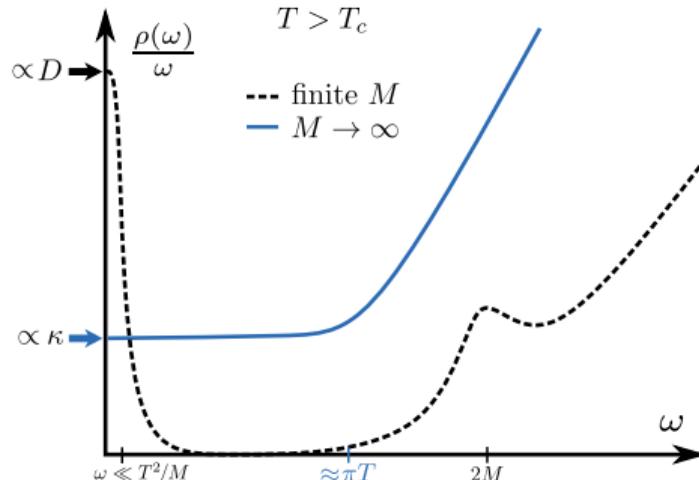
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Gluonic color-electric correlator ⌀ Caron-Huot, Laine, Moore (2009)

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

$\downarrow$

Weak-coupling structure (LO)
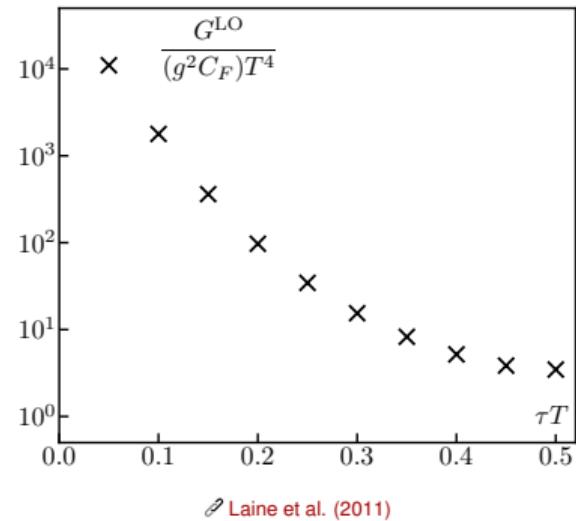
⌀ Laine et al. (2011)

Drawback of $M \to \infty$

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

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

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

$$\downarrow$$
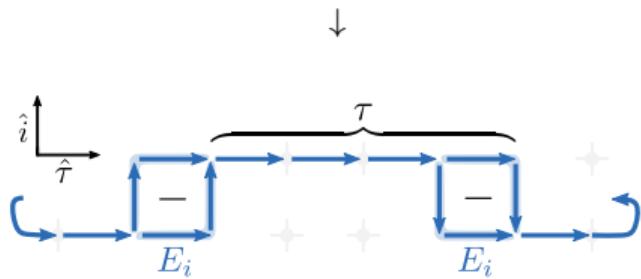
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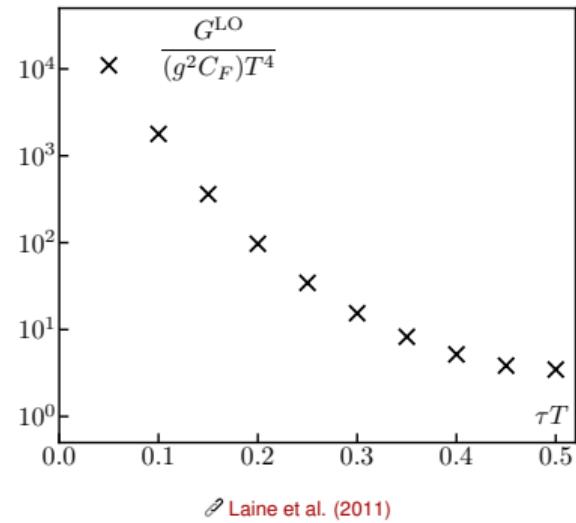
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## Noise reduction via gradient flow 🔗 Lüscher (2010)

- supports nonlocal actions! (e.g. 2+1 flavor HISQ)
- new gaugefield parameter: "flow time" τ_{F}

Flow = smooth regulator:

- links continuously smeared, $\boxed{\text{width} \simeq \sqrt{8\tau_{\mathrm{F}}}}$, "flow radius"

- lattice renorm. artifacts suppressed if $\boxed{\sqrt{8\tau_{\mathrm{F}}} \gtrsim a}$

- $G(\tau)$ free of distortion if $\boxed{\sqrt{8\tau_{\mathrm{F}}} \lesssim \tau/3}$
  (next slide)

Idea:

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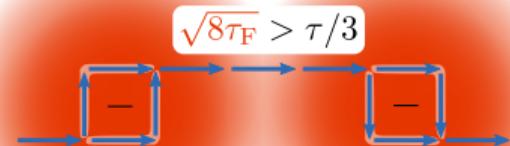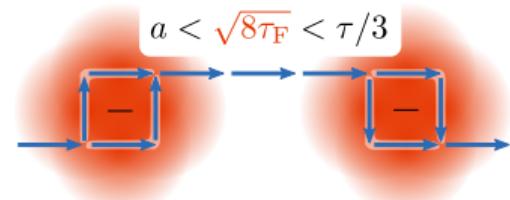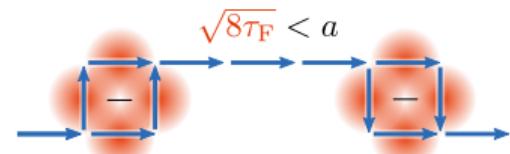
Weak coupling + Wilson flow

$$\frac{G^{\mathrm{LO}}}{(g^2 C_F) T^4}$$

$\sqrt{8\tau_{\mathrm{F}}}\, T =$
- —— 0.00
- – – 0.05
- ⋯⋯ 0.10

τT

Eller, Moore (2018)
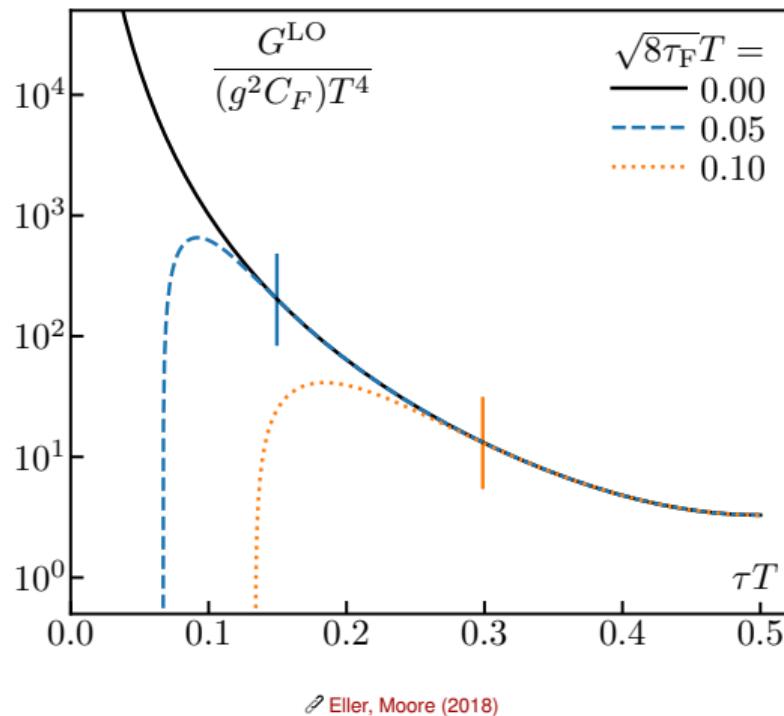
Flow limit = lower bound for τ

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

Enhance nonpert. lattice data:

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

Pure gauge, $1.5\,T_c$, Wilson action
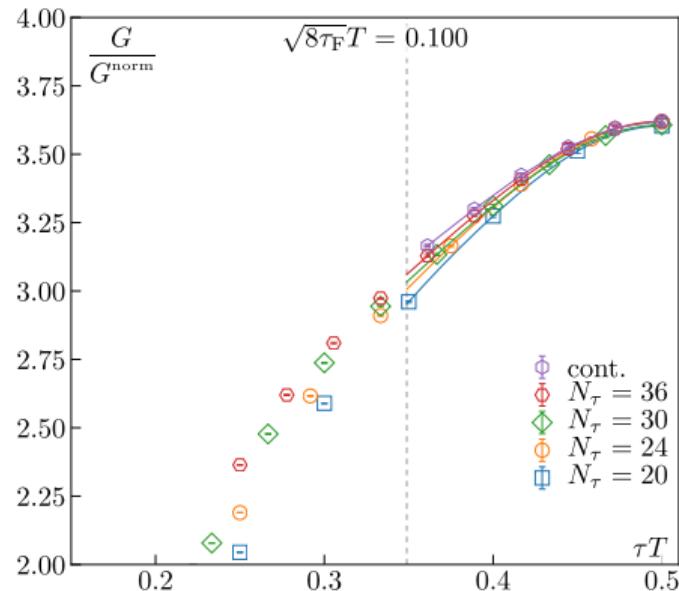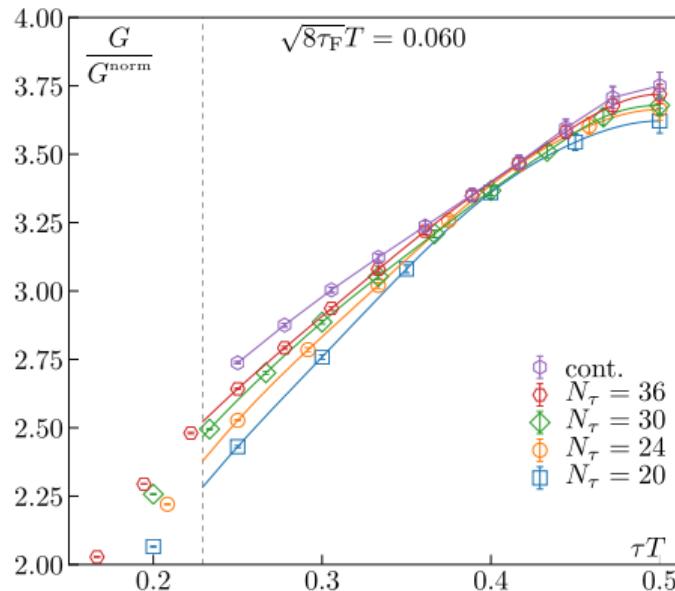
Lattice & flow setup

$N_\sigma^3 \times N_\tau$	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

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

- **1. Continuum extrapolation** (linear in a^2)
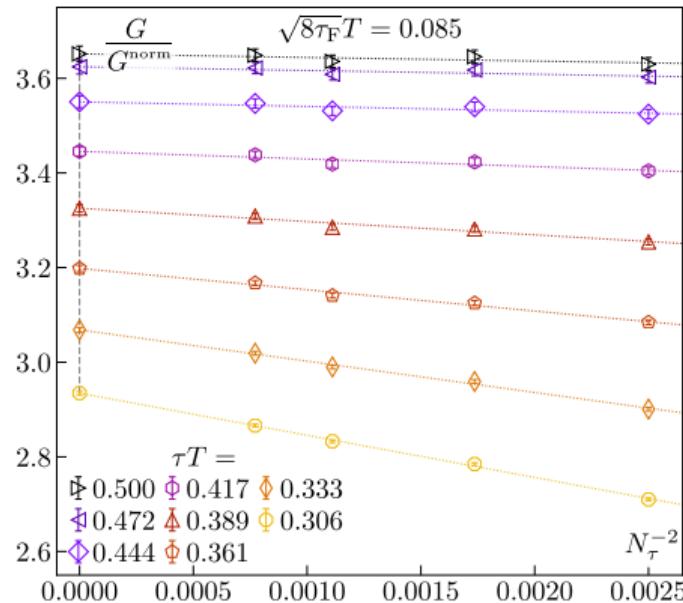
- **2. Flow-time-to-zero extrapolation** (linear in τ_F)
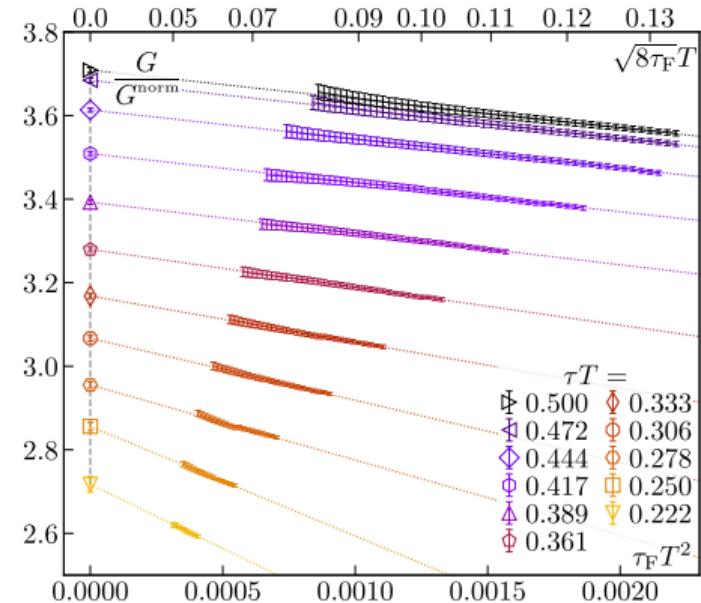
- ansatz from weak-coupling NLO Eller 2021

 LA et al. 2021

Pure gauge, $1.5\,T_c$
$a \to 0, \tau_{\mathrm{F}} \to 0$

$\frac{G}{G^{\mathrm{norm}}}$

τT

Gradient flow method
Multi-level method

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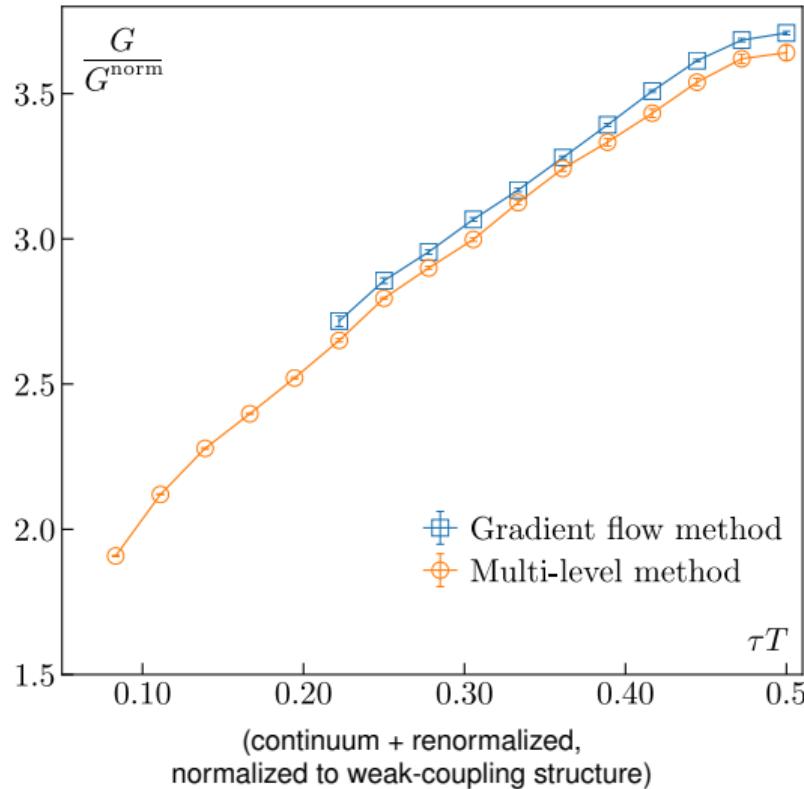
Comparison to previous method

■ 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

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

Strategy: use spectral function models

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

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

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

  ⇨ obtain κ/T^3 by fitting

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

✎ LA et al. 2021
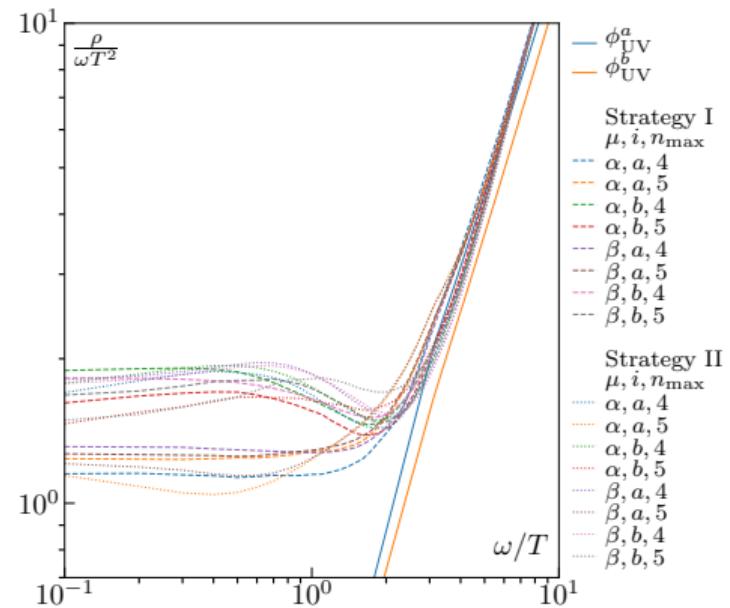
Pure gauge, $1.5 T_c$
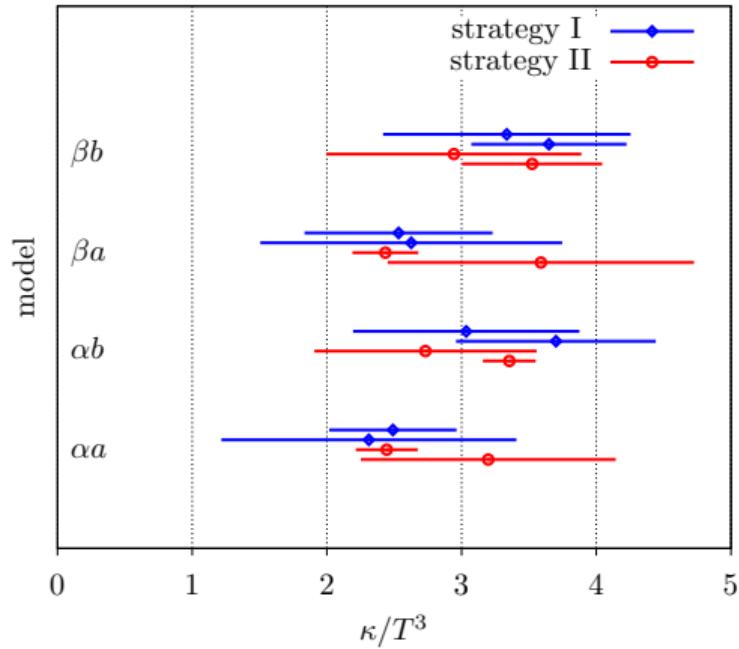
Final estimate:

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

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

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

2+1 flavor QCD, HISQ action

■ $T \approx 200 \ldots 350\,\mathrm{MeV}, \quad m_\pi \approx 310\,\mathrm{MeV}$

■ no $a \to 0$ and $\tau_\mathrm{F} \to 0$ yet

Intermediate strategy

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

⇨ 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	$T\,[\mathrm{MeV}]$	$N_\sigma^3 \times N_\tau$	$a\,[\mathrm{fm}]$
$m_s/5$	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	$64^3 \times 24$	
	$\ldots$		

2 + 1 flavor QCD

Dashed lines: fit with model $\rho(\omega) = \sqrt{[\kappa\omega/2T]^2 + [c\,\phi_{\mathrm{UV}}(\mu)]^2}$, $\mu = \sqrt{[2\pi T]^2 + \omega^2}$

Legend (left plot):

N_τ, $\sqrt{8\tau_{\mathrm{F}}}/\tau$, T

- 36, 0.25, 196 MeV
- 32, 0.25, 220 MeV
- 28, 0.25, 251 MeV
- 24, 0.25, 296 MeV
- 20, 0.25, 352 MeV

$\frac{G}{G^{\mathrm{norm}}}$

Fit $\tau T \geq 0.35$

τT

HotQCD preliminary

Right plot:

κ/T^3

AdS/CFT estimate

$T\,[\mathrm{MeV}]$

HotQCD preliminary
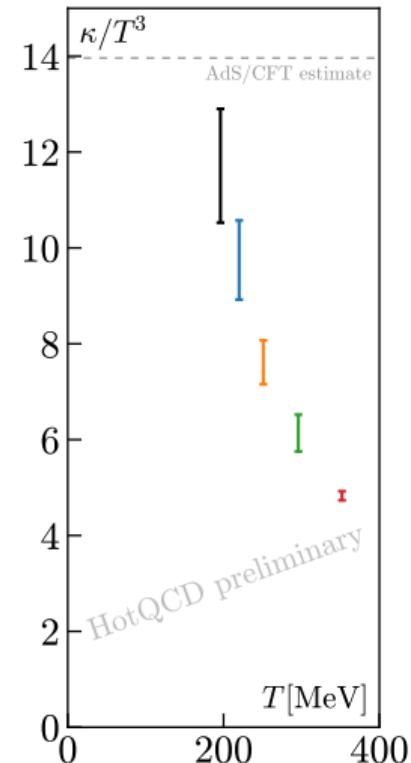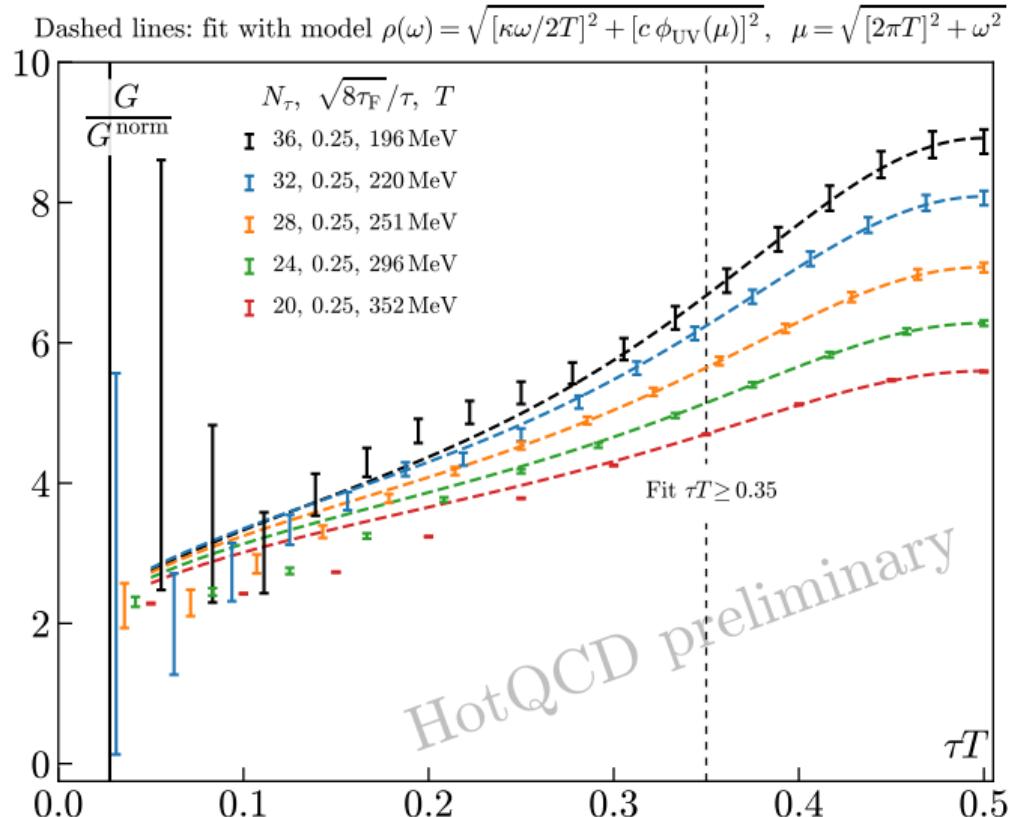
Comparison to other results

- Reminder:
$$\frac{4\pi}{\kappa/T^3} = 2\pi TD \sim \frac{T^2}{M}\tau_{\text{heavy}}$$
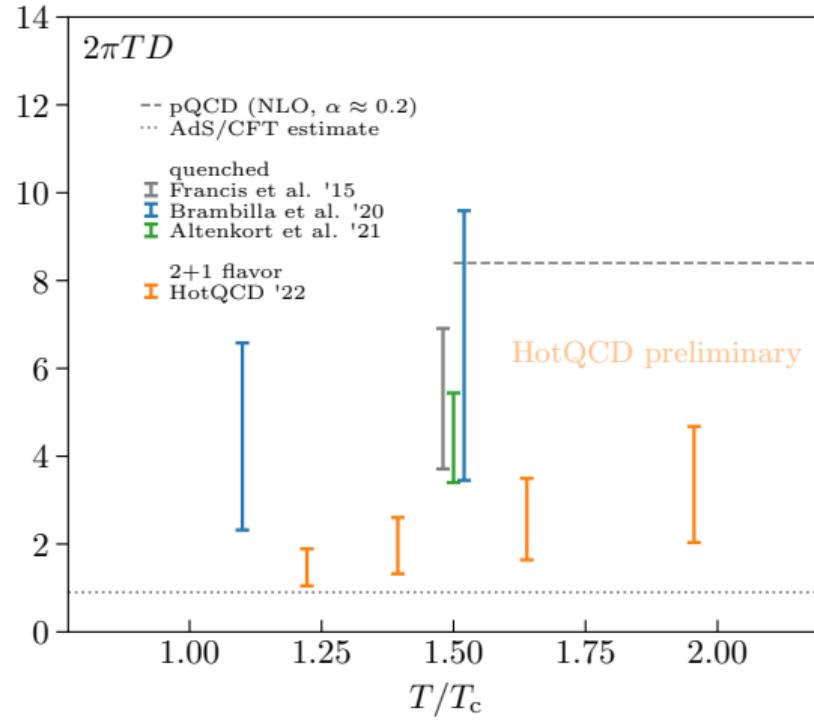
🔗 pQCD: Caron-Huot, Moore (2008)
🔗 AdS/CFT: Casalderrey-Solana, Teaney (2006)

Pure gauge, $1.5\,T_c$: $\mathcal{O}(T/M)$ correction

- $\boxed{\kappa \simeq \kappa_E + \frac{2}{3}\langle \mathbf{v}^2 \rangle \kappa_B}$ 🖉 Bouttefeux, Laine (2020)   🖉 Laine (2021)

  ⇰ color-**magnetic** correlator G_B

- Problem: anomalous dimension
  → logarithm in $G_B(\tau_F)$

- Solution: consider $\boxed{Z_B^2(Z_K^2 Z_f^2 G_B)_{\tau_F \to 0}}$

  → cancel scale-dependence

  → match flow to $\overline{MS}$ scheme

  → $\overline{MS}$ renorm. factor

  ⇰ $\boxed{Z_f^2(\tau_F, g_{\tau_F}^2)}$ obtained by integrating RG
  equation, ($g_{\tau_F}^2$ measured at $T = 0$)

  - expect $Z_K^2 \sim 1$, calculation in progress

$\tau_F \to 0$ for $Z_f^2 G_B$

$\sqrt{8\tau_F}\,T$

preliminary

$\frac{Z_f^2 G_B}{G^{\mathrm{norm}}}$

$\tau T =$

$\tau T =$	
0.500	0.361
0.472	0.333
0.444	0.306
0.417	0.278
0.389	

$\tau_F T^2$
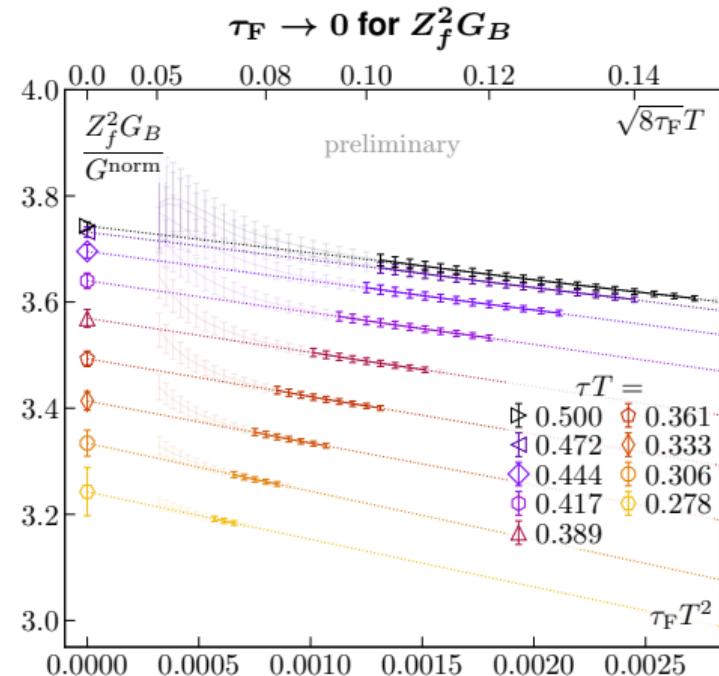
EE vs BB correlator ($a \to 0$, $\tau_F \to 0$)
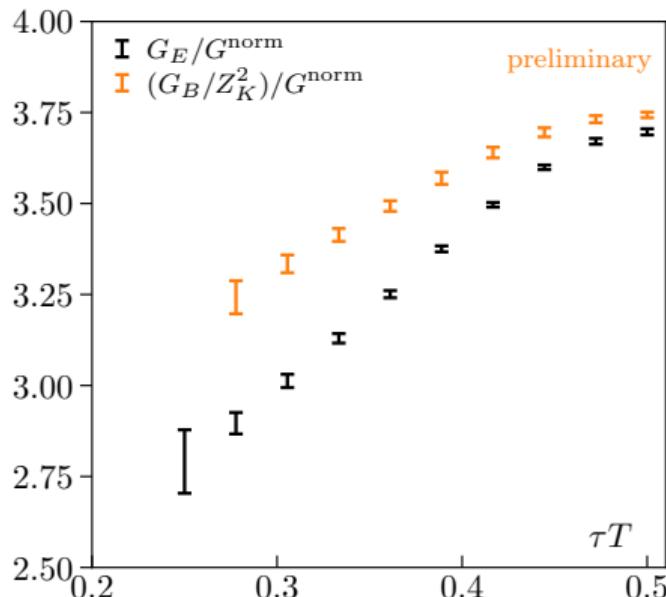
Comparison to other works (pure gauge)
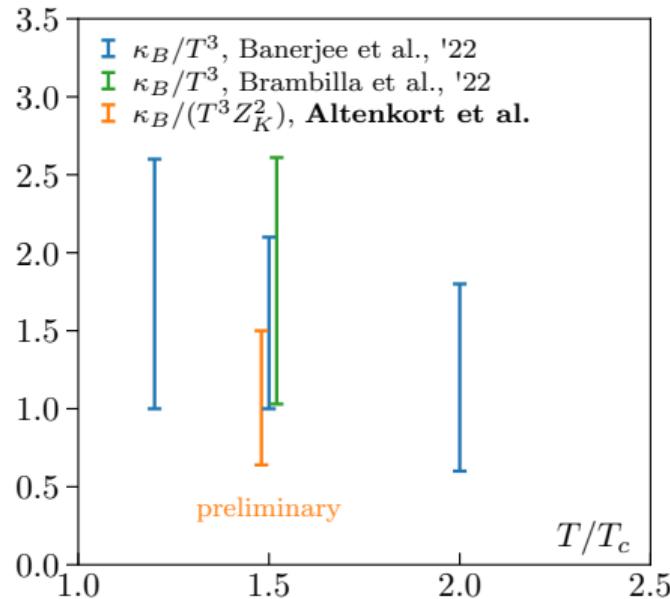
Quenched QCD
- proof-of-concept for gradient flow method ⌖ LA et al. 2021
- results serve as crosscheck for systematics of 2+1 flavor data
- **Next:**
  determine finite-mass correction (color-magnetic correlator) ⌖ Bouttefeux, Laine 2021

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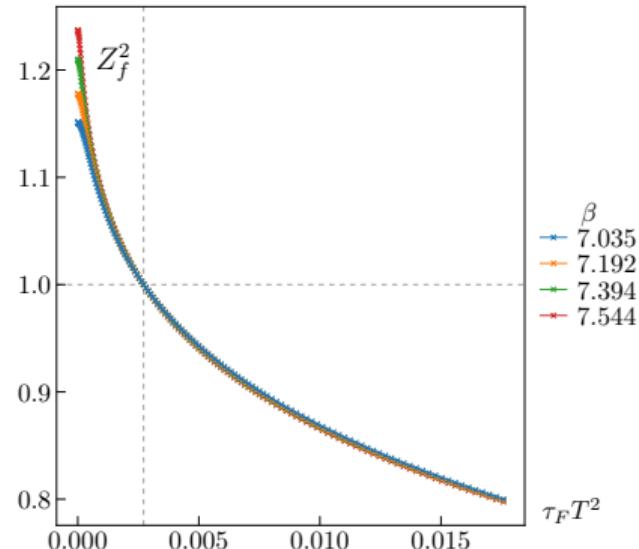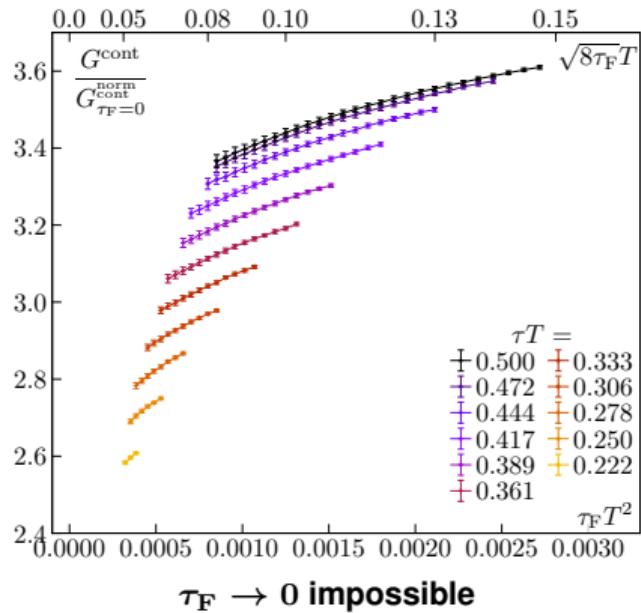
Quenched, $1.5 T_c$:   systematics of simple model fits

Dashed lines: fit with model $\rho(\omega) = \sqrt{[\kappa\omega/2T]^2 + [c\,\phi_{\mathrm{UV}}(\mu)]^2}$, $\mu = \sqrt{[2\pi T]^2 + \omega^2}$
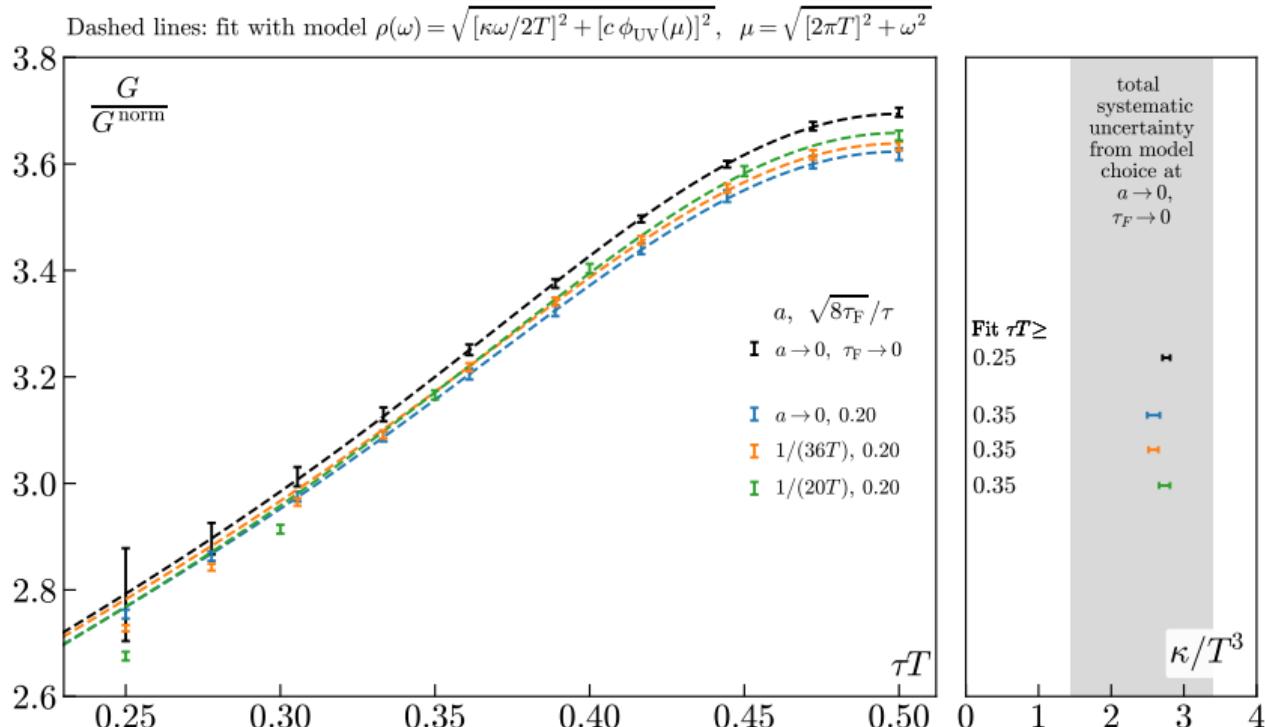
Conclusions

■ 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, $1.5T_c$)
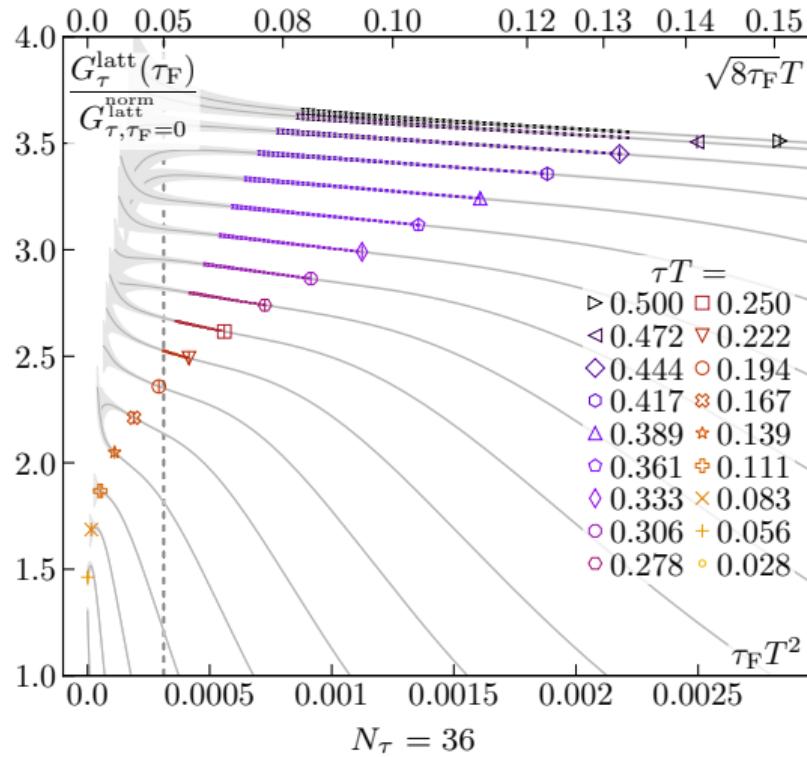
- inside extrapolation window: single colorful data points. outside: data points connected via grey lines.
- markers at $\sqrt{8\tau_F} \approx \tau/3$
- dashed line: minimum flow such that $\sqrt{8\tau_F} \gtrsim a$ for our coarsest lattice
- small τ_F: strong flow dependence (suppress noise and renorm. artifacts)
- intermediate τ_F: minor dependence (for large τ)

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

LO spectral function:

$$\rho_E^{(2)}(\omega, \tau_F) = \frac{g^2 C_R}{6\pi}\omega^3$$

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

$$G_E(\tau, \tau_F) \neq \int\limits_0^\infty \frac{d\omega}{\pi}\rho(\omega, \tau_F)\frac{\cosh\left[\omega(\frac{\beta}{2} - \tau)\right]}{\sinh\left[\frac{\beta\omega}{2}\right]}$$
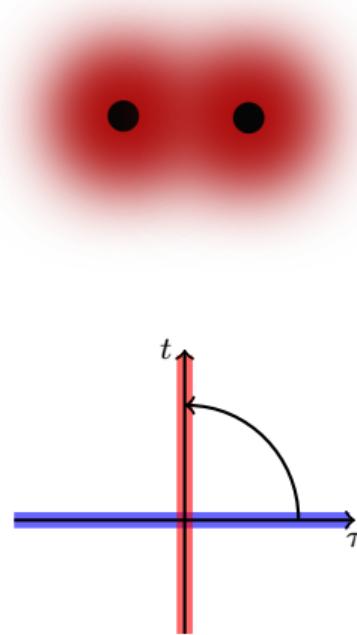
Physical: Contact terms **break causality** of theory

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

Integration kernel effect
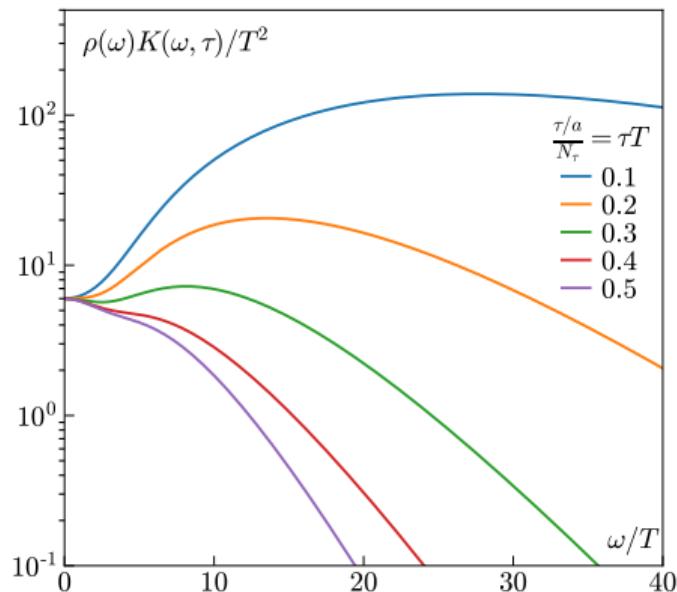
Gradient flow equations

- 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:
  $\Rightarrow$ Formal solution:

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

  $\langle A(\mathbf{k},\omega) \rangle = \frac{i}{\omega + iD\mathbf{k}^2} \langle A(\mathbf{k},t=0) \rangle$

- Approach II, Linear response th.
  Hamiltonian:
  $\Rightarrow$ Formal solution ($\mathcal{O}(h)$):

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

  $\delta\langle A(\mathbf{k},\omega) \rangle = \frac{1}{i\omega} \left[\frac{G_R(\mathbf{k},\omega)}{\chi(\mathbf{k})} - 1 \right] \delta\langle A(\mathbf{k},t=0) \rangle$

- Comparison (for small ω, $|\mathbf{k}|$):

  $\Rightarrow G_R(\mathbf{k},\omega) = \frac{iD\mathbf{k}^2}{\omega + iD\mathbf{k}^2} \chi(\mathbf{k})$

- $\Rightarrow$ **Kubo**-type **formula**

  $\Leftrightarrow D = \frac{1}{\chi_s} \lim\limits_{\omega \to 0} \left[\lim\limits_{k \to 0} \frac{\omega}{k^2} \rho(k,\omega) \right]$

- diffusion physics encoded in **spectral function** $\rho(k,\omega) \sim \int_{\mathbf{x},t} e^{i(\omega t - \mathbf{k}\mathbf{x})} \langle [A(\mathbf{x},t), A(\mathbf{0},0)] \rangle_{\text{eq.}}$

- directly relates **macroscopic <u>non-eq.</u> evolution** and **microscopic <u>in-eq.</u> 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 $A(\mathbf{x})$, $\langle A(\mathbf{x})\rangle_{\mathrm{eq}} = 0$
  - 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:
  $\Rightarrow \partial_t\langle A(\mathbf{x},t)\rangle = D\nabla^2\langle A(\mathbf{x},t)\rangle$

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

- How to identify D here?

Heavy Ion Collision **QGP** **Expansion+Cooling** **Hadronization**
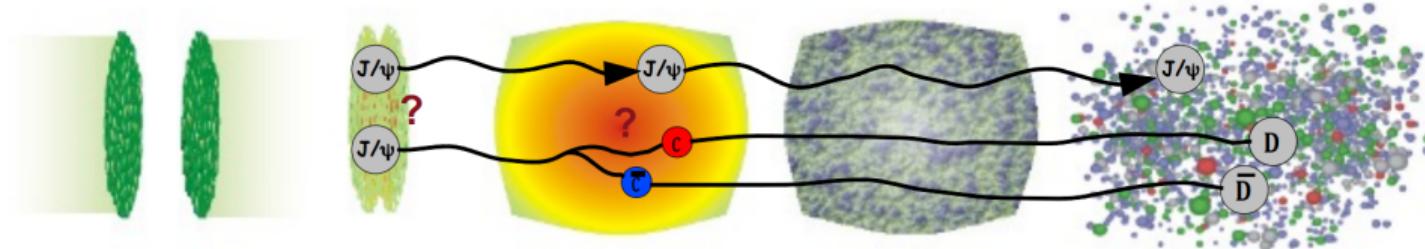
- Heavy quarkonia mainly produced in early hard collisions ($M \gg T$)
  - some remain as bound states (J/Ψ, Υ)
  - some melt into constituents
    - travel through medium, thermalize to some extent via **diffusion**
    - form $D\bar{D}$ or $B\bar{B}$ meson pairs, decay into dileptons
- Evidence of 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	$\mathrm{W\,m^{-1}\,K^{-1}}$
Particle diffusion	Mass	Diffusion coefficient	$\mathrm{m^2\,s^{-1}}$
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