UNIVERSITÄT BIELEFELD
Faculty of Physics

CRC-TR 211
Strong-interaction matter under extreme conditions

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DFG Deutsche Forschungsgemeinschaft
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Lattice QCD results for the heavy quark diffusion coefficient

How fast do heavy quarks thermalize in the QGP?

1. Precise calculation in quenched QCD at $1.5\,T_c$ 10.1103/PhysRevD.103.014511 (2021)

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

2. First impressions from $2+1$ flavor QCD

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

Luis Altenkort
Bielefeld University

June 15, 2022
SQM2022

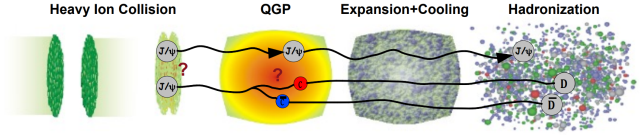


Figure: Steffen Bass, mod. by O. Kaczmarek

What does heavy quark diffusion tell us about the QGP?

- Hydrodynamics → 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)! → $\tau_{\text{kin}}^{\text{heavy}} \overset{?}{\approx} \frac{1}{T}$ → $\tau_{\text{kin}}^{\text{light}} \overset{?}{\ll} \frac{1}{T}$
- Knowledge of $\tau_{\text{kin}}^{\text{heavy}}$ essential to understand collisional energy loss and explain exp. data
- Crucial input for quarkonium production models

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

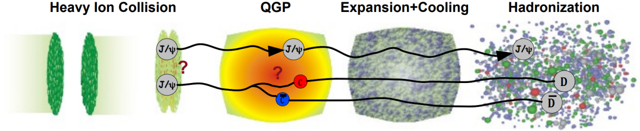
- Consider non-relativistic limit $M \gg T$
  → Langevin dynamics Moore, Teaney (2005)

$$(\tau_{\text{kin}}^{\text{heavy}})^{-1} = \frac{\kappa}{2MT}$$

$$D = 2T^2/\kappa$$

- **Problem:**
  perturbative series for D or κ ill-behaved!
  Caron-Huot, Moore (2008)

  → **nonperturbative first-principles** approach: **lattice QCD**



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How to calculate diffusion coefficients from the lattice?

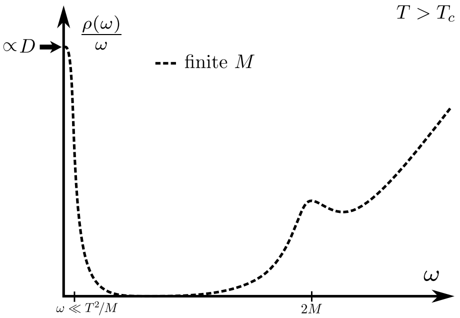
Petreczky, Teaney (2005) Caron-Huot, Laine, Moore (2009)

- Linear response theory: diffusion physics ⇔ low-energy **in-equilibrium spectral functions** (SPF)
- SPF of HQ vector current:

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

- reconstruct from **Euclidean correlation functions**:

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



- fluct.-dissipation: consider Kubo-formula for **momentum diffusion coeff.** κ instead of D
- utilize **HQET**: HQ mass $M \to \infty$, expansion in $1/M$, replace $\hat{\mathcal{J}}^i$ with LO versions

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

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

⇒ smooth $\omega \to 0$ limit expected: **no transport peak** (much easier to reconstruct)

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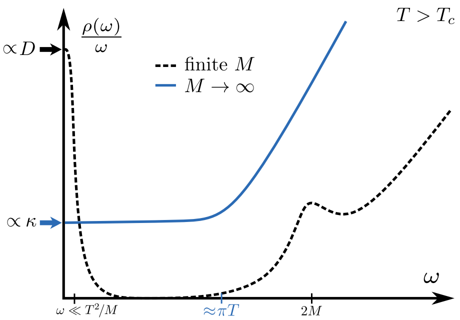

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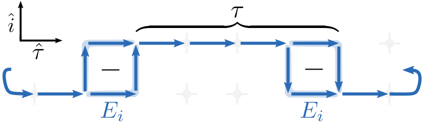
Gluonic color-electric correlator

Caron-Huot, Laine, Moore (2009)

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

$$= \int_0^\infty \mathrm{d}\omega\, \boldsymbol{\rho}(\omega) \underbrace{\frac{\cosh\left(\omega(\tau-\frac{\beta}{2})\right)}{\sinh\left(\omega\frac{\beta}{2}\right)}}_{K(\omega,\tau)}, \qquad \boldsymbol{\kappa} = \lim_{\omega\to 0} 2T\frac{\boldsymbol{\rho}(\omega)}{\omega}$$

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



The drawback of the $M\to\infty$ limit

- $G(\tau)$ is purely gluonic
  - ⇛ UV gauge fluctuations dominate for large τ
- $K(\omega,\tau)$: large τ are most sensitive to $\omega\to 0$
  - ⇛ need noise reduction method

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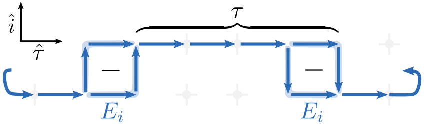

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Solution to gauge noise problem: gradient flow Lüscher 2010

- applicable to nonlocal actions (e.g. 2+1 flavor QCD)
- 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”

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

On the lattice:

- links replaced by well-defined local averages ⇒ noise suppression
- suppression of renormalization artifacts
- ...but contact terms contaminate $G(\tau)$ for $\sqrt{8\tau_\mathrm{F}} \gtrsim \tau/3$ (LO pert. theory Eller, Moore 2018)

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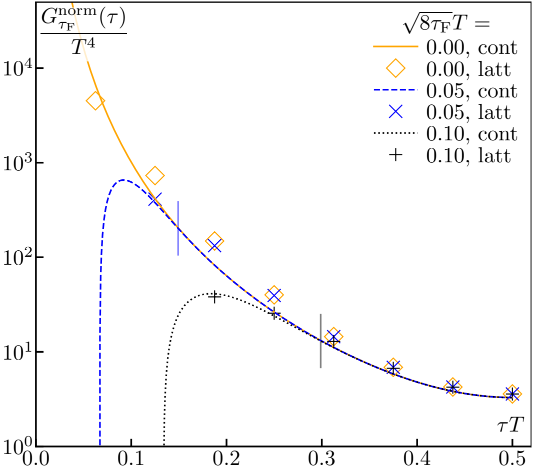
LO perturbative EE correlator (Wilson flow)



continuum corr. from Eller, Moore 2018,
lattice corr. from Eller, Moore, LA et al. 2021

Flow limit = lower bound for τ

- cont. correlator deviates $< 1\%$ for $\tau \gtrsim 3\sqrt{8\tau_F}$ (vertical lines)

Use to enhance nonpert. lattice results:

- get rid of log-scale by normalizing to this
- comparison of LO cont. and LO latt. correlators
  - → remove tree-level discretization errors

Measurement & double-extrapolation

- Measure correlator, integrate flow equation, repeat. . .
- $a \to 0$ extrapolation at each flow time τ_{F}, then $\tau_{\mathrm{F}} \to 0$ at each separation τ
  - for details see backup or LA et al. 2021

Result & comparison

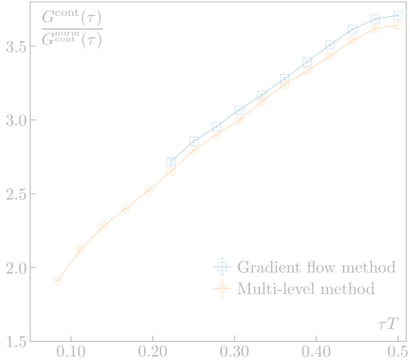
- double-extrapolated EE correlator
- shape consistent with Multi-level results (only pert. renormalized)
  Francis et al. 2015 , Christensen, Laine 2016
- Overall shift due to...
  - nonperturbative renormalization
  - better statistics
  - systematic uncertainty introduced by flow extr.
- Note: only large-τ correlator can be obtained

Lattice setup (quenched, $1.5T_c$)

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

Renormalized continuum EE correlator (quenched, $1.5T_c$)



LA et al. 2021

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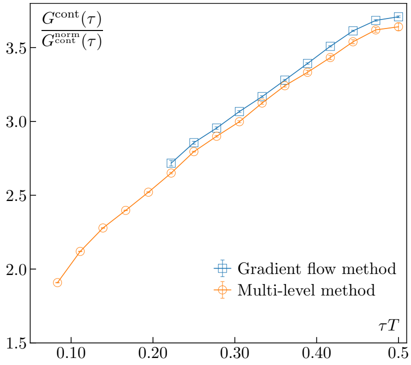


LA et al. 2021

Spectral reconstruction through model fits

Integral inversion problem:

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

Strategy:

- constrain $\boldsymbol{\rho}(\omega)$ using IR and UV **asymptotics**:

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

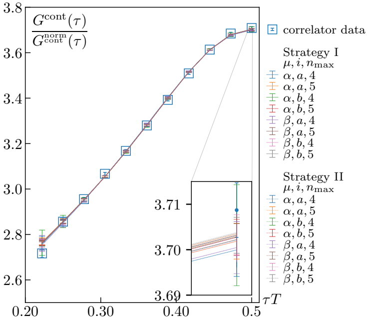
  and various **interpolations** $I(w)$:

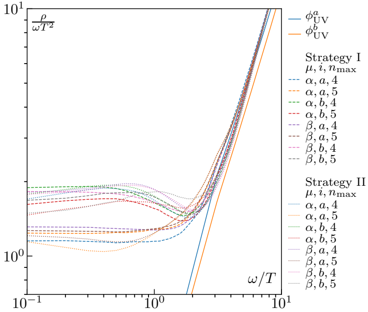
  ⇒ $\rho_{\mathrm{model}}(\omega) \equiv I(\omega)\sqrt{[\phi_{\mathrm{IR}}(\omega)]^2 + [\phi_{\mathrm{UV}}(\omega)]^2}$

⇒ **well-defined fit** with parameters $\boldsymbol{\kappa}/T^3$ and c_n via

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

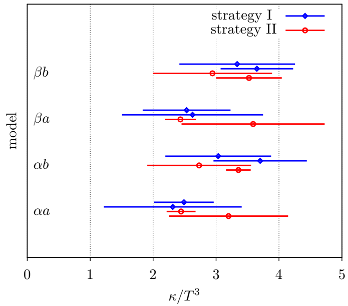
- for details see LA et al. 2021





LA et al. 2021

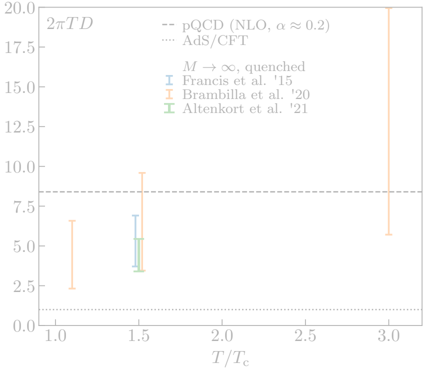
HQ momentum diffusion coefficient
(quenched, $1.5T_c$)



- We find $\boldsymbol{\kappa}/T^3 = 2.31 \ldots 3.70$
  - agrees with previous studies
    e.g. Francis et al. 2015 (multi-level method + pert. renorm.)
- convert via $2\pi TD = \dfrac{4\pi}{\boldsymbol{\kappa}/T^3}$: $2\pi TD = 3.40 \ldots 5.44$
- kinetic equilibration time:

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

Comparison to previous studies



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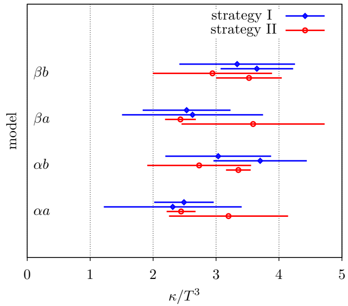

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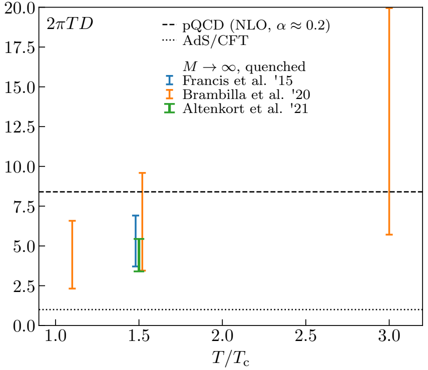


LA et al. 2021

Setup & strategy for $2+1$ flavor QCD

Lattice setup (in progress)

- $2+1$ flavor HISQ fermions
- physical m_s, with $m_l = m_s/5$ $(m_\pi \approx 320\,\mathrm{MeV})$

T [MeV]	$N_\sigma^3 \times N_\tau$	a [fm]
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

+ three temp. $\leq 195\,\mathrm{MeV}$ with **physical masses** $(64^3 \times 24)$

Current situation

- no continuum and flow-time-to-zero extrapolation

However:

- long-distance correlator insensitive to finite (a, τ_F)
- to keep flow corrections small, use τ_F relative to each τ:

$$\frac{\sqrt{8\tau_F}}{\tau} = \text{const.} < \frac{1}{3}$$

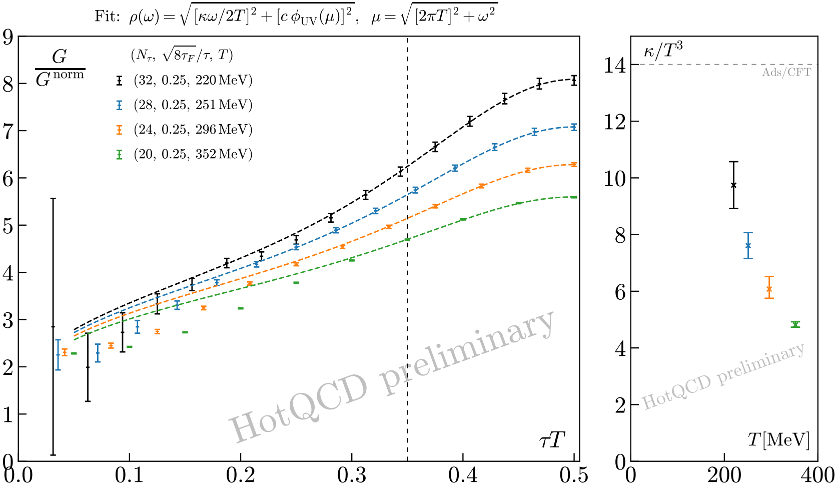
⇒ quenched data suggests that's enough to constrain κ! (see backup)

So, in the meantime:

- treat finite (a, τ_F) as systematic uncertainties
- use quenched data to estimate additional systematic error

$2+1$ flavor: simple model fits at finite a and τ_F

- Fit range: $\tau T \geq 0.35$ (dashed vertical line)



Lattice setup

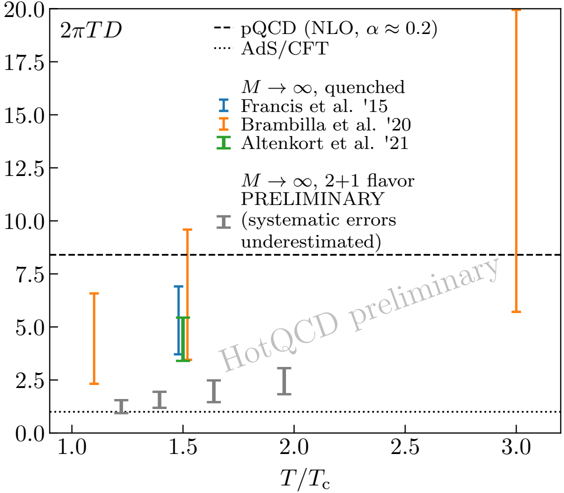
T [MeV]	$N_\sigma^3 \times N_\tau$	a [fm]	#
220	$96^3 \times 32$	0.028	1700
251	$96^3 \times 28$	0.028	1600
296	$96^3 \times 24$	0.028	1375
352	$96^3 \times 20$	0.028	4600

- $2+1$ flavor HISQ fermions
- $m_l = m_s/5$ (pion mass ≈ 320 MeV)

First impressions

- much larger κ/T^3 compared to quenched ($\sim 2\times$)
- κ/T^3 seems to decrease with increasing T

Comparison of first impressions from 2+1 flavor QCD



- preliminary: systematic errors underestimated (first impressions from a few simple model fits)
- Reminder: $2\pi TD = \dfrac{4\pi}{\kappa/T^3} \propto \tau_{\text{kin}} \dfrac{T^2}{M}$

Recap

What do we want?

- a first-principles nonpert. estimate from full QCD for the **HQ momentum diffusion coefficient** κ (or in turn D, τ_{kin})

Why?

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

What did we achieve so far?

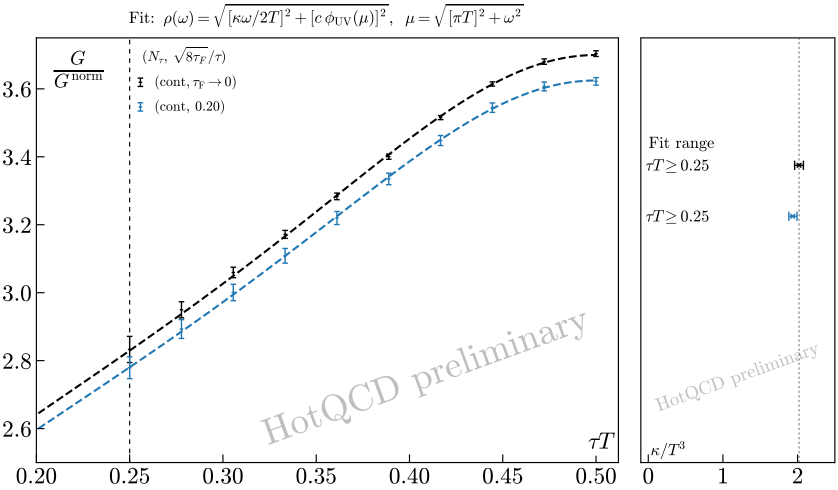
- quenched QCD
  - proof-of-concept for gradient flow method LA et al. 2021 with consistent results for κ
  - $(a, \tau_F) \to 0$ data serves as benchmark for systematics of finite (a, τ_F) data
- 2+1 flavor QCD
  - preliminary explorations to constrain κ

What to do next?

- 2+1 flavor QCD
  - increase statistics, add lattice spacings, study quark mass effects
  - estimate systematic errors
- determine finite-mass correction (color-magnetic correlator) Bouttefeux, Laine 2021

Backup

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



Conclusions

- shape of correlator preserved at fixed small $\sqrt{8\tau_F}/\tau$

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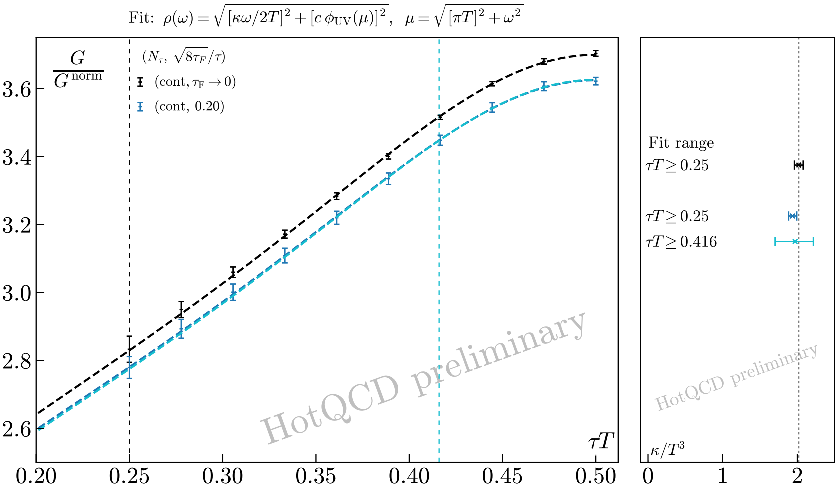

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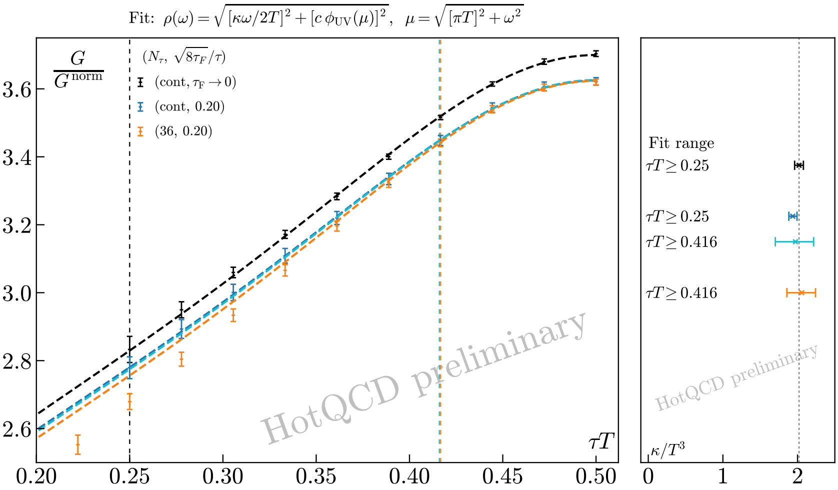

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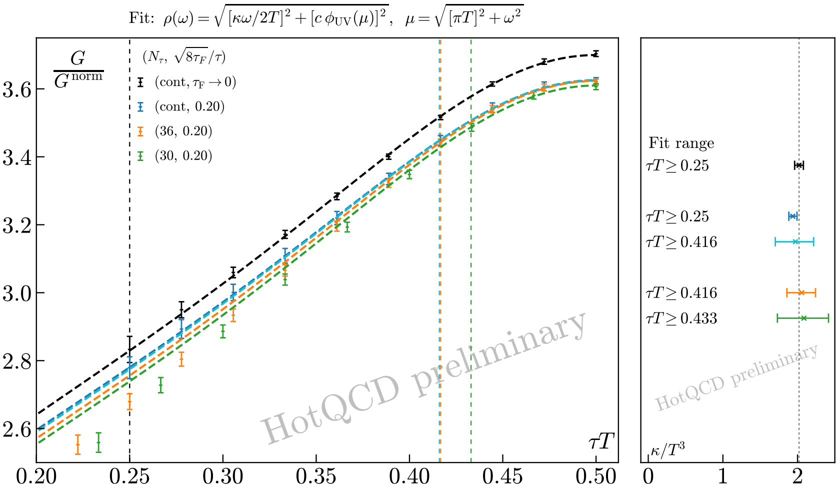

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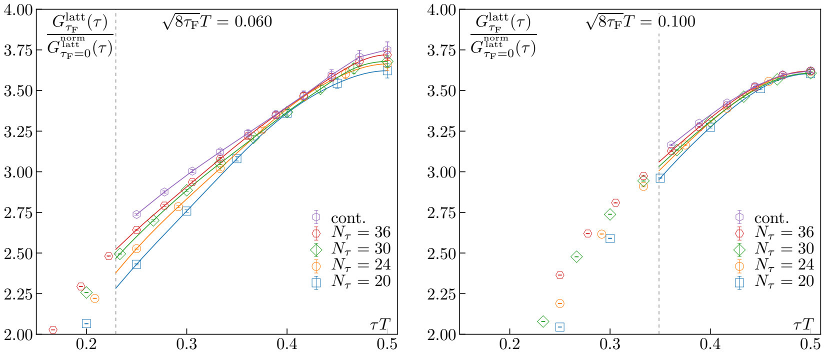
$80^3 \times 20$	0.0213
$96^3 \times 24$	0.0176
$120^3 \times 30$	0.0139
$144^3 \times 36$	0.0116

- 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

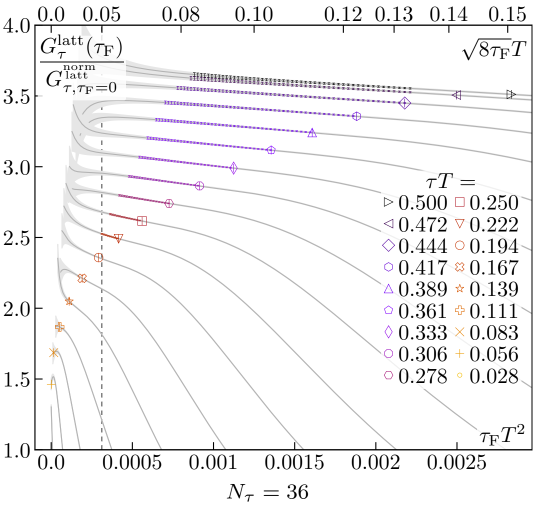
Nonpert. EE correlator (normalized to pert.)



- dashed lines at $\tau \approx 3\sqrt{8\tau_F}$
- → more flow = higher precision, but smaller window of noncontaminated data
- interpolation in τ through cubic splines (no smoothing)

LA et al. 2021

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)

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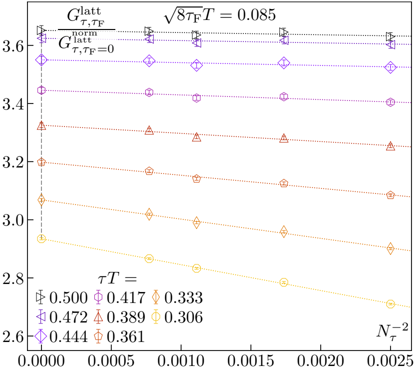
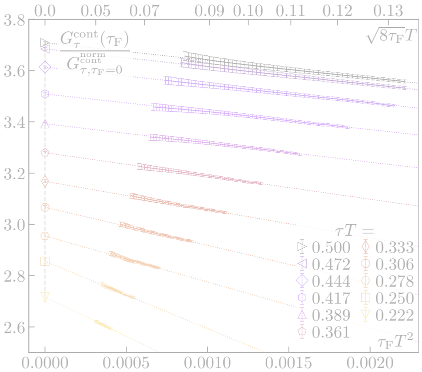
(Quenched, $1.5T_c$)

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



- ansatz motivated by gauge action discretization
- taken separately for each flow time
- take continuum limit first to control a^2/τ_F-type corrections

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



- ansatz motivated by NLO pert. theory Eller 2021
- flow time window depends on:
  - signal-to-noise
  - $\sqrt{8\tau_F} \gtrsim a$ (suppression of latt. artifacts)
  - $\sqrt{8\tau_F} \lesssim \tau/3$ (flow limit)

LA et al. 2021

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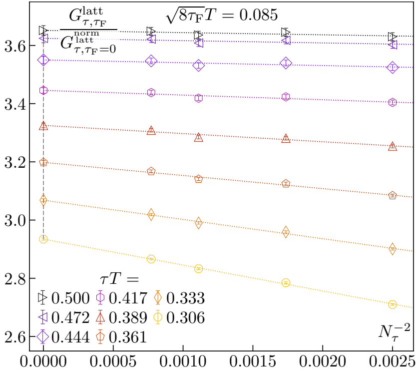

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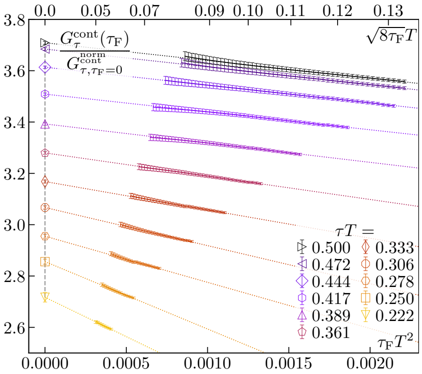

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LA et al. 2021