

# Lattice calculations of the heavy quark diffusion coefficient in quenched QCD

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Viljami Leino  
Helmholtz Institute Mainz, JGU Mainz

Based on:

Nora Brambilla, V.L., Peter Petreczky, Antonio Vairo: PRD. 102 (2020) [hep-lat/2007.10078]  
Nora Brambilla, V.L., Julian Mayer-Stedte, Peter Petreczky: hep-lat/2206.02861

Heavy Flavor Production in Heavy-Ion and Elementary Collisions  
INT, Seattle  
24.10.2022

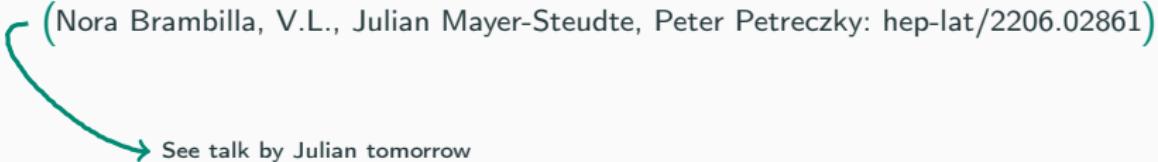
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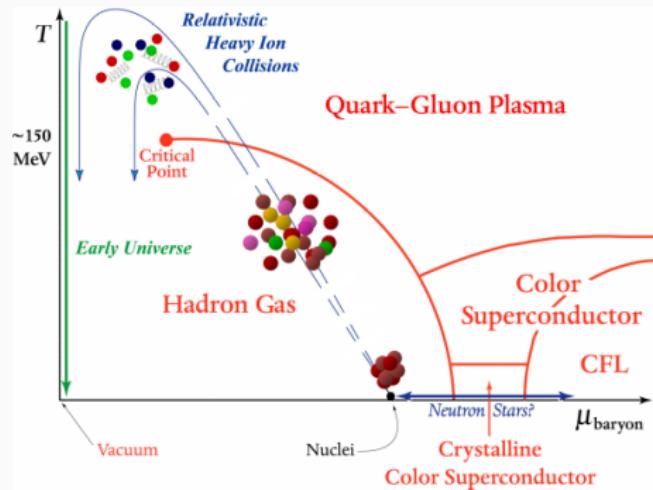
# Outline

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- Introduction
- Diffusion in strongly coupled plasma
  - Heavy Quarks
  - Heavy Quarkonium
- Lattice basics
- Measurements
- Results
- Conclusions

# Introduction: QCD and QGP

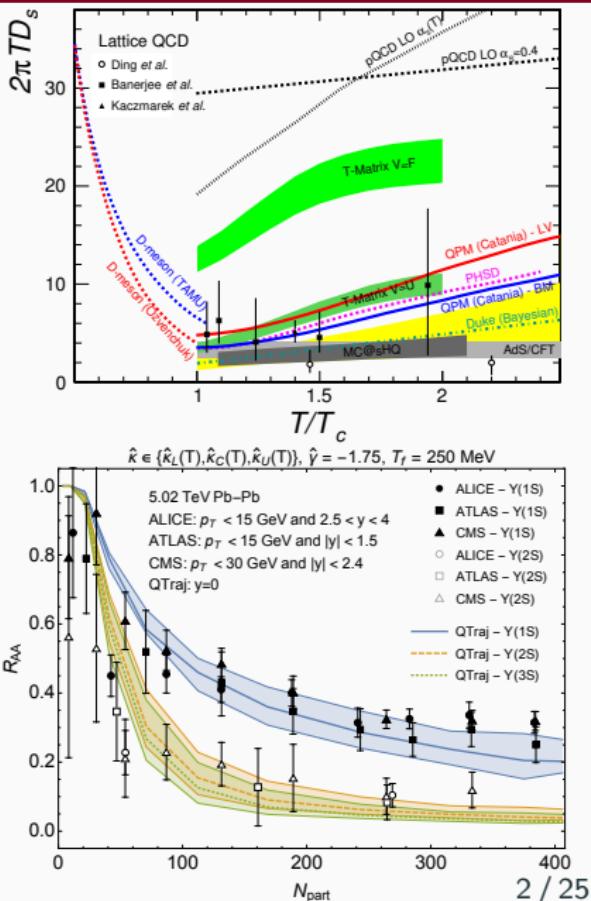
- We aim to understand the strongly coupled Quark Gluon Plasma (QGP)
- QGP generated at particle accelerators such as LHC/RHIC



- The QGP can be described in terms of transport coefficients
- In this talk we focus on the heavy quark momentum diffusion coefficient  $\kappa$

# Motivation: diffusion coefficient

- Nuclear modification factor  $R_{AA}$  and elliptic flow  $v_2$  described by spatial diffusion coefficient  $D_x$
- Multiple theoretical models predicting wide range of values
- Non-perturbative lattice simulations needed
- $\kappa(\gamma)$  dominant source of variation in  $R_{AA}$  in some models



# Heavy Quark in medium

- Heavy quark energy changes only little when colliding with medium

$$E_k \sim T, \quad p \sim \sqrt{MT} \gg T$$

- HQ momentum is changed by random kicks from the medium  
→ Brownian motion; Follows Langevin dynamics

$$\frac{dp_i}{dt} = -\frac{\kappa}{2MT} p_i + \xi_i(t), \quad \langle \xi(t) \xi(t') \rangle = \kappa \delta(t - t')$$

- Heavy quark momentum diffusion coefficient  $\kappa$  related also to:

Spatial diffusion coefficient  $D_s = 2T^2/\kappa$ ,

Drag coefficient  $\eta_D = \kappa/(2MT)$ ,

Heavy quark relaxation time  $\tau_Q = \eta_D^{-1}$

- Considering full Lorentz force:

$$F(t) = \dot{p} = q(E + v \times B)(t)$$

- $\langle v^2 \rangle \sim \mathcal{O}(\frac{T}{M})$  correction to HQ momentum diffusion

$$\kappa_{\text{tot}} \simeq \kappa_E + \frac{2}{3} \langle v^2 \rangle \kappa_B$$

## Quarkonium in medium

- Quarkonium in QGP (environment energy scale  $\pi T$ )

$$M \gg \frac{1}{a_0} \gg \pi T \gg E, \quad \tau_R \gg \tau_E \sim 1/\pi$$

- HQ mass  $M$ , Bohr radius  $a_0$ , binding energy  $E$ , correlation time  $\tau_E$
- Quarkonium in fireball can be described by Limbland equation

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_{n,m} h_{nm} \left( L_i^n \rho L_i^{m\dagger} - \frac{1}{2} \{ L_i^{m\dagger} L_i^n, \rho \} \right)$$

- All terms depend on two free parameters  $\kappa$  and  $\gamma$
- Described by adjoint correlator
- $\kappa$  turns out to be the heavy quark diffusion coefficient and related to thermal width  $\Gamma(1S) = 3a_0^2\kappa$
- $\gamma$  is correction to the heavy quark-antiquark potential and related to mass shift  $\delta M(1S) = 2a_0^2\gamma/3$
- Unquenched lattice measurements of  $\Gamma(1S)$  and  $\delta M(1S)$  available

## $\kappa$ from perturbation theory

- From kinetic theory we can derive

$$\kappa^{\text{LO}} = \frac{g^4 C_F}{12\pi^3} \int_0^\infty q^2 dq \int_0^{2q} \frac{p^3 dp}{(p^2 + \Pi_{00}^2)^2} \times N_c n_B(q)(1 + n_B(q)) \left( 2 - \frac{p^2}{q^2} + \frac{p^4}{4q^4} \right)$$

- Solution depends on assumptions

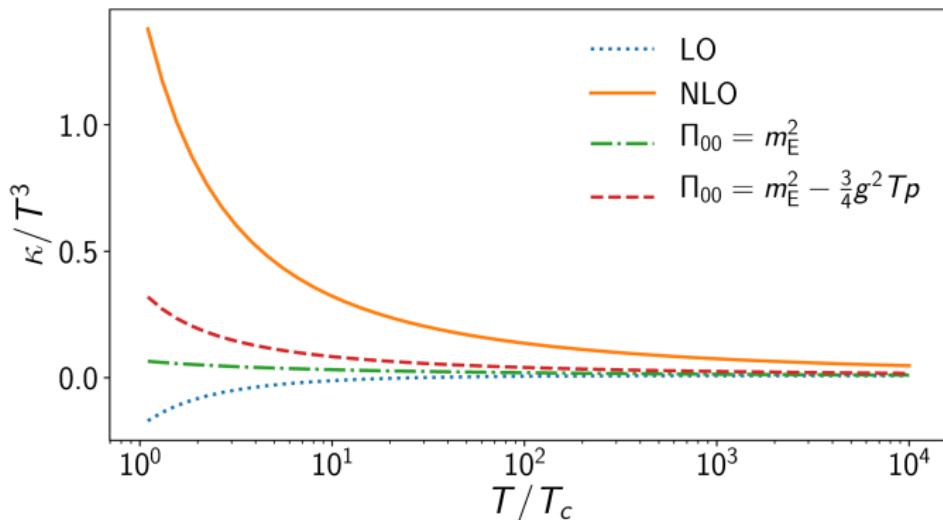
- Is  $m_E \ll T$
- How to expand the temporal gluon self-energy  $\Pi_{00} \simeq m_E$

- Alternatively from Kubo formula:

$$\frac{\kappa}{T^3} = \frac{g^4 C_F N_c}{18\pi} \left[ \left( \ln \frac{2T}{m_E} + \xi \right) + \frac{m_E}{T} C \right], \quad \xi \simeq -0.64718$$

- Truncated LO:  $C = 0$ , NLO:  $C \simeq 2.3302$
- $N_f = 0$  assumed here

## $\kappa$ from perturbation theory



- Clearly  $m_E \ll T$  is too strict assumption on small  $T$
- Huge perturbative variation  
⇒ needs non-perturbative measurements
- Also huge scale dependence through  $m_E = g(\mu)T$
- Here we have scale from NLO EQCD  $\mu \sim 2\pi T$

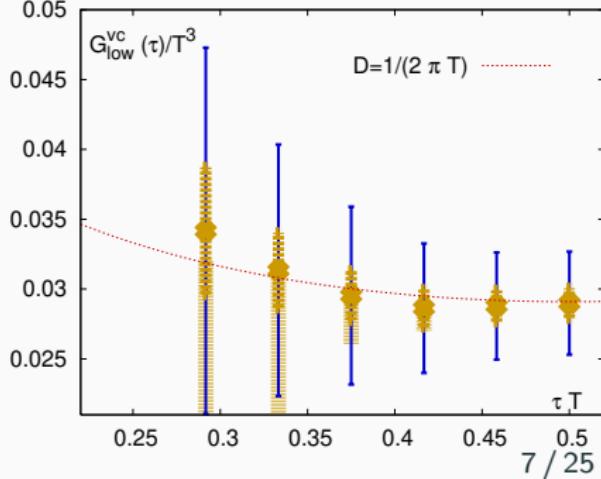
# Current-Current correlator

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

- Above spectral function with heavy quark current correlator  $\mathcal{J} = \bar{Q}\gamma^i Q$  has a pole at  $\omega = -iD_x k^2$ . Solving the pole position leads to Kubo formula with susceptibility  $\chi$ :

$$D_x = \frac{1}{3\chi^{00}} \lim_{\omega \rightarrow \infty} \sum_{i=1}^3 \frac{\rho_V^{ii}(\omega)}{\omega}, \quad \chi^{00} = \beta \int dx^3 \left\langle \frac{1}{2} [\mathcal{J}^0(t, 0), \mathcal{J}^0(0, 0)] \right\rangle$$

- Very narrow transport peak at zero
- Heavier quark  $\Rightarrow$  narrower peak
- Very weak signal insensitive to  $D$   
(Petreczky and Teaney PRD 73 (2006),  
Petreczky EPJC62 (2008))
- Better approach:  
Integrate out heavy quarks



# Heavy Quark limit

- In the  $M \rightarrow \infty$  limit we can define:

$$\kappa = \frac{1}{3T\chi} \sum_{i=1}^3 \lim_{\omega \rightarrow 0} \left[ \lim_{M \rightarrow \infty} \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} \int d^3x \left\langle \frac{1}{2} \left\{ \mathcal{F}^i(t, x), \mathcal{F}^i(0, 0) \right\} \right\rangle \right]$$

- Where  $\mathcal{F} = M \frac{\hat{\mathcal{J}}^i(0, 0)}{dt}$  and  $\hat{\mathcal{J}}^i(x) = \bar{\psi}(x)\gamma^\mu\psi(x)$  is the heavy quark current
- The heavy quark force in static limit:

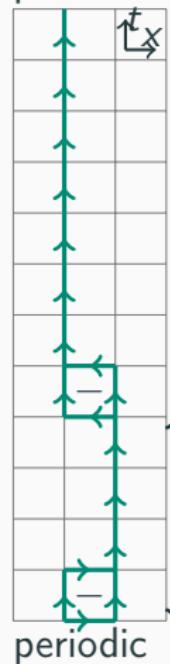
$$M \frac{d\hat{\mathcal{J}}^i}{dt} = \left\{ \phi^\dagger E^i \phi - \theta^\dagger E^i \theta \right\} + \phi^\dagger \left\{ \frac{[D^i, D^2 + \sigma \cdot B]}{2M} + \dots \right\} \phi$$

- Where  $\phi, \theta$  are HQ and H $\bar{Q}$  operators,  $E^i$  chromoelectric field
- Now the euclidean correlator is defined as:

$$\kappa = \sum_{i=1}^3 \lim_{M \rightarrow \infty} \frac{\beta}{3\chi} \int dt dx^3 \left\langle \frac{1}{2} \left\{ [\phi^\dagger g E^i \phi - \theta^\dagger g E^i \theta](t, x), [\phi^\dagger g E^i \phi - \theta^\dagger g E^i \theta](0, 0) \right\} \right\rangle$$

# Euclidean correlator

periodic



- Switch to Euclidean electric fields  $G_E =$

$$-\frac{1}{3T\chi} \sum_{i=1}^3 \lim_{M \rightarrow \infty} \int d^3x \left\langle [\phi^\dagger gE_i \phi - \theta^\dagger gE_i \theta] (\tau, x) [\phi^\dagger gE_i \phi - \theta^\dagger gE_i \theta] (0, 0) \right\rangle$$

- After simplifying the propagators of  $\phi$  and  $\theta$  in  $M \rightarrow \infty$ :

$$G_E(\tau) = -\frac{1}{3} \sum_{i=1}^3 \frac{\langle \text{Re Tr } [U(\beta, \tau) gE_i(\tau, 0) U(\tau, 0) gE_i(0, 0)] \rangle}{\langle \text{Re Tr } [U(\beta, 0)] \rangle}$$

$$G_B(\tau) = \sum_{i=1}^3 \frac{\langle \text{Re Tr } [U(1/T, \tau) B_i(\tau, 0) U(\tau, 0) B_i(0, 0)] \rangle}{3 \langle \text{Re Tr } U(1/T, 0) \rangle}$$

- Free of transport peak at zero
- Field strength tensor components need discretization
- Choose corner discretization for this study
- On lattice there is a self-energy contribution that generates a multiplicative renormalization

## Connecting $G_E$ to $\kappa$

$$G_E(\tau) = \int_0^\infty \frac{d\omega}{\pi} \rho(\omega) \frac{\cosh\left(\frac{\omega}{T}[\tau T - \frac{1}{2}]\right)}{\sinh \frac{\omega}{2T}} \quad \kappa = \lim_{\omega \rightarrow 0} \frac{2T}{\omega} \rho(\omega)$$

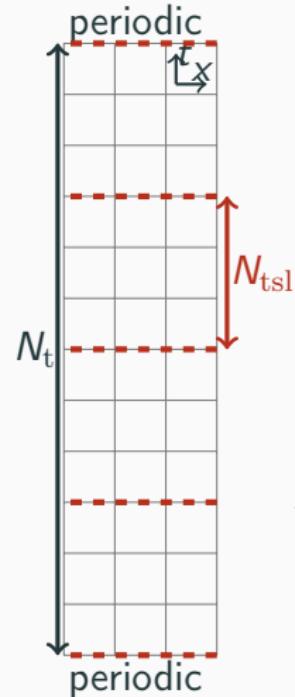
- Euclidean correlator related to spectral function
- Needs inversion of integral equation
- We use simple procedure of modeling  $\rho(\omega)$  and comparing to lattice data
  - $\rho(\omega)$  known at IR and UV
  - Connect IR and UV with i) step ii) line

$$\begin{aligned}\rho_{E,B}^{\text{step}}(\omega, T) &= \rho_{E,B}^{\text{IR}}(\omega, T) \theta(\Lambda - \omega) + \rho_{E,B}^{\text{UV}, T=0}(\omega, T) \theta(\omega - \Lambda), \\ \rho_{E,B}^{\text{line}}(\omega, T) &= \rho_{E,B}^{\text{IR}}(\omega, T) \theta(\omega^{\text{IR}} - \omega) + \\ &\quad \left[ \frac{\rho_{E,B}^{\text{IR}}(\omega^{\text{IR}}, T) - \rho_{E,B}^{\text{UV}}(\omega^{\text{UV}}, T)}{\omega^{\text{IR}} - \omega^{\text{UV}}} (\omega - \omega^{\text{IR}}) + \rho_{E,B}^{\text{IR}}(\omega^{\text{IR}}, T) \right] \\ &\quad \times \theta(\omega - \omega^{\text{IR}}) \theta(\omega^{\text{UV}} - \omega) + \rho_{E,B}^{\text{UV}}(\omega, T) \theta(\omega - \omega^{\text{UV}}),\end{aligned}$$

- Related:  $\gamma$  not measured yet

$$\gamma = -\frac{1}{3N_c} \int_0^\infty \frac{d\omega}{2\pi} \frac{\rho(\omega)}{\omega} = -\int_0^\infty d\tau G_E(\tau)$$

# Algorithms

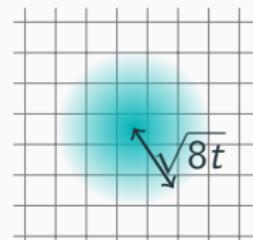


## Multilevel

- Algorithm for quenched simulations
  - At large  $N_t$  observable like Polyakov loop can have poor signal
  - Idea: Divide the lattice to temporal slices of size  $N_{tsl}$
  - Update each sub-lattice independently keeping boundaries fixed
  - Average over different boundary configurations
- Allows reaching better statistics with less configurations

## Gradient flow

- Automatically renormalizing smearing
- Can be generalized to unquenched
- Needs zero flow time limit



# Lattice parameters for the multilevel study

$T/T_c$	$N_t \times N_s^3$	$\beta$	$N_{\text{conf}}$	$T/T_c$	$N_t \times N_s^3$	$\beta$	$N_{\text{conf}}$	$T/T_c$	$N_t \times N_s^3$	$\beta$	$N_{\text{conf}}$
1.1	$12 \times 48^3$	6.407	1350	3	$12 \times 48^3$	7.193	1579	10	$12 \times 48^3$	8.211	1807
	$16 \times 48^3$	6.621	2623		$16 \times 48^3$	7.432	1553		$16 \times 48^3$	8.458	2769
	$20 \times 48^3$	6.795	2035		$20 \times 48^3$	7.620	1401		$20 \times 48^3$	8.651	2073
	$24 \times 48^3$	6.940	2535		$24 \times 48^3$	7.774	1663		$24 \times 48^3$	8.808	2423
1.5	$12 \times 48^3$	6.639	1801	6	$12 \times 48^3$	7.774	1587	$10^4$	$12 \times 48^3$	14.194	1039
	$16 \times 48^3$	6.872	2778		$16 \times 48^3$	8.019	1556		$16 \times 48^3$	14.443	1157
	$20 \times 48^3$	7.044	2081		$20 \times 48^3$	8.211	1258		$20 \times 48^3$	14.635	1139
	$24 \times 48^3$	7.192	2496		$24 \times 48^3$	8.367	1430		$24 \times 48^3$	14.792	1375
2.2	$12 \times 48^3$	6.940	1535	$2 \times 10^4$	$12 \times 48^3$	14.792	1948				

- Quenched multilevel simulations

Code from: [Banerjee et.al. PRD85 \(2012\)](#)

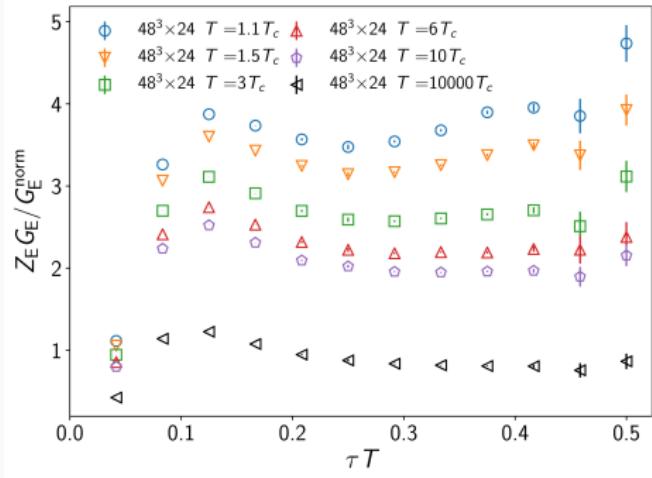
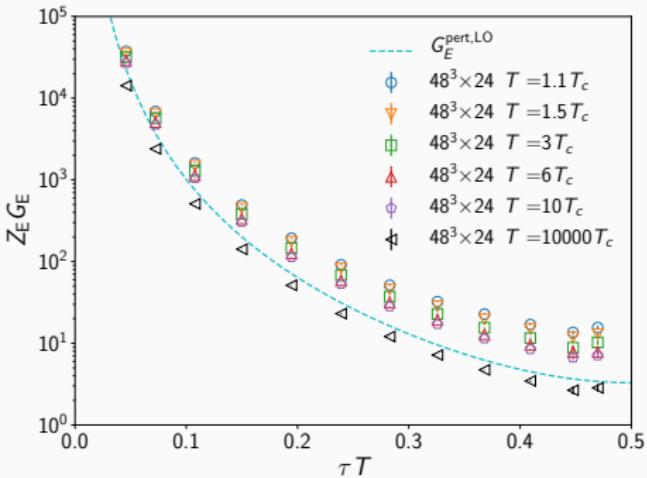
- 4 sublattices with 2000 updates
- Temperatures between  $1.1 T_c - 10^4 T_c$
- Scale setting with

(Francis et.al. PRD91 (2015))

- Other lattice results

[Meyer NJP13 \(2011\)](#),  
[Ding et.al. JPG38 \(2011\)](#),  
[Banerjee et.al. PRD85 \(2012\)](#),  
[Francis et.al. PRD92 \(2015\)](#),  
[Brambilla et.al. PRD102 \(2020\)](#),  
[Altenkort et.al. PRD103 \(2021\)](#),  
[Banerjee et.al. hep-lat/2204.14075](#),  
[Banerjee et.al. hep-lat/2206.15471](#)

# Lattice correlator



$$G_E^{\text{norm}} = \frac{G_E^{\text{pert,LO}}}{g^2 C_f} = \pi^2 T^4 \left[ \frac{\cos^2(\pi \tau T)}{\sin^4(\pi \tau T)} + \frac{1}{3 \sin^2(\pi \tau T)} \right]$$

- Chromoelectric field  $E$  needs discretization
- On Lattice  $E$  has non-physical self-energy contribution

$$Z_E = 1 + g_0^2 \times 0.137718569 \dots + \mathcal{O}(g_0^4)$$

(Christensen and Laine PLB02 (2016))

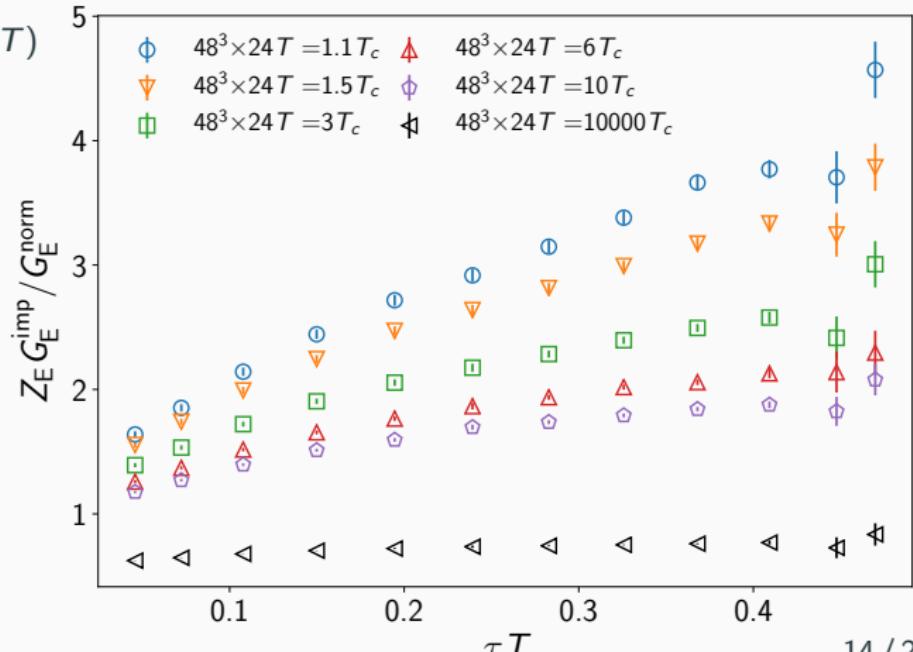
Caron-Huot et.al.JHEP04 (2009), Francis et.al.PoSLattice (2011)

# Tree level improvement

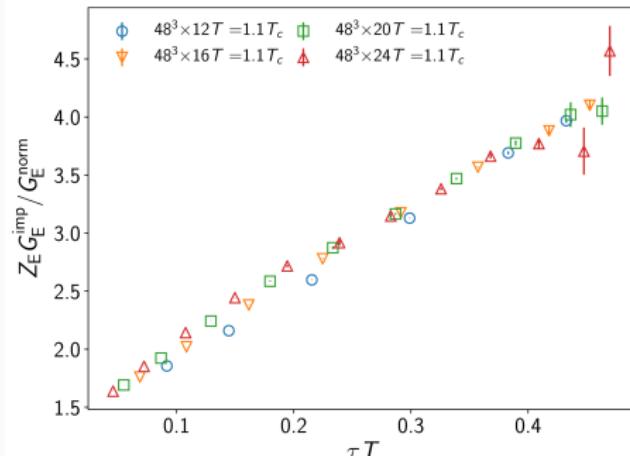
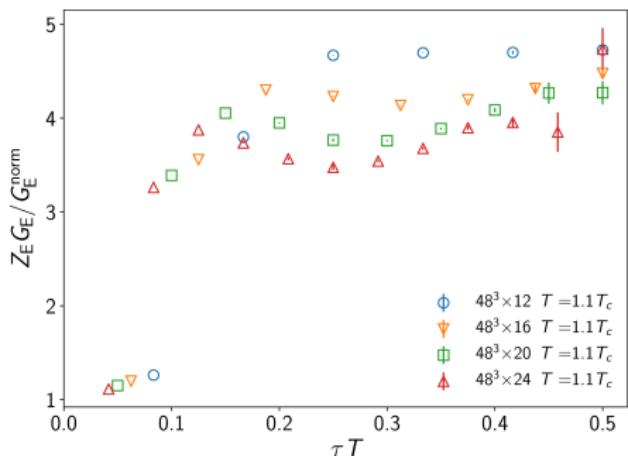
$$G_{E, \text{LOlat}} = \frac{1}{3a^4} \int_{-\pi}^{\pi} \frac{d^3 q}{(2\pi)^3} \frac{e^{\bar{q}N_\tau(1-\tau T)} + e^{\bar{q}N_\tau\tau T}}{e^{\bar{q}N_\tau} - 1} \frac{\tilde{q}^2}{\sinh \bar{q}},$$

$$\bar{q} = 2 \operatorname{arsinh} \left( \frac{\tilde{q}}{2} \right), \quad \tilde{q}^2 = \sum_{i=1}^3 4 \sin^2 \left( \frac{q_i}{2} \right)$$

$$G_{E, \text{pert}}(\bar{\tau} \bar{T}) = G_{E, \text{LOlat}}(\tau T)$$

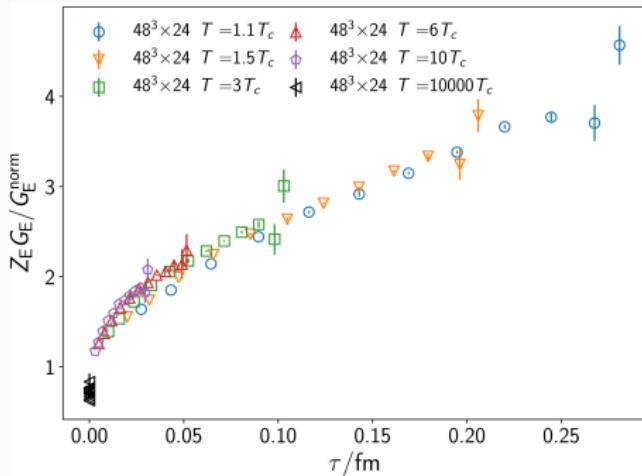
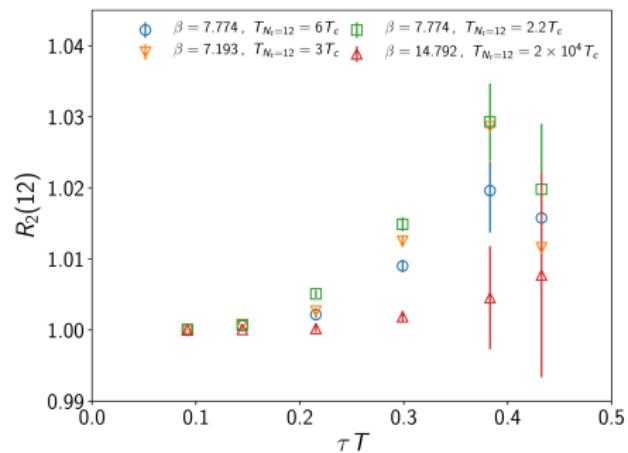


# The effect of tree-level improvement



- Greatly decreases  $N_t$  dependence
- From now on we only use tree-level improved  $\tau T$  without further indication

# When do thermal effects start



$$R_2(N_t) = \frac{G_E(N_t, \beta)}{G_E^{\text{norm}}(N_t)} \Bigg/ \frac{G_E(2N_t, \beta)}{G_E^{\text{norm}}(2N_t)} .$$

- On small physical separation every  $T$  shares a scaling (apart from finite size effects)
- Thermal effect nonexistent for  $\tau < 0.10$ , then grow

## Spectral function basics: LO

$$G_E(\tau) = \int_0^\infty \frac{d\omega}{\pi} \rho(\omega) \frac{\cosh\left(\frac{\omega}{T}[\tau T - \frac{1}{2}]\right)}{\sinh \frac{\omega}{2T}}$$
$$\kappa = \lim_{\omega \rightarrow 0} \frac{2T}{\omega} \rho(\omega), \quad \gamma = -\frac{1}{3N_c} \int_0^\infty \frac{d\omega}{2\pi} \frac{\rho(\omega)}{\omega}$$

- Assume simple behavior on IR ( $\omega \ll T$ ):

$$\rho_{\text{IR}}(\omega) = \frac{\kappa\omega}{2T}$$

- Perturbative behavior in UV in LO ( $\omega \gg T$ ):

$$\rho_{\text{UV}}^{\text{LO}}(\omega) = \frac{g^2(\mu_\omega) C_F \omega^3}{6\pi}, \quad \mu_\omega = \max(\omega, \pi T)$$

- Use 5-loop running for the coupling

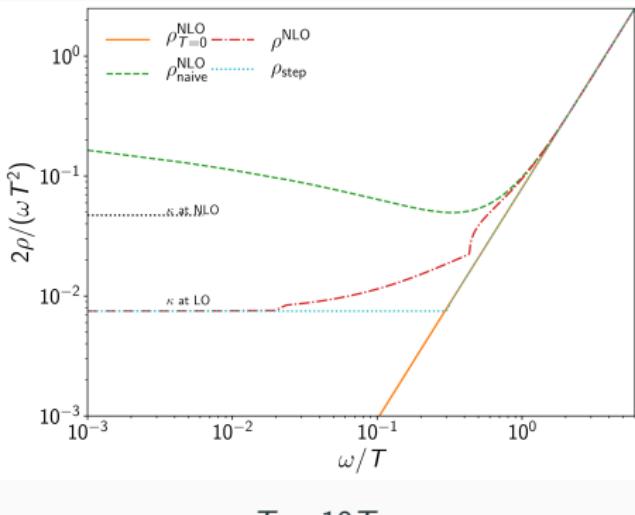
## Spectral function: NLO

- NLO  $\rho(\omega)$  known from ([Burnier et.al. JHEP08 \(2010\)](#))
- Full HTL resummed NLO  $\rho$  over corrects and gives negative  $\kappa$  at small  $T$
- Naive QCD NLO  $\rho(\omega)$  diverges logarithmically:

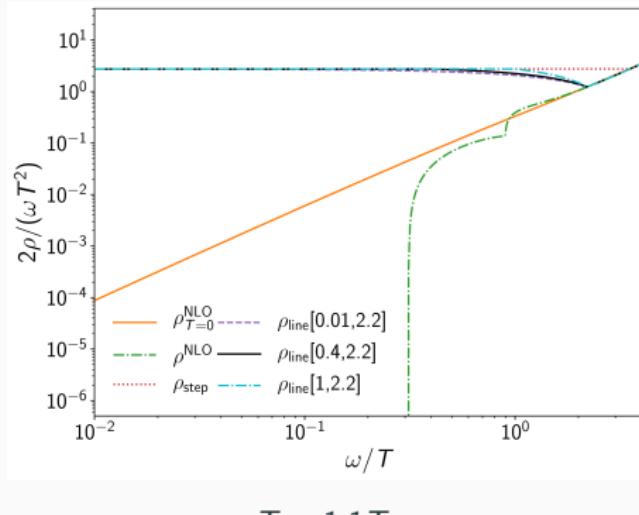
$$\begin{aligned}\rho_{\text{QCD,naive}}(\omega) &= \frac{g^2 C_F \omega^3}{6\pi} \left\{ 1 + \frac{g^2}{(4\pi)^2} \left[ N_c \left( \frac{11}{3} \ln \frac{\mu^2}{4\omega^2} + \frac{149}{9} - \frac{8\pi^2}{3} \right) \right] \right\} \\ &+ \frac{g^2 C_F}{6\pi} \frac{g^2}{2\pi^2} \left\{ N_c \int_0^\infty dq n_B(q) \left[ (q^2 + 2\omega^2) \ln \left| \frac{q+\omega}{q-\omega} \right| + q\omega \left( \ln \frac{|q^2 - \omega^2|}{\omega^2} - 1 \right) \right. \right. \\ &\quad \left. \left. + \frac{\omega^4}{q} \mathbb{P} \left( \frac{1}{q+\omega} \ln \frac{q+\omega}{\omega} + \frac{1}{q-\omega} \ln \frac{\omega}{|q-\omega|} \right) \right] \right\},\end{aligned}$$

- We will use the  $T = 0$  naive QCD  $\rho(\omega)$  as our normalization
- set scale: UV:  $\rho_{T=0}^{\text{LO}} = \rho_{T=0}^{\text{NLO}}$ , IR: from NLO EQCD

# Spectral function behavior



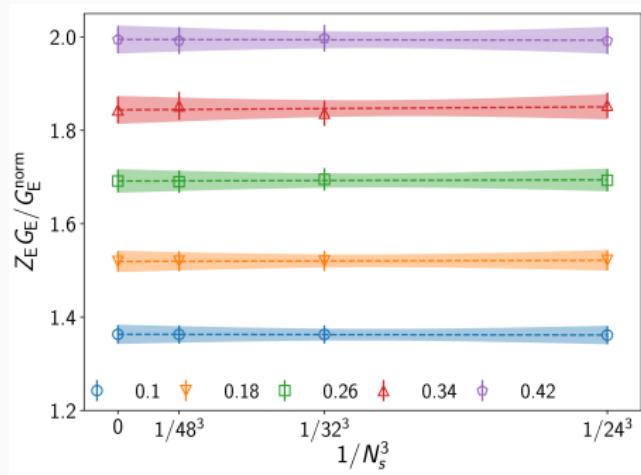
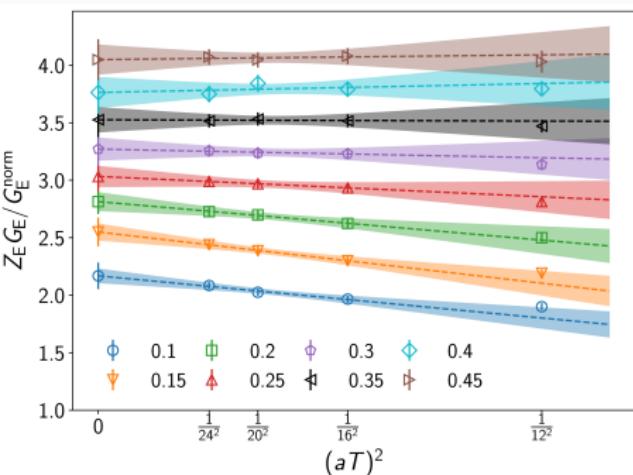
$$T = 10T_c$$



$$T = 1.1T_c$$

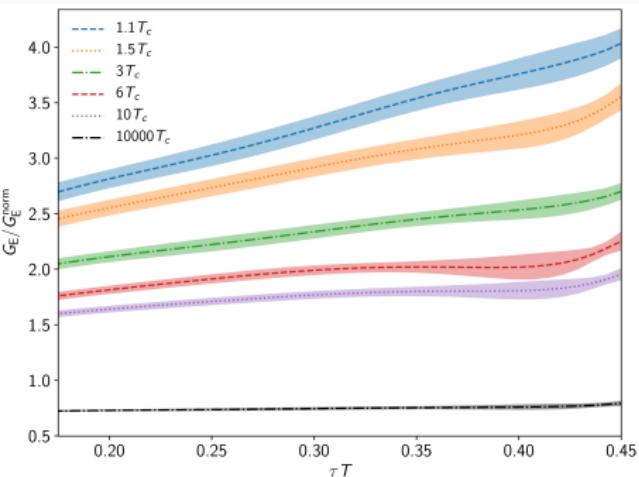
- NLO spectral function works only at very high temperatures
- Try different models for  $\omega \sim T$  behavior
- Instead of inverting integral equation, compare to ansatz

# Continuum limit and finite size effects

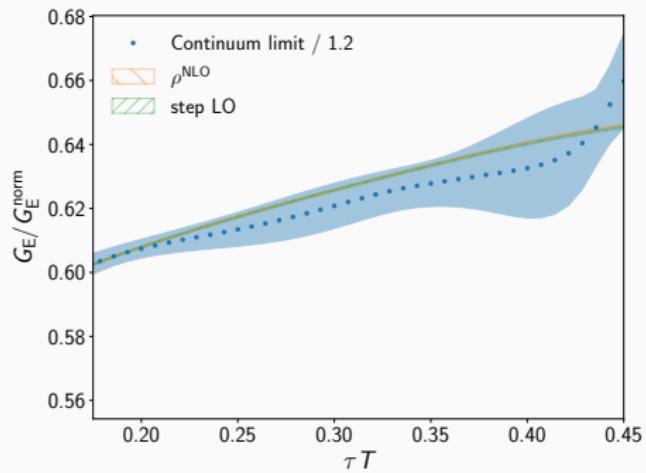


- Use 3 largest lattices for continuum limit
- Check systematics by including the  $N_t = 12$  point
- $\chi^2/\text{d.o.f.} < 5$  for  $\tau T > 0.20$  when using 3 largest lattices ( $< 10$  with  $N_t = 12$ )
- Finite size effects are negligible

# Continuum limit



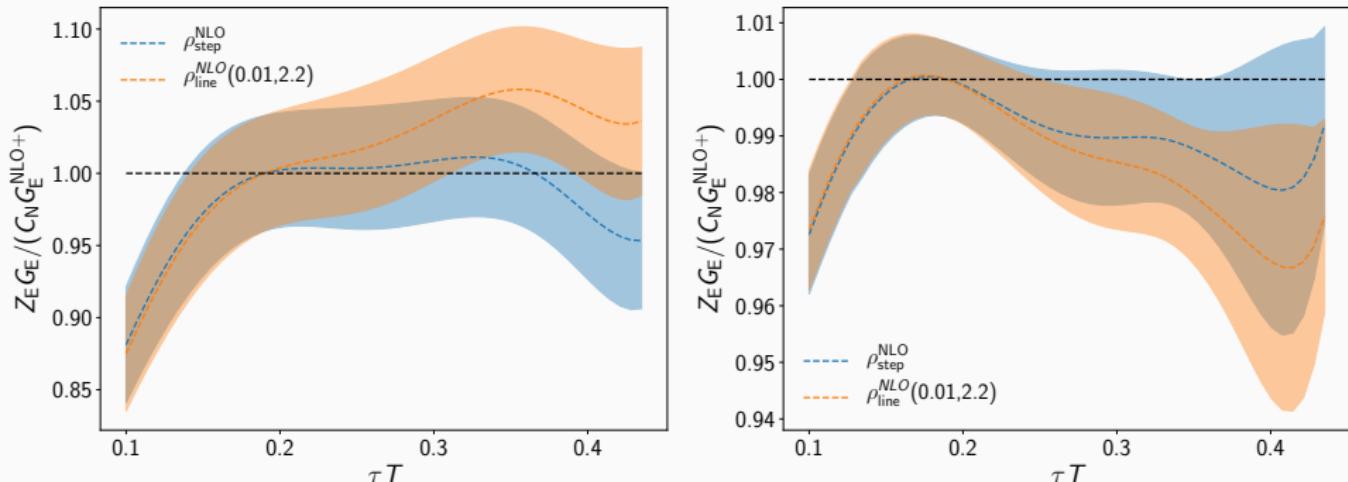
$$T = 1.1T_c$$



$$T = 10^4 T_c$$

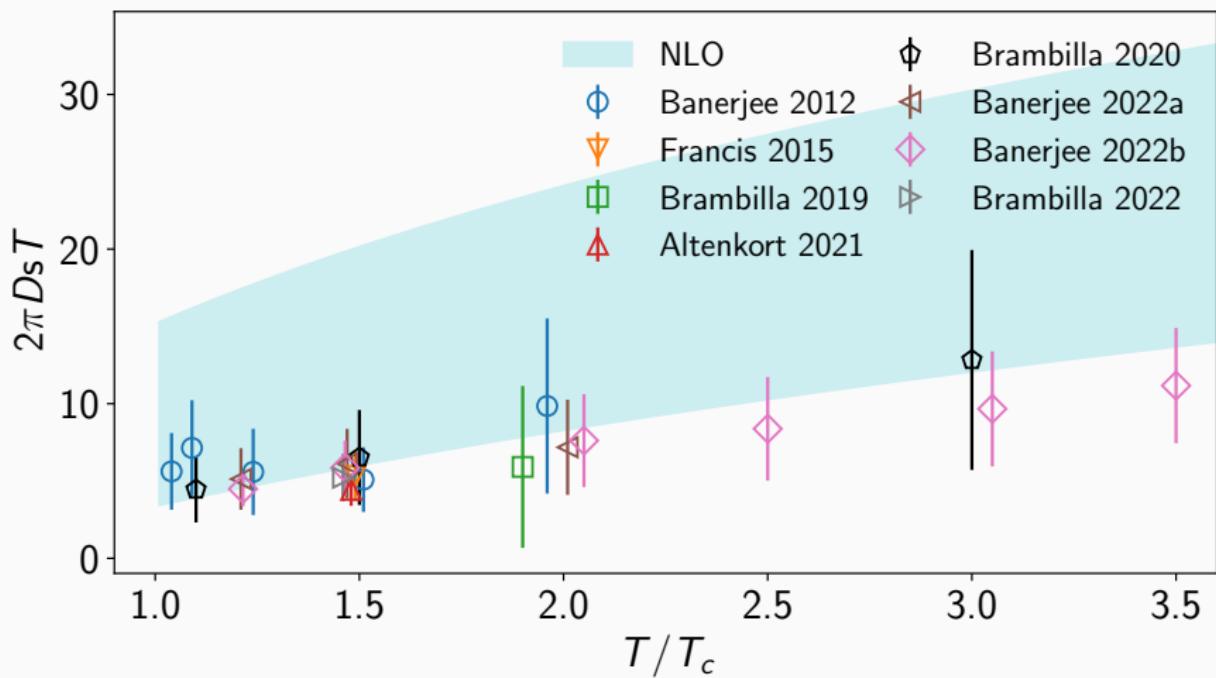
- Data needs additional normalization, do this at  $\tau T = 0.19$
- Great agreement to perturbation theory at very high temperatures

## $\kappa$ extraction

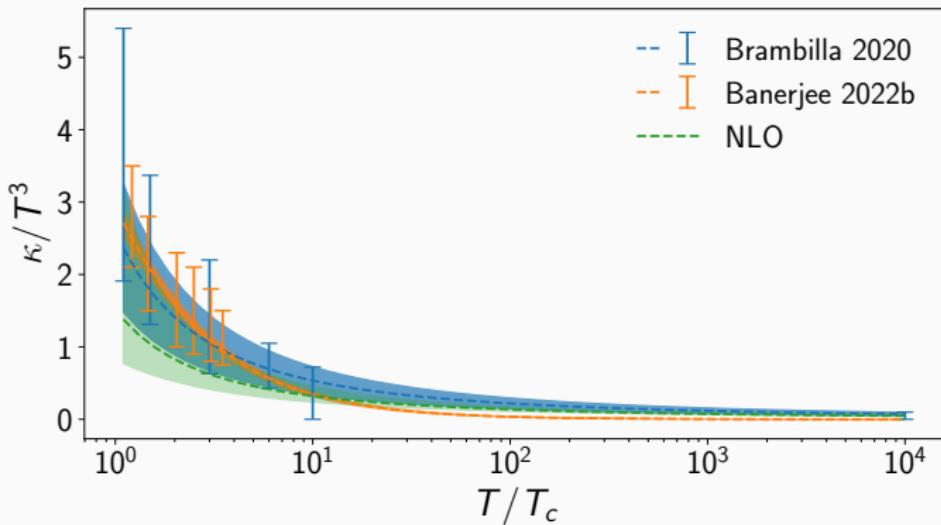


- Take continuum limit of the lattice data
- Normalize with different models for spectral function
- Extract  $\kappa$  as all values that normalize to unity in  $0.19 \leq \tau T \leq 0.45$

## Multilevel results for $D_s$



# Temperature dependence of $\kappa$



- Measure  $\kappa$  in range:  
 $T = 1.1 - 10^4 T_c$
- Fit temperature dependence to perturbatively motivated ansatz  
 $C = 3.81(1.33)$
- In [Banerjee et.al.\[2206.15471\]](#) different form is used  $2\pi TD_s \sim \alpha + \beta(T/T_c - 1)$

$$\frac{\kappa^{\text{NLO}}}{T^3} = \frac{g^4 C_F N_c}{18\pi} \left[ \ln \frac{2T}{m_E} + \xi + C \frac{m_E}{T} \right].$$

## Conclusions and Future prospects

- Measured in wide range of temperatures
- Fit temperature dependence
- Agreement to perturbation theory at high T
- Agreement to previous results at small T
- Measured  $1/M$  corrections (See Julians talk tomorrow)
- Future prospects:
  - Measure  $\gamma$  from our data
  - Check adjoint representation to study quarkonium

## Conclusions and Future prospects

- Measured in wide range of temperatures
- Fit temperature dependence
- Agreement to perturbation theory at high T
- Agreement to previous results at small T
- Measured  $1/M$  corrections (See Julians talk tomorrow)
- Future prospects:
  - Measure  $\gamma$  from our data
  - Check adjoint representation to study quarkonium

Thank you for your attention!