QCD Thermodynamics

Peter Petreczky

Brookhaven National Laboratory

BES program and RHIC

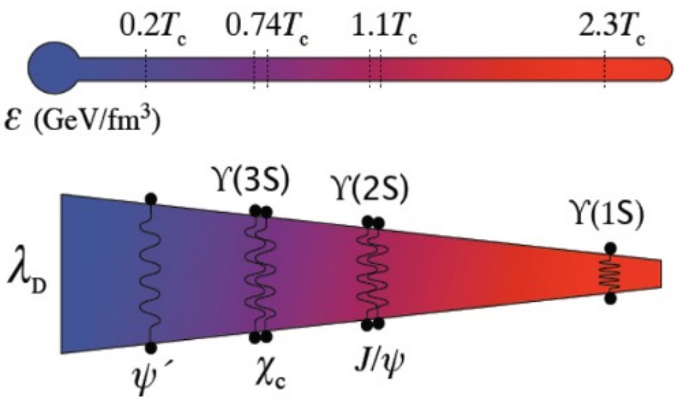
- QCD Phase Diagram and EoS

Heavy Flavor probes of sPHENIX @ RHIC, LHC heavy ion program

- Bottomonium masses and widths at $T>0$
  Larsen, Meinel, Mukherjee, PP, PLB 800 (20) 135119
- Complex potential at $T>0$
  Balla et al (HotQCD), PRD 105 (2022) 054513
- Heavy quark diffusion coefficient from lattice QCD
  Altenkort, Kaczmarek, Larsen, Mukherjee, PP, Shu, Stenbach (HotQCD), arXiv:2302.08501

Heavy flavor probes and lattice QCD

From 2015 LRP: understanding the inner workings of QGP by probing different length scales



RHIC
sPHENIX, STAR+
2023-2025

LHC Runs 3-5
ALICE 2-3, CMS+,ATLAS+,LHC+
2022-2038

White papers for the 2023 LRP:

The Present and Future of QCD, arXiv:2303.02579 — Conveners: S. Mukherjee

Hot QCD White Paper, arXiv:2303.17254 — PP

Lattice:		Phenomenology:
In-medium quarkonium masses and widths $M_\alpha(T),\ \Gamma_\alpha(T)$	⟺	Transport models for quarkonium suppression and regeneration
Complex potential at $T>0$	⟺	Langevin dynamics of quarkonium regeneration, open quantum system
Heavy quark diffusion coefficient $\kappa(T)$ (average momentum transfer to heavy quark)	⟺	Collisional energy loss, open heavy flavor suppression

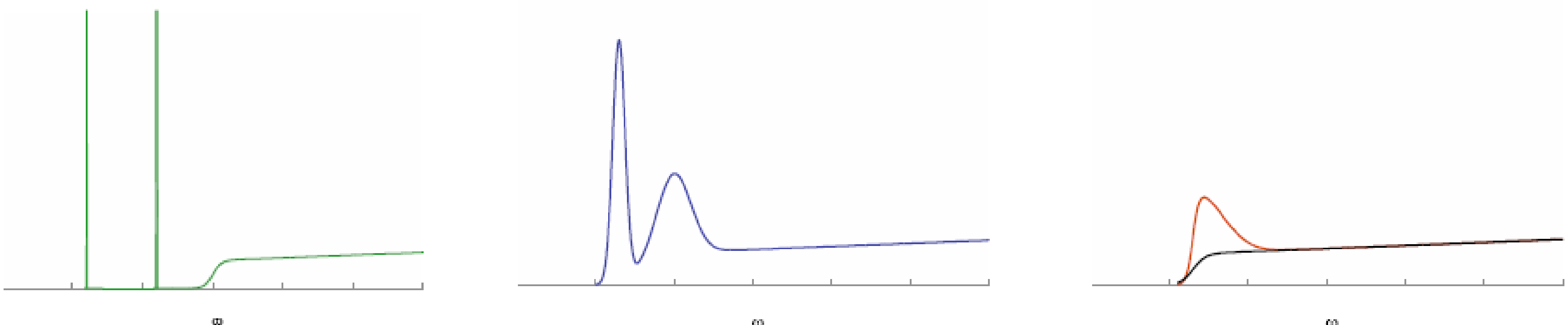
Meson correlators and spectral functions

Vacuum and in-medium properties as well as dissolution of mesons are encoded in the spectral functions:

$$\rho(\omega,p,T)=\frac{1}{2\pi}\mathrm{Im}\int_{-\infty}^{\infty}dte^{i\omega t}\int d^3xe^{ipx}\langle[O(x,t),O(0,0)]\rangle_T,\quad O(x,t)\sim\bar{Q}(x,t)\Gamma Q(x,t)$$

Melting is seen as progressive broadening and disappearance of the bound state peaks

Modifications of quarkonium yields in heavy ion collisions   Matsui and Satz, PLB 178 (1986) 416



$$C(\tau,T)=\sum_x\langle O(x,\tau)O(0,0)\rangle_T \quad\longleftrightarrow\quad C(\tau,T)=\int_{-\infty}^{+\infty}d\omega\rho(\omega,T)e^{-\tau\omega}$$

Consider large τ behavior of $C(\tau,T=0)$:

$$C(\tau,T)\sim\sum_n|\langle 0|O|n\rangle|^2e^{-M_n\tau}\simeq f_1e^{-M_1\tau}+f_2e^{-M_2\tau}+\ldots$$

$T>0:\quad \tau<1/T\Rightarrow\text{reconstruct }\rho(\omega,T)$

Strategies to obtain the spectral functions from lattice

Strategy: use EFT to simplify the problem, use appropriately chosen correlation functions to enhance sensitivity to quantities of interest, constrain the spectral function by *T=0* results

Example: NRQCD using correlation functions of optimized meson operators projecting on bottomonium states of interest

$$C_\alpha(\tau, T) = \int_{-\infty}^{\infty} d\omega \rho_\alpha(\omega, T) e^{-\omega\tau}$$

$$\alpha = \Upsilon(1S),\ \Upsilon(2S),\ \Upsilon(3S)$$

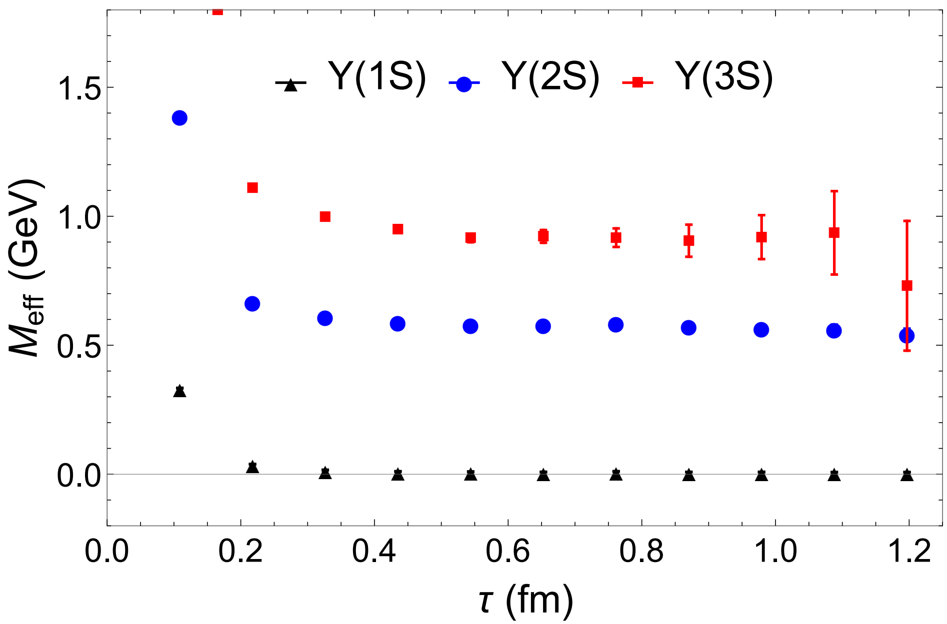
$$\rho_\alpha(\omega, T) = \rho_\alpha^{\mathrm{med}}(\omega, T) + \rho_\alpha^{\mathrm{high}}(\omega)$$

parametrized as single peak+ tail

constrained at *T=0*

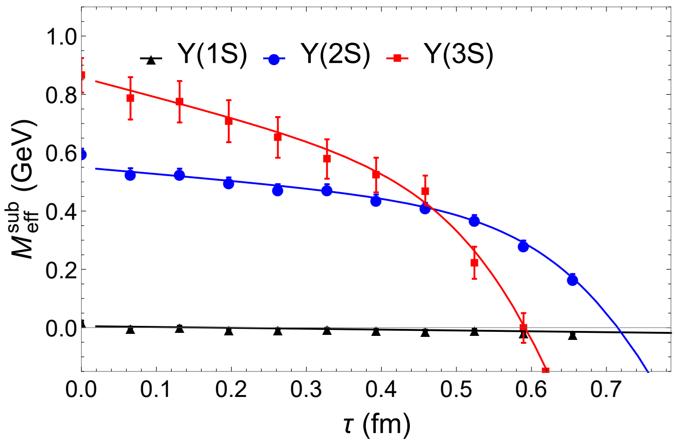
Larsen, Meinel, Mukherjee, PP, PLB 800 (20) 135119

$$M_{\mathrm{eff}}(\tau) = \frac{1}{a} \ln[C_\alpha(\tau)/C_\alpha(\tau + a)]$$



Thermal mass shift of bottomonium

Larsen, Meinel, Mukherjee, PP, PLB 800 (20) 135119

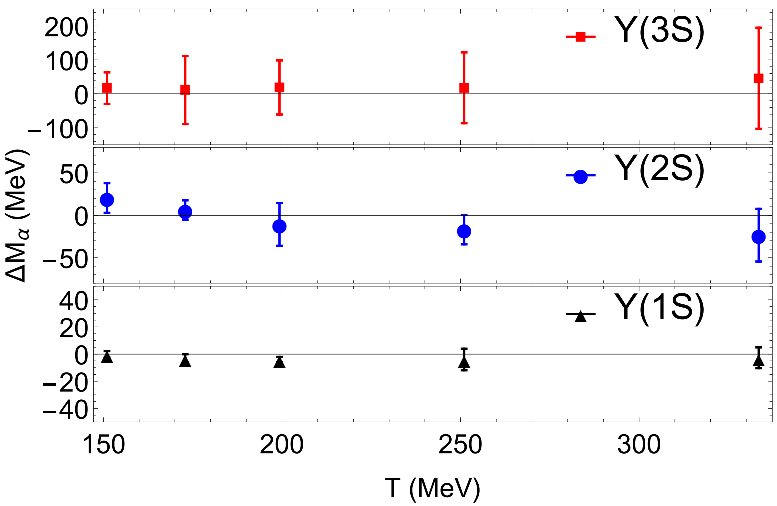


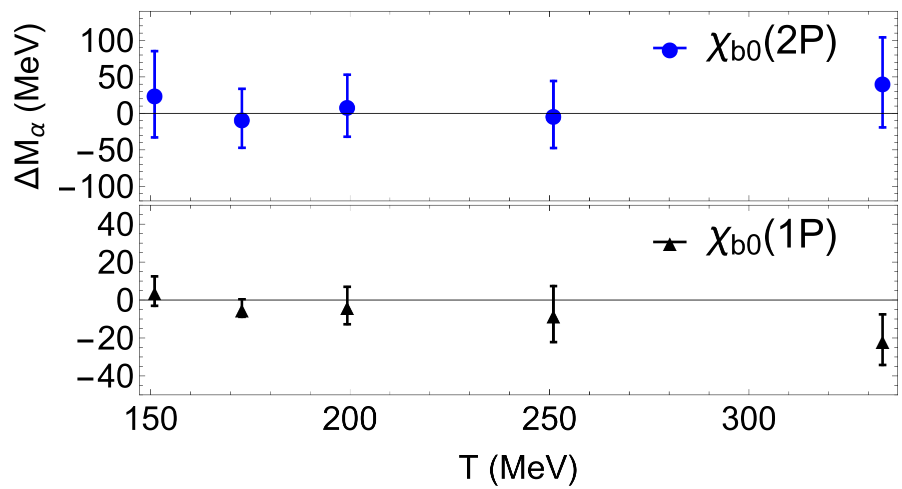
HISQ, $48^3 \times 12$ lattices with $m_l = m_s/20$ (from T_c and EoS calculations)

Fit $M_{\rm eff}^{\rm sub}(\tau, T)$ using a simple Ansatz:

$$\rho_\alpha^{\rm med}(\omega, T) = A_\alpha^{\rm cut}(T)\,\delta\left(\omega - \omega_\alpha^{\rm cut}(T)\right) + A_\alpha(T)\exp\left(-\frac{[\omega - M_\alpha(T)]^2}{2\Gamma_\alpha^2(T)}\right)$$

$$\Rightarrow M_\alpha(T), \Gamma_\alpha(T)$$

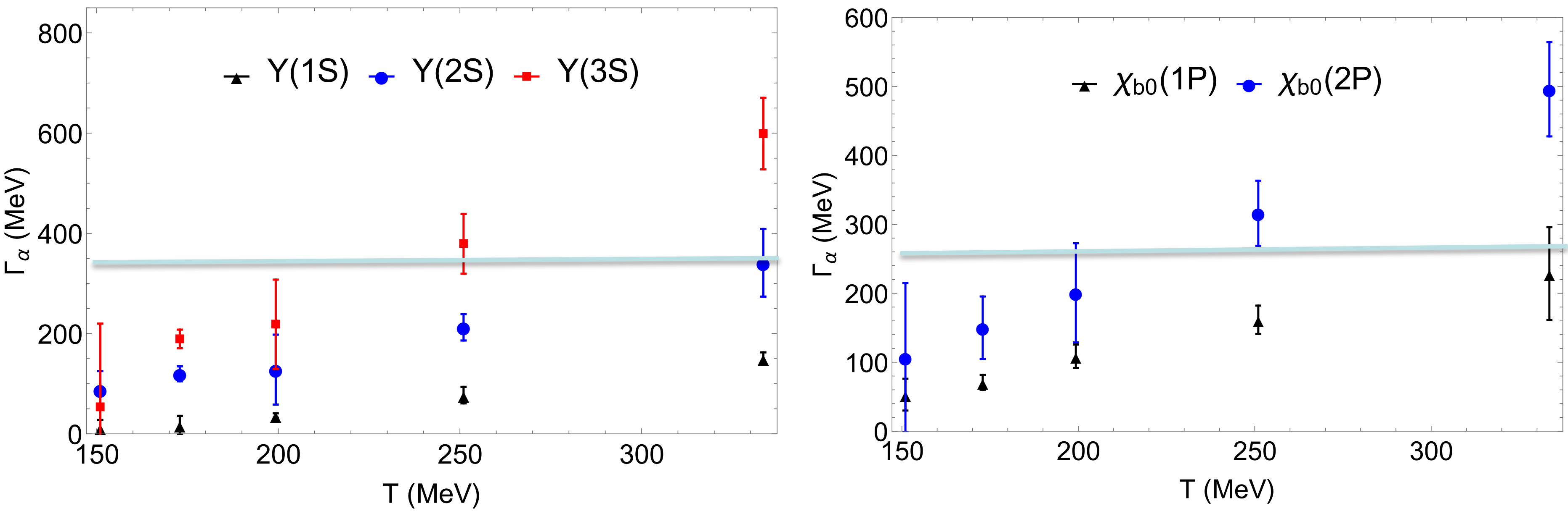




No significant thermal mass shift is observed in any of the bottomonium states contrary to expectations of the potential model with screened potential

Thermal width of bottomonium

Larsen, Meinel, Mukherjee, PP, PLB 800 (20) 135119



Significant thermal width for all bottomonium states that increases with T

Bottomonium states dissolve when thermal width is larger than the level splitting

$$\Gamma_\alpha(T) > \Delta E$$

$$T_{melt}(\Upsilon(3S)) \simeq T_{melt}(\chi_b(2P)) \simeq 220 \text{ MeV}$$

$$T_{melt}(\Upsilon(2S)) \simeq T_{melt}(\chi_b(1P)) \simeq 360 \text{ MeV}$$

Quark anti-quark potential at T>0

Conjecture, Matsui and Satz, PLB 178 (86) 416 $-\frac{4}{3}\frac{\alpha_s}{r}+\sigma r \to -\frac{4}{3}\frac{\alpha_s}{r}e^{-m_D r}, T > T_c$

Extending pNRQCD to *T>0*: the potential is complex, the real part can have thermal correction but is not necessarily screened, except when $r \sim 1/m_D >> 1/T$

Weak coupling calculation

Laine, Philipsen, Romatschke, Tassler, JHEP 03 (06) 054
Brambilla, Ghiglieri, PP, Vairo, PRD 78 (08) 014017

Calculate the potential non-perturbatively on the lattice by considering Wislon loops of size *r* x τ at *T>0*

$$W(r,\tau,T)=\int_{-\infty}^{\infty}\rho_r(\omega,T)e^{-\omega\tau}$$

If potential at $T > 0$ exists the $\rho_r(\omega,T)$ should have a well define peak at $\omega \simeq \mathrm{Re}V(r,T)$, and the width of the peak is $\mathrm{Im}V(r,T)$

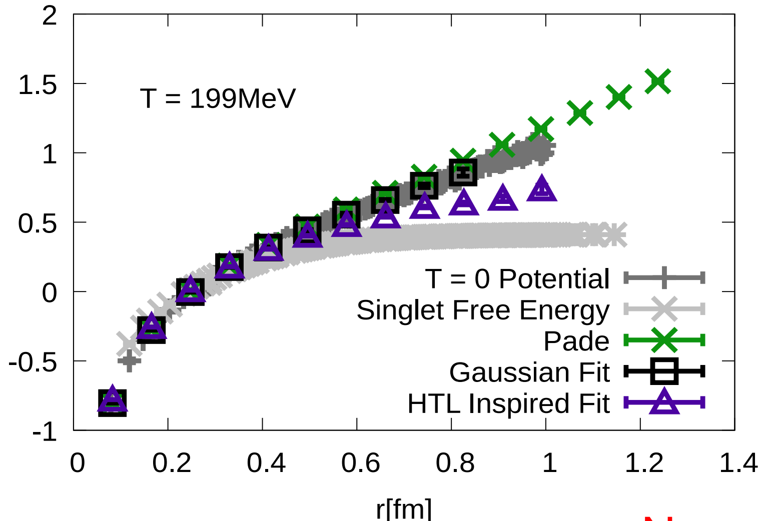
Rothkopf, Hatsuda, Sasaki, PRL 108 (2012) 162001

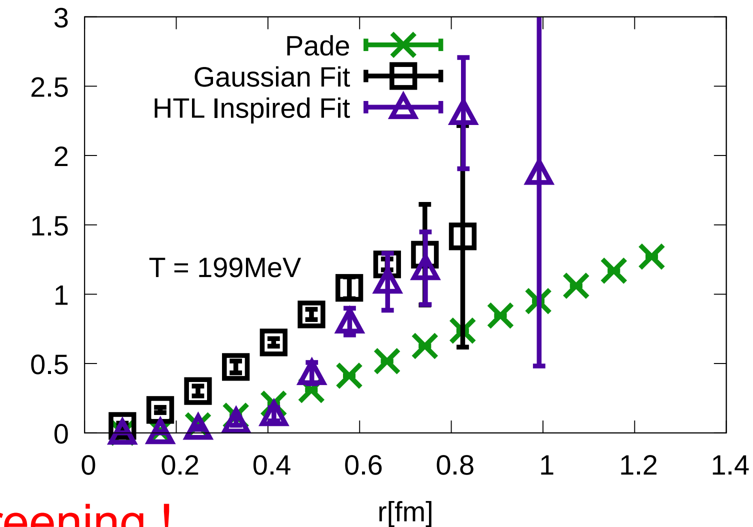
Challenge: reconstruct $\rho_r(\omega,T) \Rightarrow$ subtract the high ω part of the spectral function using $T = 0$ lattice results and model the ground state peak by a Gaussian form

Quark anti-quark potential at T>0 from the lattice

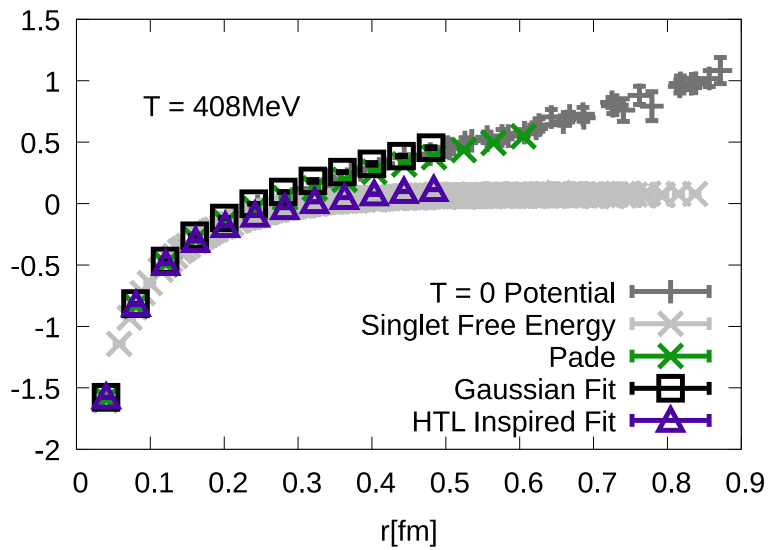
HISQ, $N_\tau = 12$

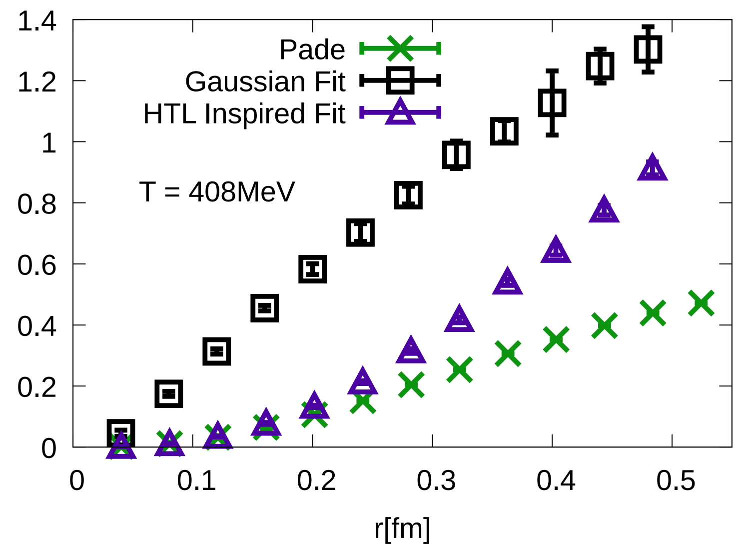
Bala et al (HotQCD), PRD 105 (2022) 054513





No color screening !





Current-current correlators and heavy quark diffusion coefficient

$$\rho_V^{\mu\nu}(\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3x \left\langle [\hat{J}^\mu(t,\vec{x}), \hat{J}^\nu(0,\vec{0})] \right\rangle$$

$$\partial_t p_i = -\eta p_i + f_i(t),$$

$$\langle f_i(t) f_j(t') \rangle = \kappa \delta_{ij} \delta(t - t')$$

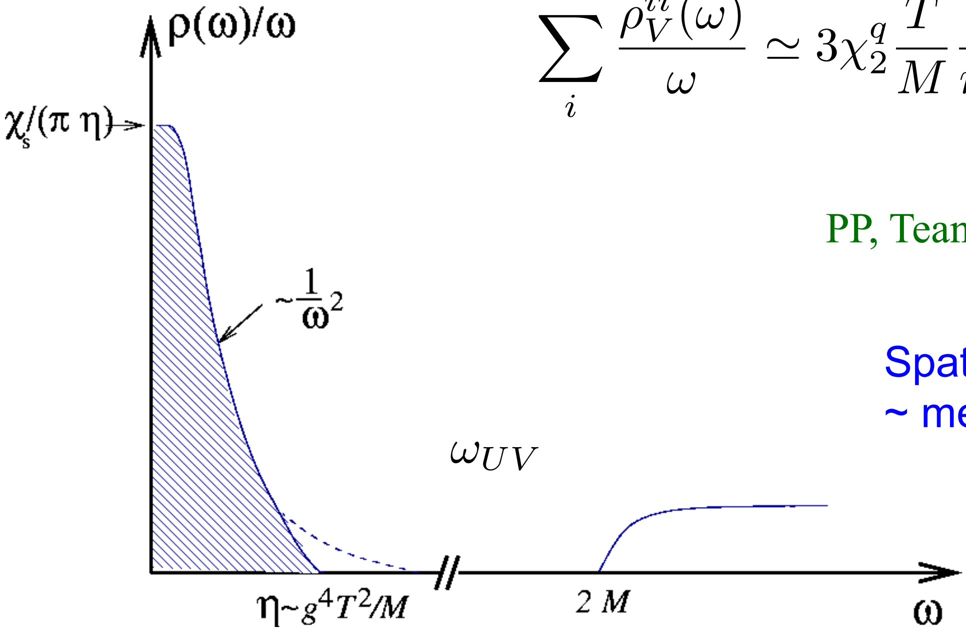
$$\kappa = 2MT\eta = 2T^2/D_s$$

Momentum diffusion coefficient

$$\sum_i \frac{\rho_V^{ii}(\omega)}{\omega} \simeq 3\chi_2^q \frac{T}{M} \frac{\eta}{\eta^2 + \omega^2}, \quad \omega < \omega_{UV}, \quad \eta = \frac{T}{M}\frac{1}{D_s}$$

drag constant

PP, Teaney, PRD 72 (2006) 014508



Spatial diffusion constant
~ mean free path (weak coupling)

$$D_s \sim \frac{1}{g^4 T}$$

area under the peak ~ $\chi_2^q \frac{T}{M}$

heavy quark coefficient ~ width of the peak

For large quark mass the transport peak is very narrow even for strong coupling and its difficult to reconstruct it accurately from Euclidean correlator calculated on the lattice

Heavy quark diffusion and lattice QCD

Obtain the momentum heavy quark transport coefficient through the force correlator

$$\langle f_i(t) f_j(t)\rangle = \langle E_i(t) E_j(t')\rangle + \frac{1}{3}\langle \mathbf{v}^2\rangle\langle \delta_{ij} B_k(t) B_k(t') - B_i(t') B_j(t)\rangle \qquad \langle \mathbf{v}^2\rangle = \frac{3T}{M}$$

$$t \to i\tau$$

Can be rigorously derived in Heavy Quark Effective Theory

Casalderrey-Solana, Teaney, PRD 74 (2006) 085012; Caron-Huot, Laine, Moore, JHEP 0904 ('09) 053

Bouttefeux, Laine, JHEP 12 (2020) 150

$$G_E(\tau) = -\frac{1}{3}\sum_{i=1}^{3} \frac{\left\langle \mathrm{ReTr}\left[U(\beta,\tau)\, gE_i(\tau,\vec{0})\, U(\tau,0)\, gE_i(0,\vec{0})\right]\right\rangle}{\left\langle \mathrm{ReTr}[U(\beta,0)]\right\rangle} \qquad \kappa_E = \lim_{\omega\to 0} \frac{2T}{\omega}\rho_E(\omega)$$

$$G_B(\tau) = -\frac{1}{3}\sum_{i=1}^{3} \frac{\left\langle \mathrm{ReTr}\left[U(\beta,\tau)\, gB_i(\tau,\vec{0})\, U(\tau,0)\, gB_i(0,\vec{0})\right]\right\rangle}{\left\langle \mathrm{ReTr}[U(\beta,0)]\right\rangle} \qquad \kappa_B = \lim_{\omega\to 0} \frac{2T}{\omega}\rho_B(\omega)$$

$$G_{E,B}(\tau) = \int_0^\infty \frac{\mathrm{d}\omega}{\pi}\rho_{E,B}(\omega)\frac{\cosh\left(\tau - \frac{1}{2T}\right)\omega}{\sinh\frac{\omega}{2T}}$$

$$\kappa = \kappa_E + \frac{2}{3}\langle \mathbf{v}^2\rangle \kappa_B$$

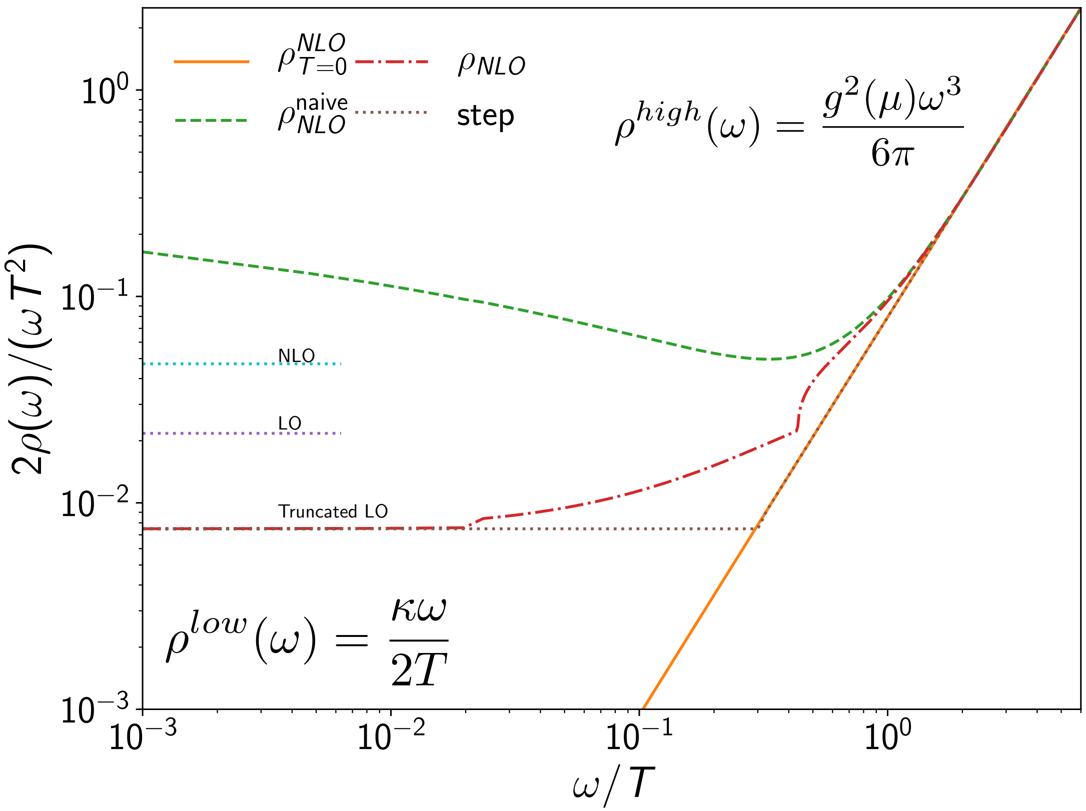
Extracting momentum diffusion coefficient from the lattice

Challenge 1: obtain precise results for chromo-electric and chromo-magnetic (very noisy)

⇒ Noise reduction via multi-level algorithm, applicable to quenched QCD (pure glue plasma)

⇒ Noise reduction by gradient flow method (new development !) , also applicable in full QCD

Challenge 2: reconstruct the spectral function from the Euclidean time lattice correlator



⇒ use known large and small energy behavior of the spectral

Parameterize $\rho(\omega, T)$ as smooth interpolation between $\rho^{low}(\omega, T)$ and $\rho^{high}(\omega)$, and treat κ as well as the additional nuisance parameters of interpolation as fit parameters

Extracting momentum diffusion coefficient from the lattice

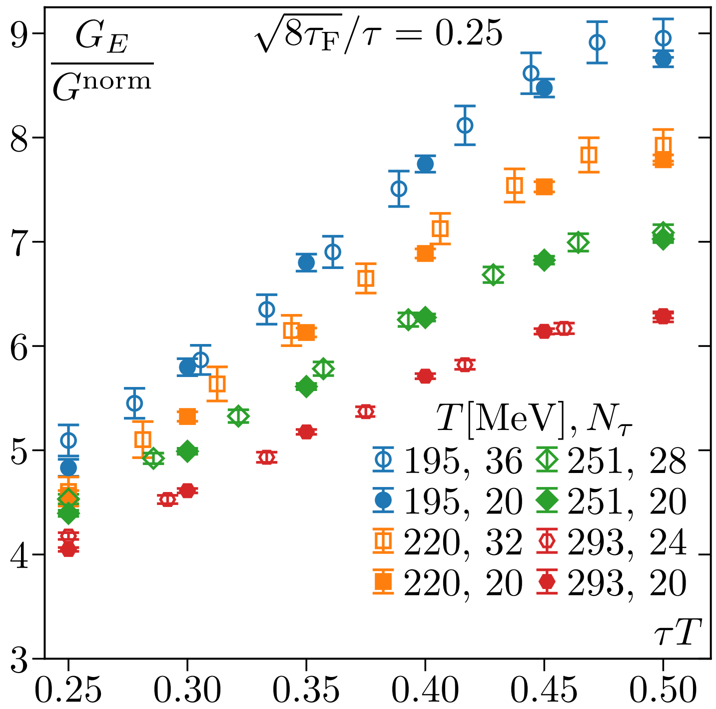
2+1 flavor QCD with $m_l = m_s/5$ ($m_\pi = 320$ MeV), $T = 195 - 354$ MeV, $96^3 \times N_\tau$ lattices with $N_\tau = 36,\ 32,\ 28,\ 24,\ 20$; additional $64^3 \times N_\tau$ lattices with $N_\tau = 20,\ 22,\ 24 \Rightarrow 3$ lattice spacings at each T; Gradient flow for noise reduction

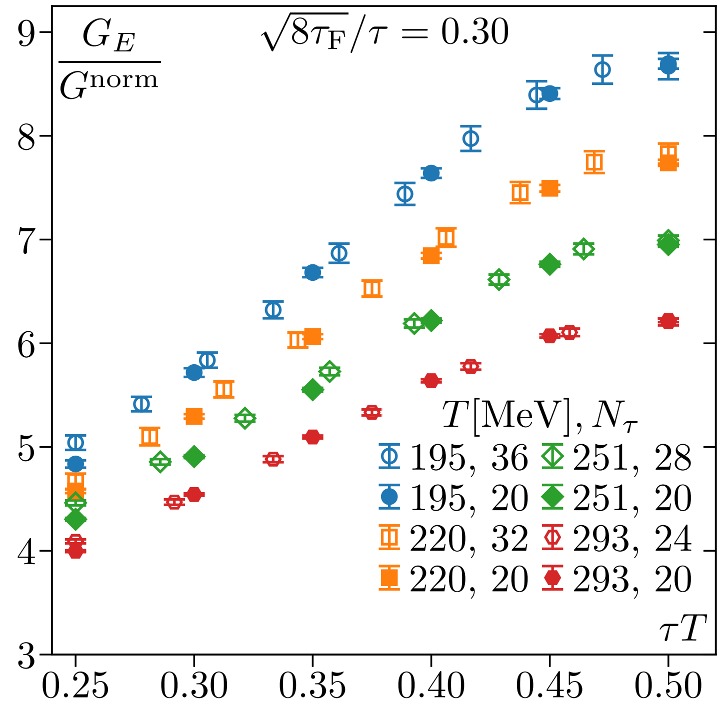
$64^3 \times N_\tau$ lattices have been partly generated using USQCD allocation (2022-2023).

Symanzik gauge action and Zeuthen flow

Gauge fields are smeared in the radius $\sqrt{8\tau_F}$

$a < \sqrt{8\tau_F} < \tau/3$





We see small cutoff effects thanks improved actions

Analysis and modeling the chromo-electric correlator

Analysis of the chromo-electric correlator:

- Extrapolate the lattice results on the chromo-electric correlator to the continuum limit
- Perform the zero flow time extrapolation

Fits to model spectral function:

$$\rho^{low}(\omega,T)=\frac{\kappa\omega}{2T} \qquad \rho^{high}(\omega)=\rho^{LO,NLO}(\omega)$$

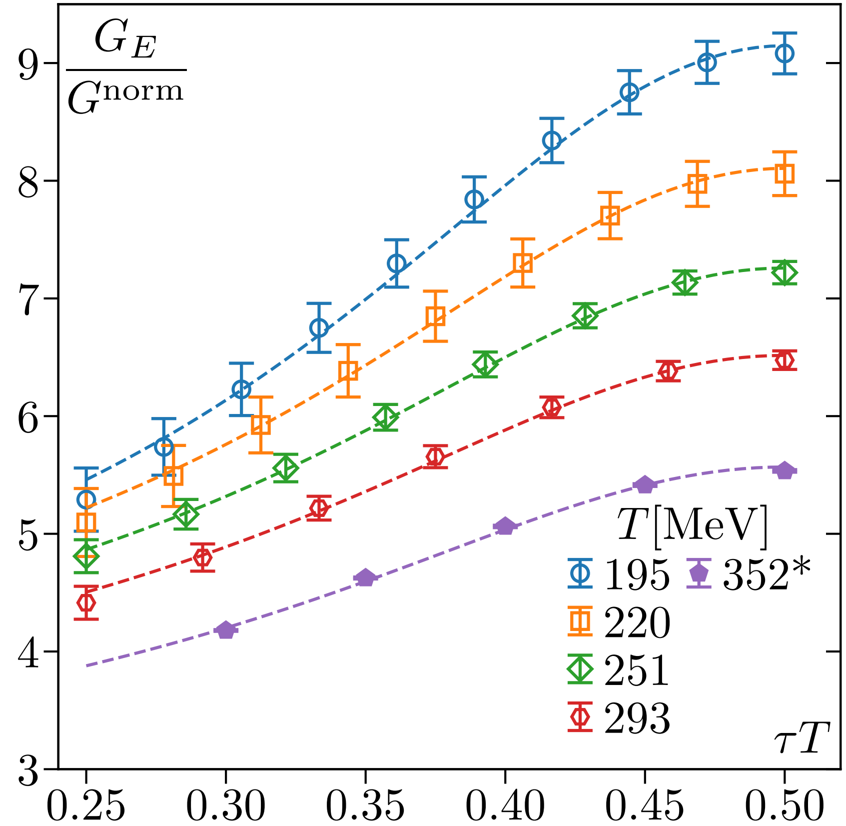
$$\rho^{max}(\omega,T)=max(\rho^{low}(\omega,T),\rho^{high}(\omega))$$

$$\rho^{smax}(\omega,T)=\sqrt{(\rho^{low})^2+(\rho^{high})^2}$$

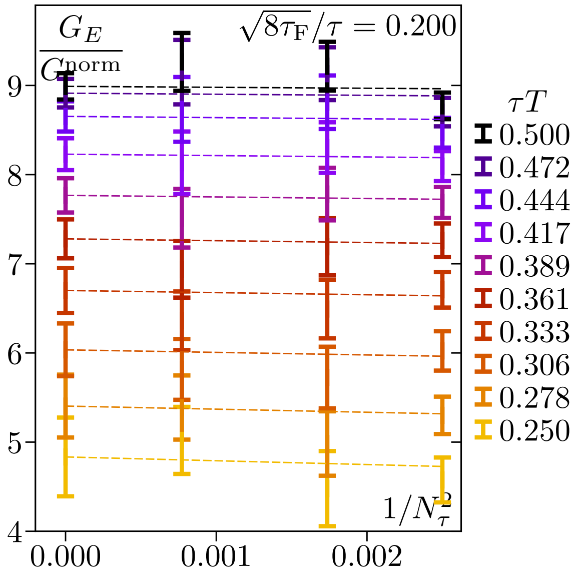
$$\rho^{pow}(\omega,T)=\rho^{low}(\omega,T),\ \omega\leq\omega_{IR}$$

$$\rho^{pow}(\omega,T)=A\omega^{\alpha},\ \omega_{IR}<\omega<\omega_{UV}$$

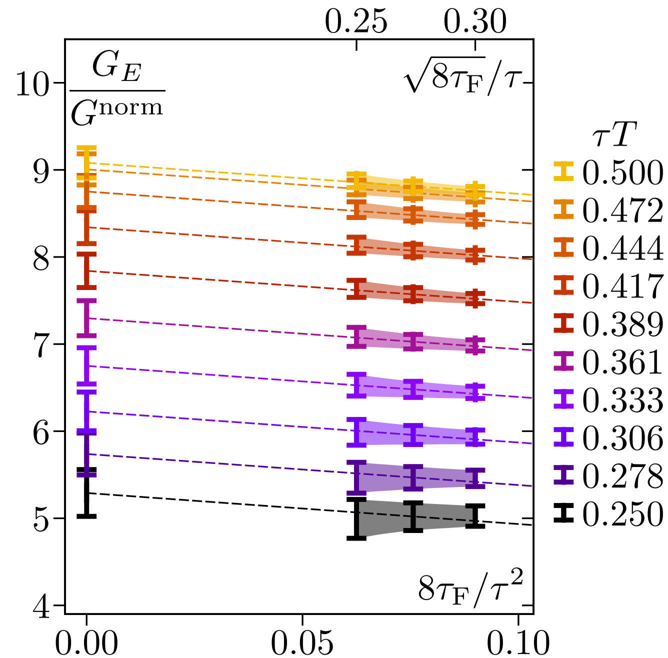
$$\rho^{pow}(\omega)=\rho^{high}(\omega),\ \omega\geq\omega_{UV}$$



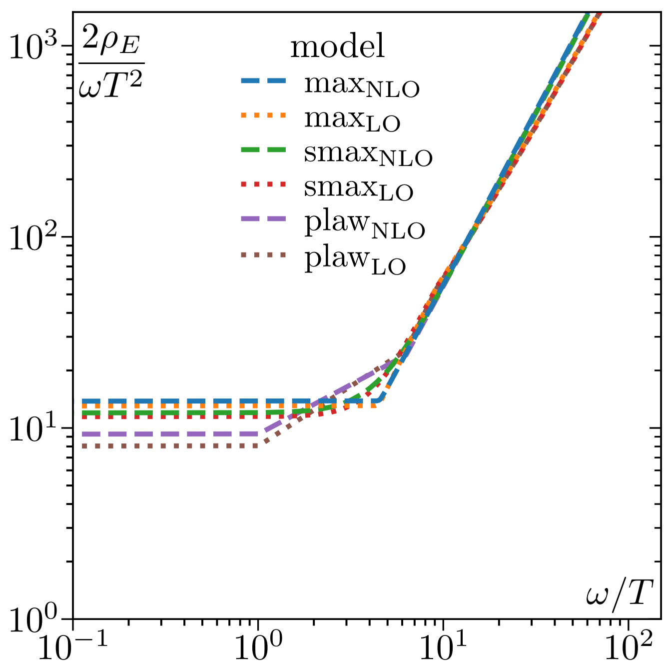
T=195 MeV:



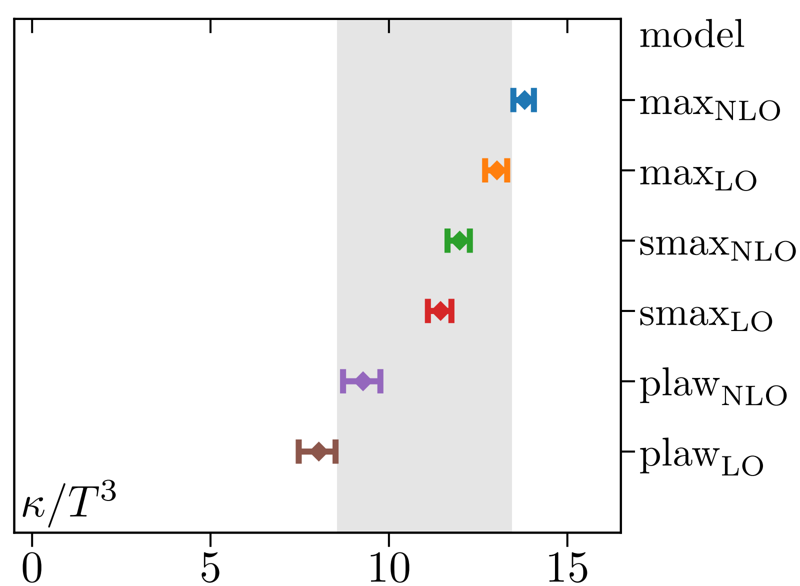
$\frac{G_E}{G^{\text{norm}}}$
$\sqrt{8\tau_F}/\tau = 0.200$
τT
0.500
0.472
0.444
0.417
0.389
0.361
0.333
0.306
0.278
0.250
$1/N_\tau^2$
0.000
0.001
0.002
4
5
6
7
8
9



0.25
0.30
$\frac{G_E}{G^{\text{norm}}}$
$\sqrt{8\tau_F}/\tau$
τT
0.500
0.472
0.444
0.417
0.389
0.361
0.333
0.306
0.278
0.250
$8\tau_F/\tau^2$
0.00
0.05
0.10
4
5
6
7
8
9
10

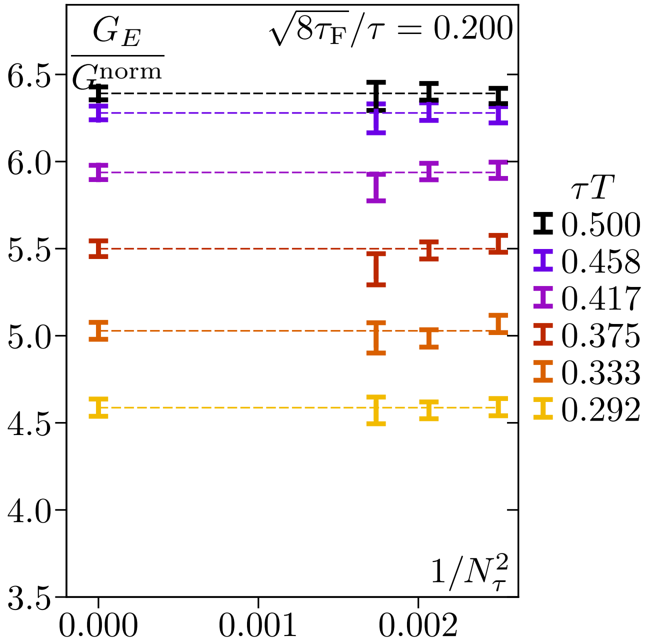


$\frac{2\rho_E}{\omega T^2}$
model
max_{NLO}
max_{LO}
smax_{NLO}
smax_{LO}
plaw_{NLO}
plaw_{LO}
ω/T
10^{0}
10^{1}
10^{2}
10^{3}
10^{-1}

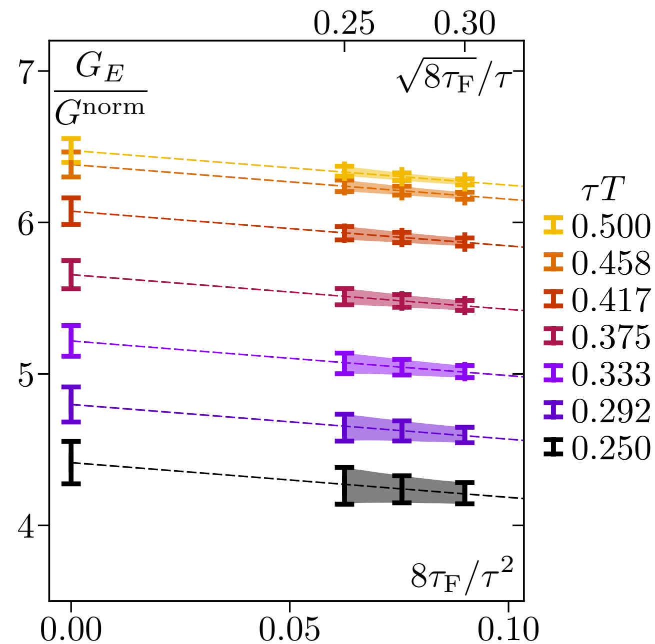


model
max_{NLO}
max_{LO}
smax_{NLO}
smax_{LO}
plaw_{NLO}
plaw_{LO}
κ/T^3
0
5
10
15

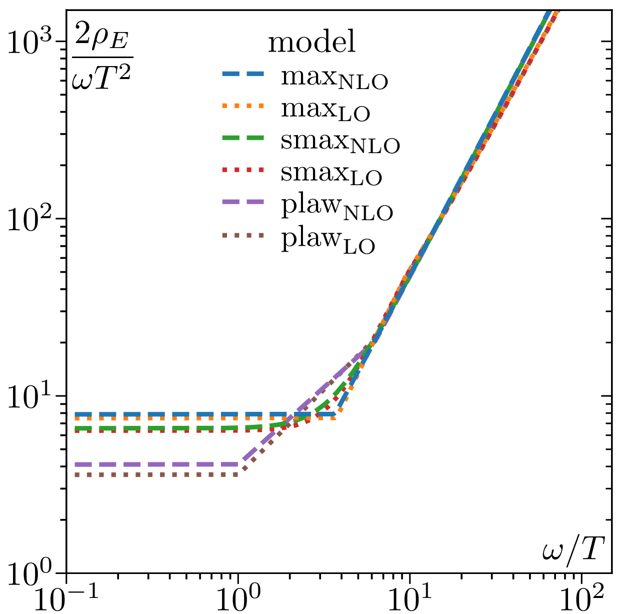
T=293 MeV:



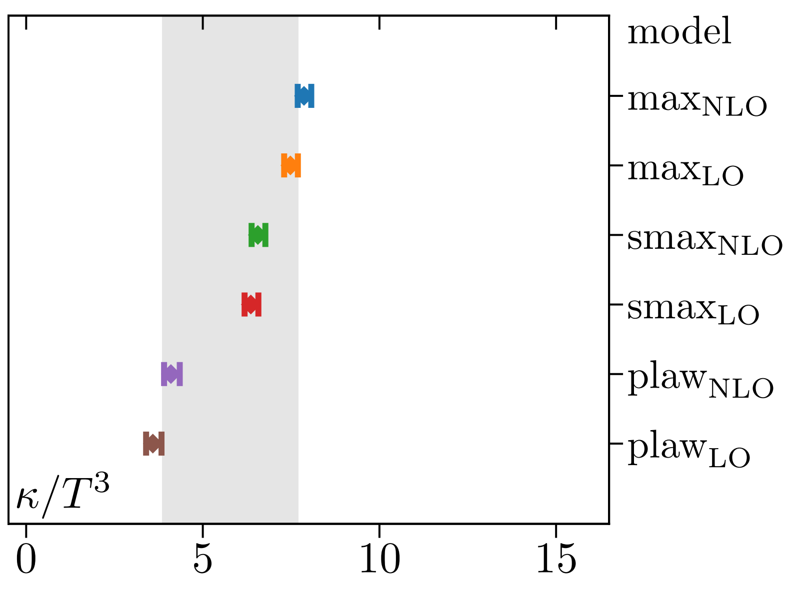
$\frac{G_E}{G^{\mathrm{norm}}}$
$\sqrt{8\tau_F}/\tau = 0.200$
6.5
6.0
5.5
5.0
4.5
4.0
3.5
0.000
0.001
0.002
$1/N_\tau^2$
τT
0.500
0.458
0.417
0.375
0.333
0.292



0.25
0.30
$\frac{G_E}{G^{\mathrm{norm}}}$
$\sqrt{8\tau_F}/\tau$
7
6
5
4
0.00
0.05
0.10
$8\tau_F/\tau^2$
τT
0.500
0.458
0.417
0.375
0.333
0.292
0.250



$\frac{2\rho_E}{\omega T^2}$
model
$\mathrm{max_{NLO}}$
$\mathrm{max_{LO}}$
$\mathrm{smax_{NLO}}$
$\mathrm{smax_{LO}}$
$\mathrm{plaw_{NLO}}$
$\mathrm{plaw_{LO}}$
10^3
10^2
10^1
10^0
10^{-1}
10^0
10^1
10^2
ω/T



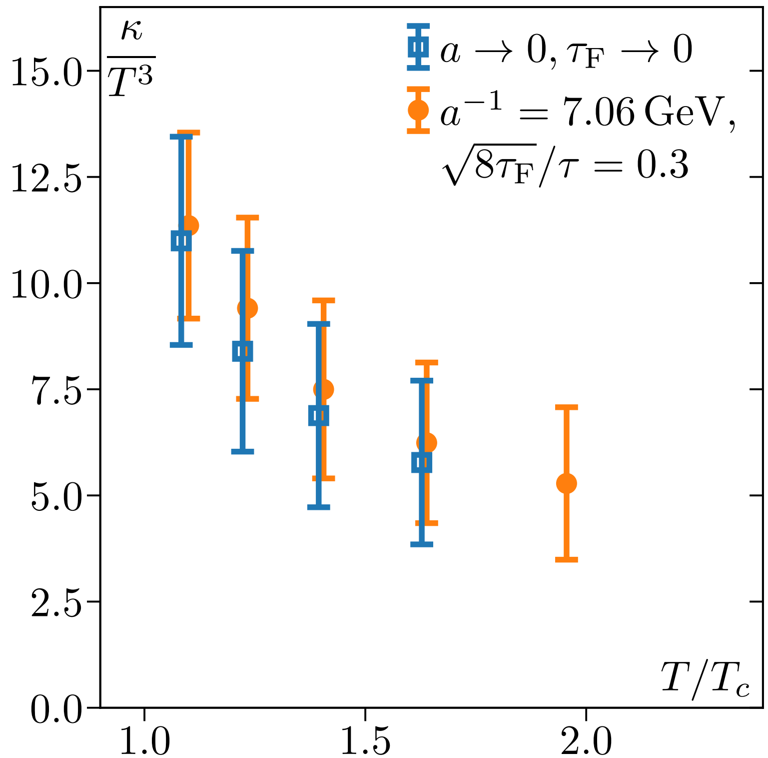
model
$\mathrm{max_{NLO}}$
$\mathrm{max_{LO}}$
$\mathrm{smax_{NLO}}$
$\mathrm{smax_{LO}}$
$\mathrm{plaw_{NLO}}$
$\mathrm{plaw_{LO}}$
κ/T^3
0
5
10
15

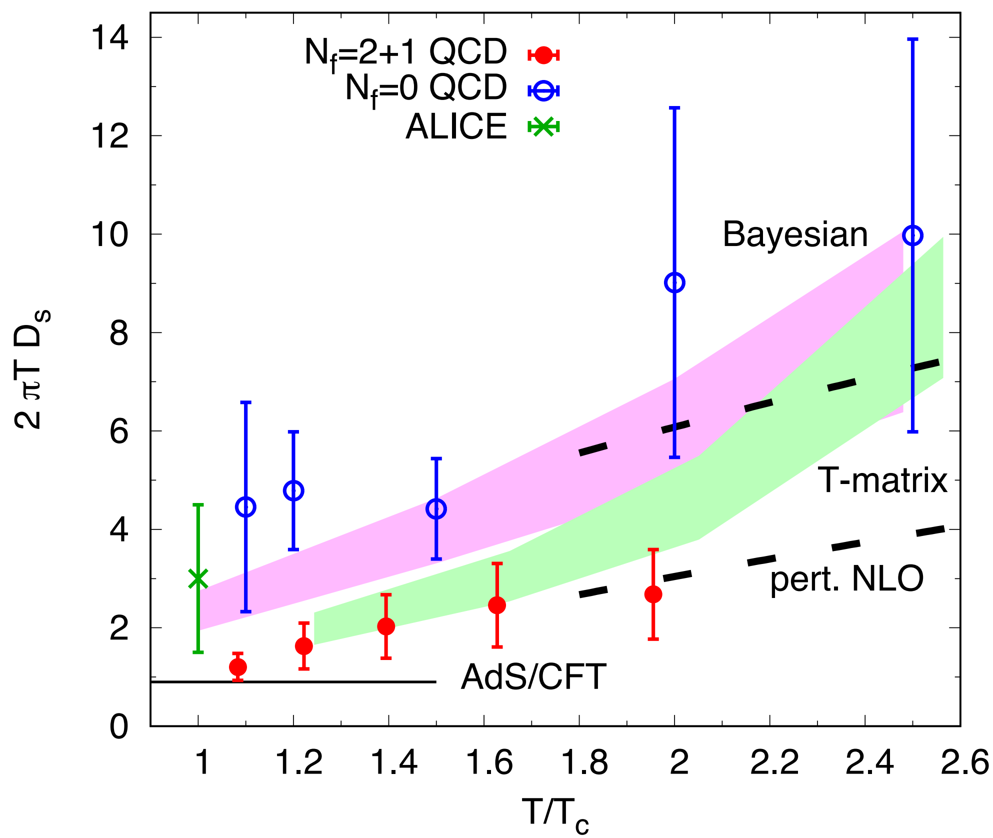
Heavy quark diffusion coefficient in QCD

- κ/T^3 has significant temperature dependence
- D_s is significantly smaller in 2+1 flavor QCD than in quenched QCD and is close to the AdS/CFT limit

$T_c \simeq 180$ MeV

$$D_s = \frac{2T^2}{\kappa}$$





Extend the calculations to smaller T and physical quark light quark masses

USQCD proposals

2005-2021 All Type-A proposal focused on EoS and various aspects of QCD phase diagram, a few Type-B proposals on spectral function

2022-2023 Type-A proposal "The heavy quark diffusion coefficient in (2+1)-flavor QCD from lattice"

Goal : generate $64^3 \times N_\tau$ lattices, $N_\tau = 20,\ 22,\ 24$ for $m_l = m_s/5$ and $m_l = m_s/20$ for the calculation of the heavy quark diffusion coefficient

Requested: 28.8 M KNL core hours, 0.22M MI100 GPU hours

Awarded: 16M KNL core hours, 0.175M MI100 GPU hours

2022-2023 Type-A continuation proposal "The heavy quark diffusion coefficient in (2+1)-flavor QCD from lattice"

Goal : generate $64^3 \times N_\tau$ lattices, $N_\tau = 18,\ 20,\ 22,\ 24,\ 26,\ 28$ for $m_l = m_s/20$ for the calculation of the heavy quark diffusion coefficient

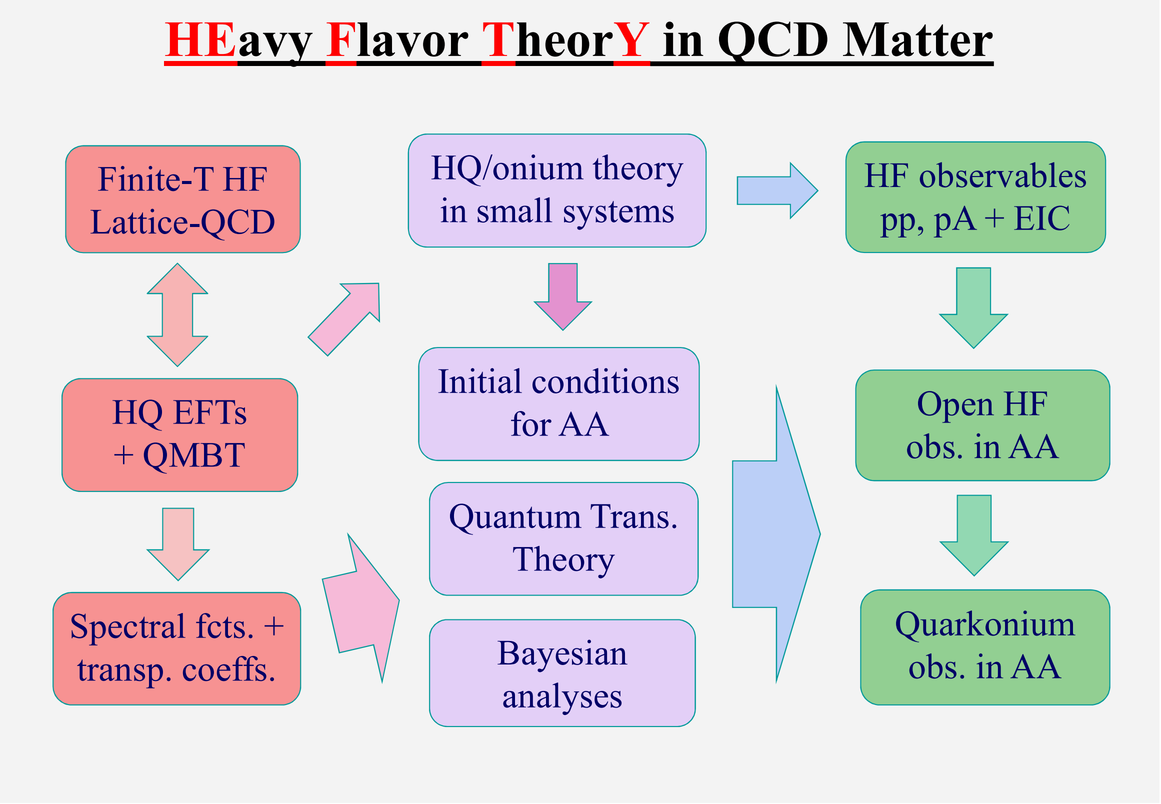
Requested: 40.3 M KNL core hours, 0.315M MI100 GPU hours

The generated gauge configurations will be also used to estimate meson spectral functions and the complex potential at *T>0*

Lattice QCD and phenomenology of heavy flavor probes

New topical collaboration
In nuclear theory

Ralf Rapp(PI), P. Petreczky,
R. Vogt (co-spokespersons),
S. Bass, X. Dong, Frawley,
Y-J. Lee T. Mehen, S. Mukherjee,
J. Qiu, M. Strickland, I. Vitev



INT program
Heavy Flavor Production in Heavy-Ion and Elementary Collisions (22-3)
Z. Meziani, P. Petreczky, R. Vogt

Summary

- The thermal width of bottomonium increases with T and leads to melting:

  $T_{melt}(\Upsilon(3S)) \simeq T_{melt}(\chi_b(2P)) \simeq 220$ MeV
  $T_{melt}(\Upsilon(2S)) \simeq T_{melt}(\chi_b(1P)) \simeq 360$ MeV

  Consistent with analysis of spatial meson correlators

- No significant thermal modification of bottomonium masses have been found in contrast with the expectations based on potential models with screened potential

- Lattice calculations confirm the existence of the imaginary part of the potential; There is no evidence for the screening of the real part of the potential $\Rightarrow$ Matsui and Satz picture is not correct, quarkonium melting is not related to color screening

- First full QCD calculation of the heavy quark diffusion coefficient become available now and indicate that κ/T^3 is larger than un quenched QCD and close to the Ads/CFT bound

- Extend the lattice calculations to larger N_τ and physical quark masses (Goal of the 2022 and 2023 USQCD proposals)

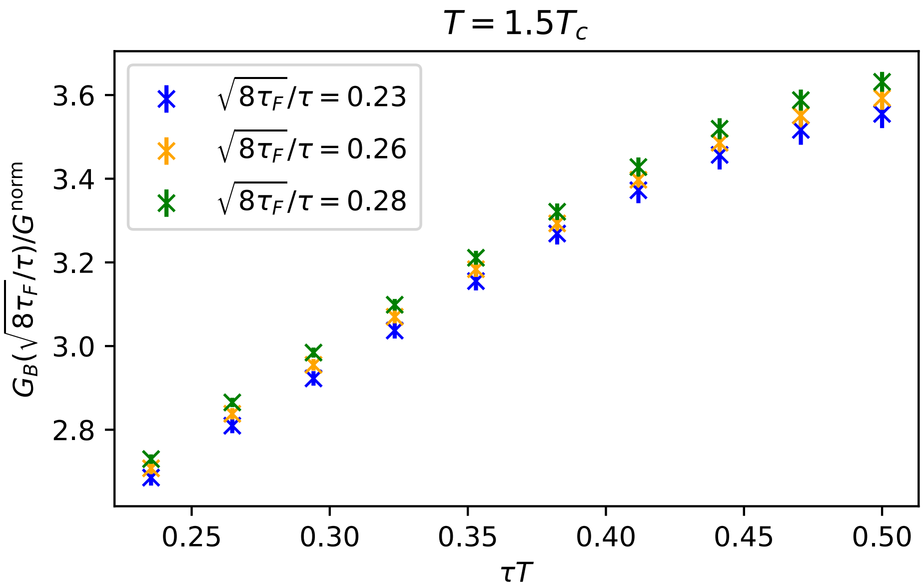
- Interface between lattice QCD and phenomenology $\Rightarrow$ Theory Topical Collaboration

Back-up: Mass suppressed correction to heavy quark diffusion coefficient

$1/M$ correction to the momentum heavy quark diffusion coefficient $\Rightarrow G_B(\tau, T)$
$G_B(\tau, T)$ has anomalous dimension $\Rightarrow$ additional matching to $\overline{MS}$ is needed

Quenched QCD

Gradient flow + incomplete 1-loop matching



Multi-level algorithm + non-perturbative matching via Schrödinger functional

$1.5T_c : \kappa_B = (1.23 - 2.54)T^3,$

Brambilla, Leino, Mayer-Steudte, PP (TUMQCD), PRD 107 (2023) 054508

$\kappa_B = (1.0 - 2.1)T^3$

Banerjee, Datta, Laine JHEP 08 (2022) 128

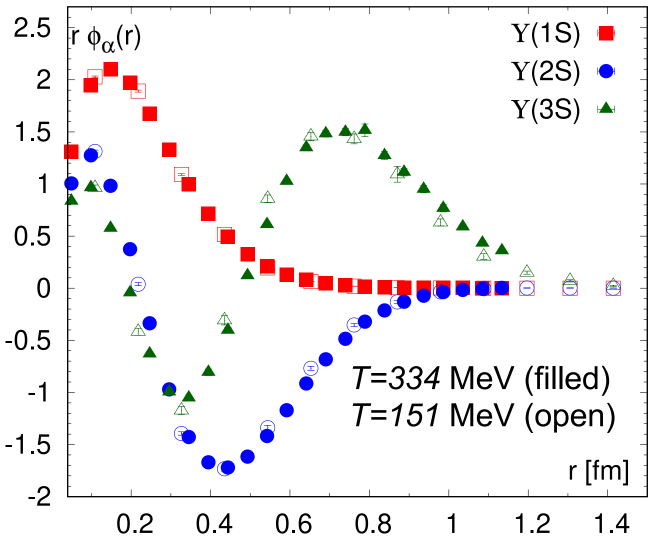
$\langle v^2 \rangle$ is taken from PP, EPJC 62 (2009) 85

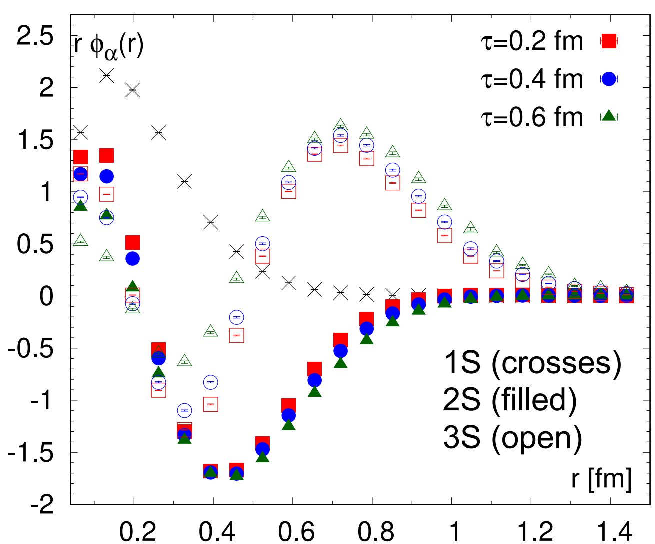
10-20% correction for bottom quark, ~30% correction for charm quark

Back-up: Bethe-Salpeter amplitude at *T>0* and potential model

Larsen, Meinel, Mukherjee, PP, PRD 102 ('20) 114508

Shi et al, PRD 105 ('22) 014017





potential model
with inverse problem
+
Thermal width
from lattice
+
Machine learning

No color screening