Lattice QCD for RHIC and LHC

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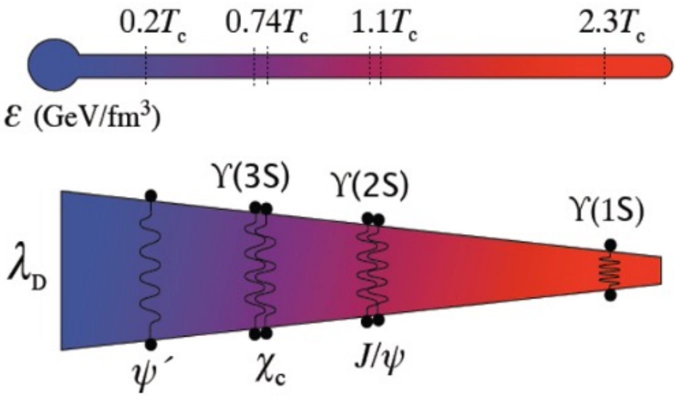
- Challenges for lattice QCD:
  1) Phase diagram and EoS at non-zero baryon density, see talk by Claudia Ratti
  2) Properties of heavy quark and quarkonia at $T>0$
     => heavy flavor probes of high T QCD matter
     => inner workings of QGP, this talk
- Lattice QCD: complex potential at $T>0$ *(is Matsui-Satz conjecture on screening and quarkonium melting correct ?),*
  in-medium quarkonium masses and widths, heavy quark diffusion coefficient

- Connecting lattice QCD to phenomenology => Theory Topical Collaborations
- Computational needs

Hot and Cold QCD Town Hall Meeting, September 23-25, 2022

Heavy flavor probes and lattice QCD

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



<u>RHIC</u>	<u>LHC Runs 3-5</u>
sPHENIX, STAR+	ALICE 2-3, CMS+,ATLAS+,LHC+
2023-2025	2022-2038

<u>Lattice:</u>		<u>Phenomenology:</u>
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

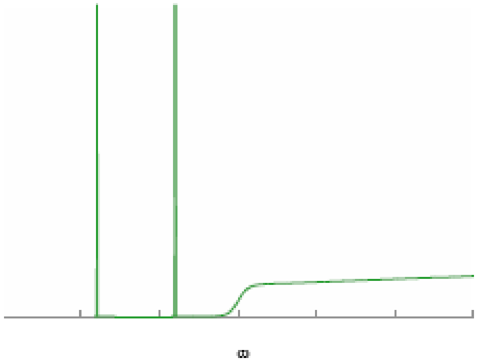
Meson correlators and spectral functions

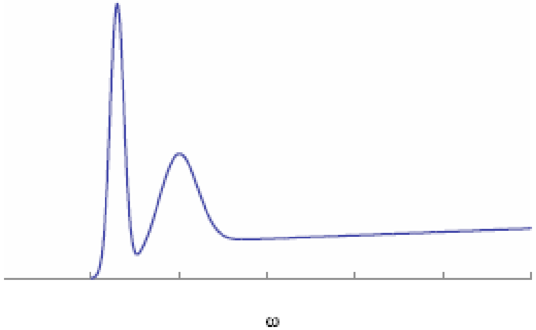
Vacuum and in-medium properties as well as dissolution of mesons are encoded in the spectral functions:

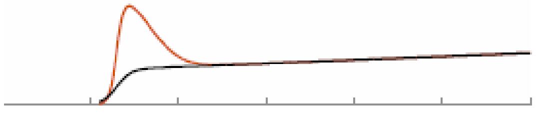
$$\rho(\omega,p,T)=\frac{1}{2\pi}\mathrm{Im}\int_{-\infty}^{\infty}dt e^{i\omega t}\int d^3x e^{ipx}\langle[O(x,t),O(0,0)]\rangle_T,\quad O(x,t)\sim\bar{Q}(x,t)\Gamma Q(x,t)$$

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







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

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

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

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

Very difficult problem !

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

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

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

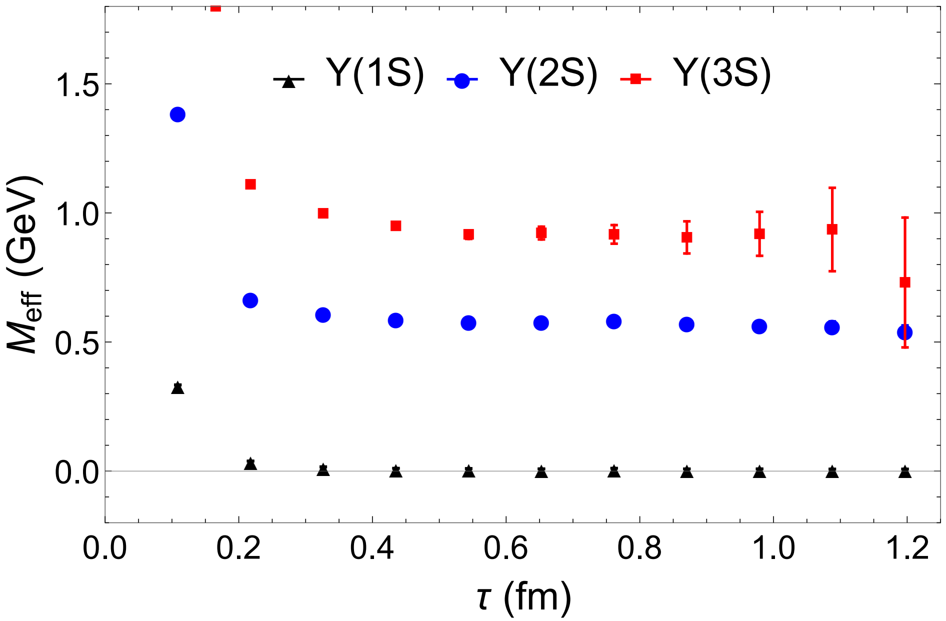
$$\rho_\alpha(\omega,T)=\rho_\alpha^{\text{med}}(\omega,T)+\rho_\alpha^{\text{high}}(\omega)$$

parametrized
as single peak+ tail

constrained at
T=0

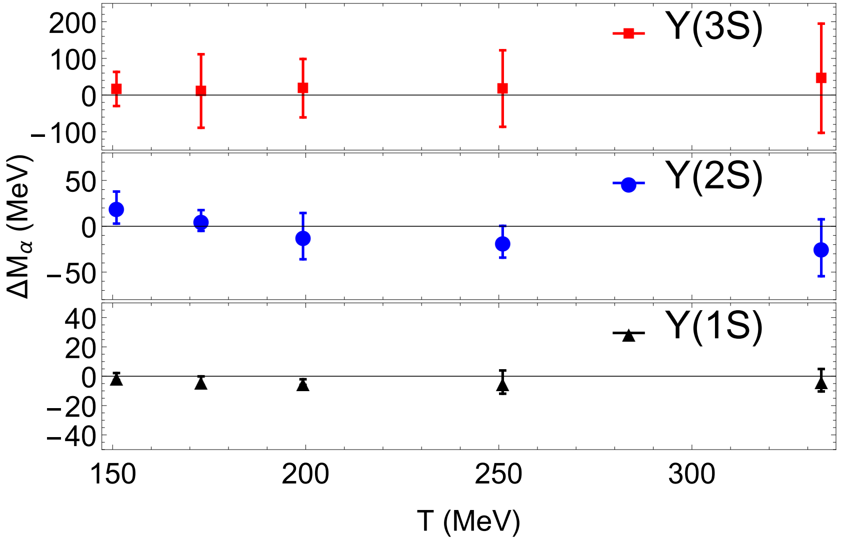
Larsen, Meinel, Mukherjee, PP, PLB 800 (20) 135119

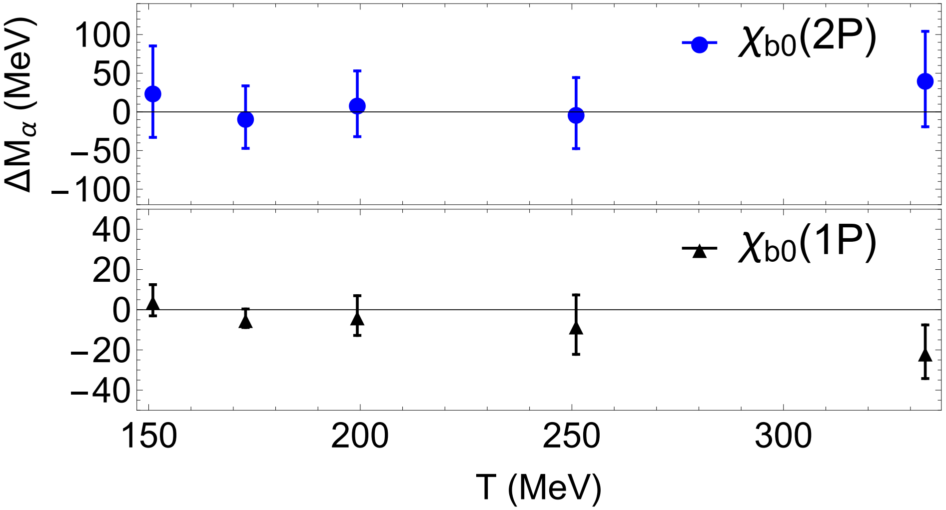
$$M_{\text{eff}}(\tau)=\frac{1}{a}\ln[C_\alpha(\tau)/C_\alpha(\tau+a)]$$



Thermal mass shift of bottomonium

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

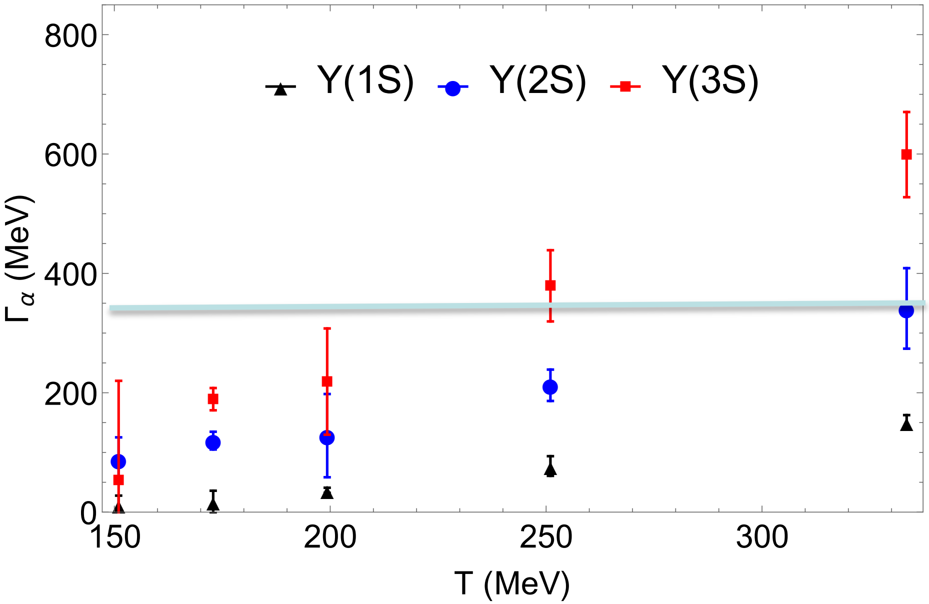


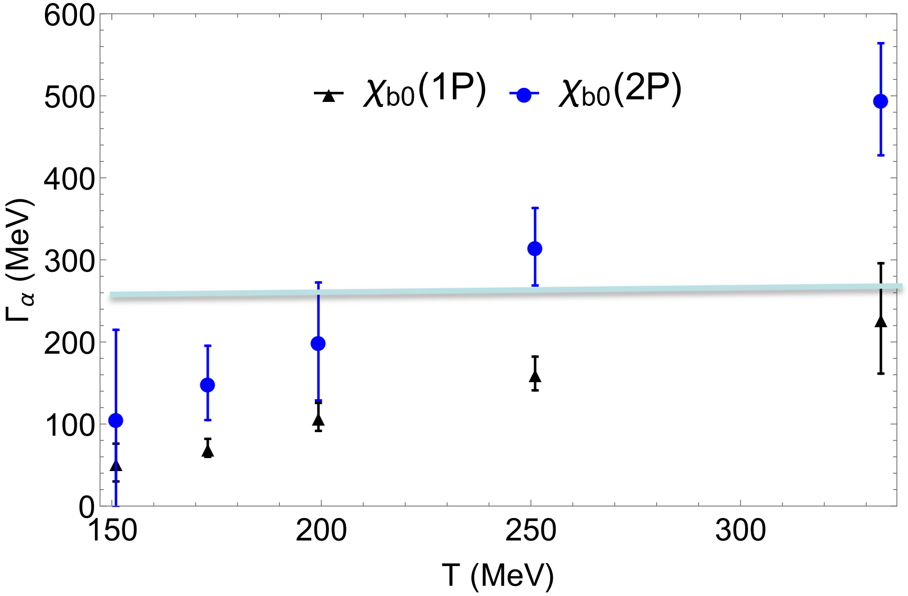


No significant thermal mass shift is observed in any of the bottomonium states contrary to expectations of the potential model with screened potential

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 $r \sim 1/m_D$

Based on weak coupling

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 $\mathrm{Im}V(r,T)$

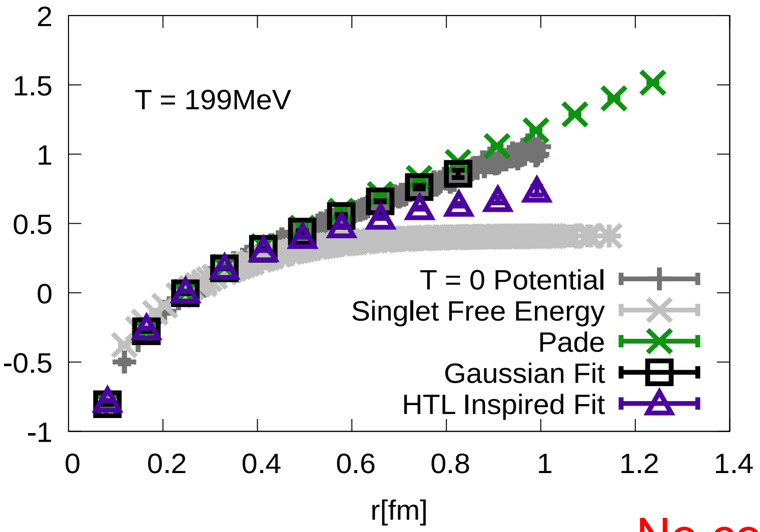
Rothkopf, Hatsuda, Sasaki, PRL 108 (2012) 162001

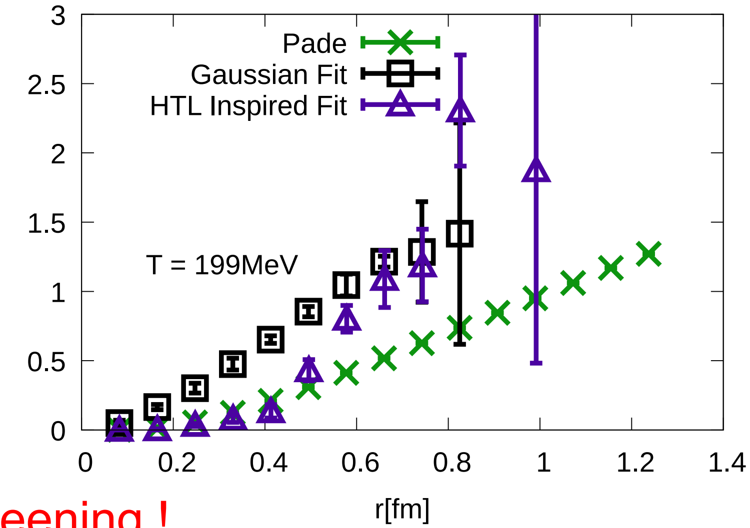
Challenge: reconstruct $\rho_r(\omega,T) \Rightarrow$ use the same approach as for reconstruction of the NRQCD bottomonium spectral functions

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

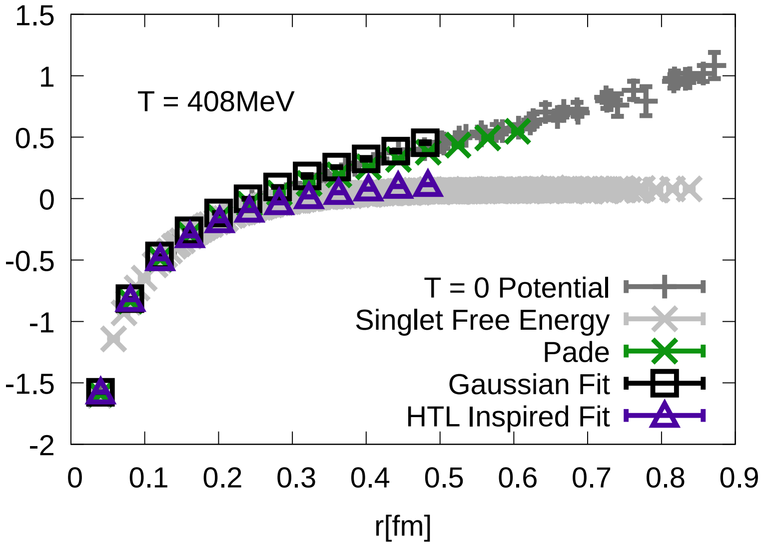
HISQ, $N_\tau = 12$

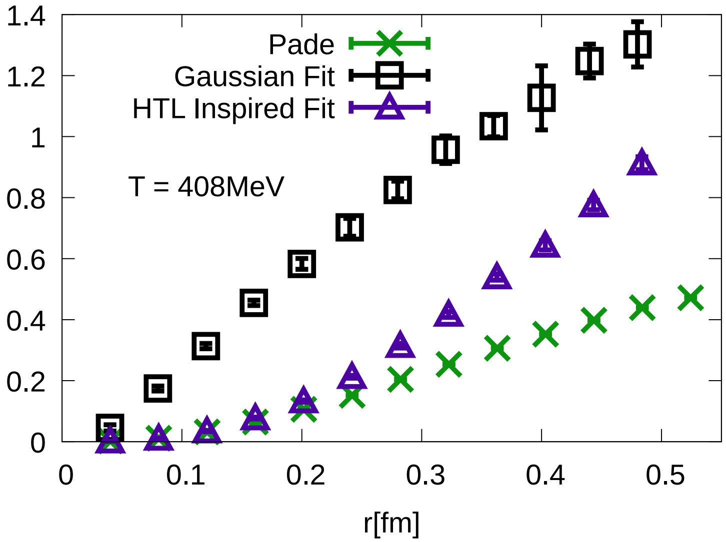
Bala et al (HotQCD), PRD 105 (2022) 054513





No color screening !

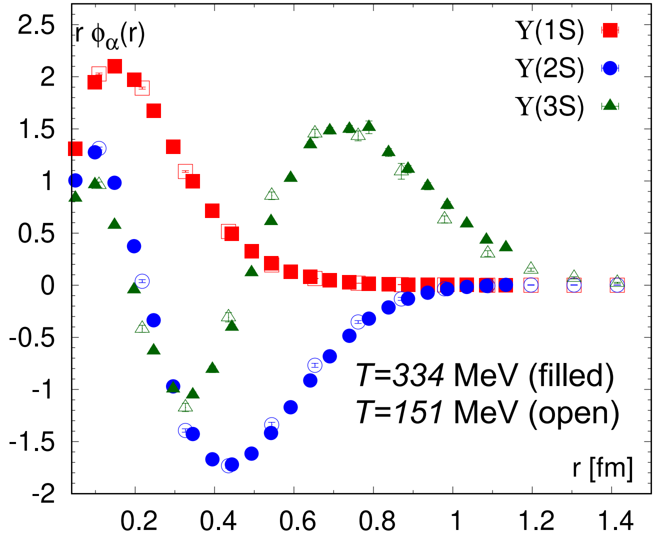


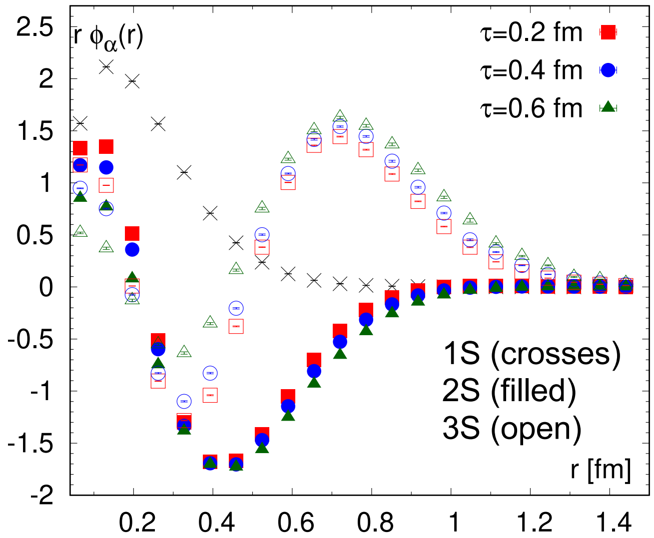


Bethe-Salpeter amplitude at *T>0* and potential model

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

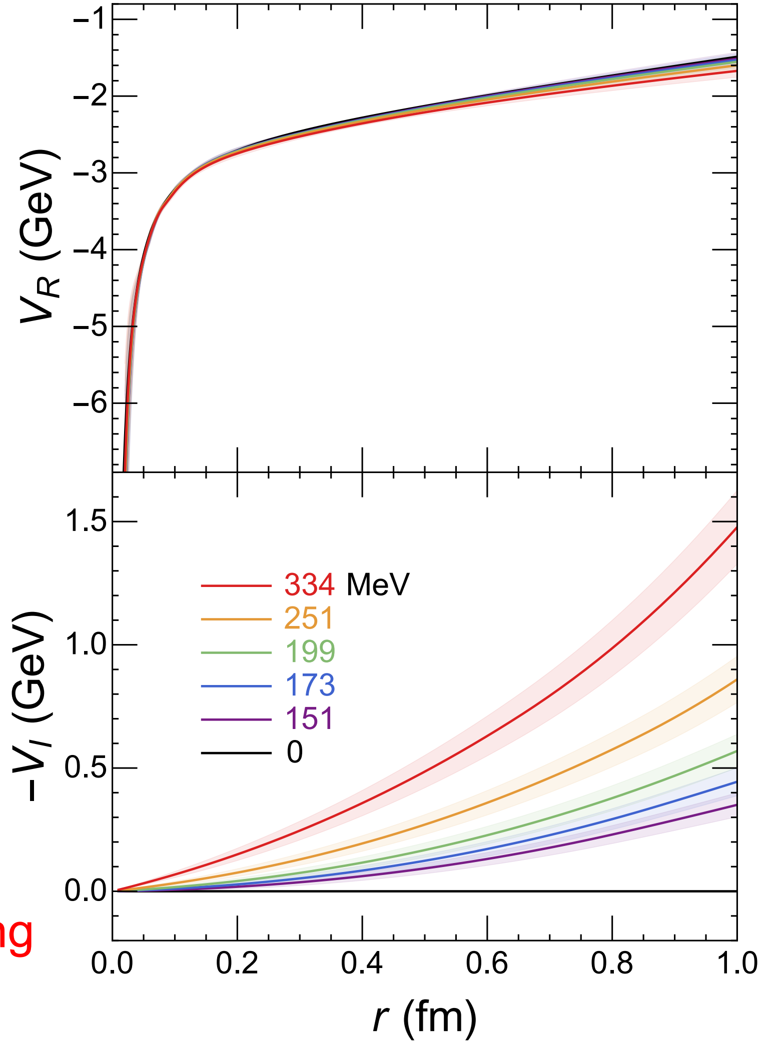
Shi et al, PRD 105 ('22) 014017





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

No color screening



Heavy quark diffusion and lattice QCD

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

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

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

Heavy quark effective theory:

$$\langle \mathbf{v}^2 \rangle = \frac{3T}{M}$$

$$t \to i\tau$$

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

Casalderrey-Solana, Teaney, PRD 74 (2006) 085012; Caron-Huot, Laine, Moore, JHEP 0904 ('09) 053
Bouttefeux, Laine, JHEP 12 (2020) 150

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

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

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

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

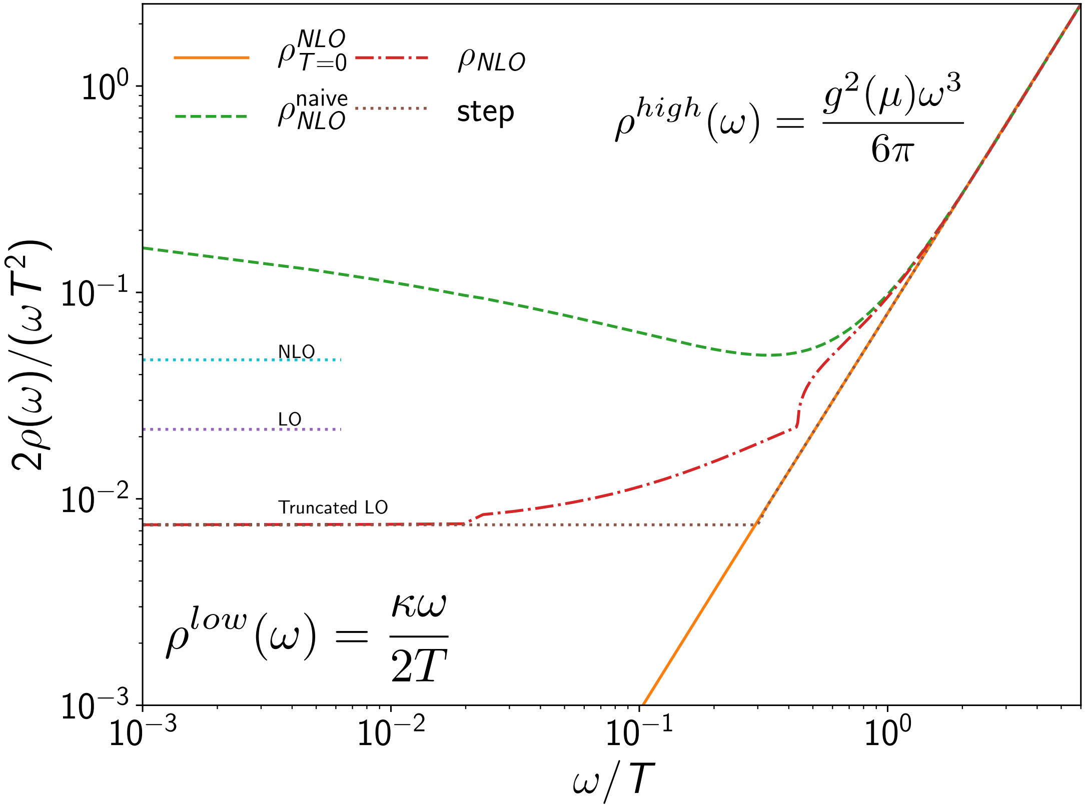
Extracting momentum diffusion coefficient from the lattice

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

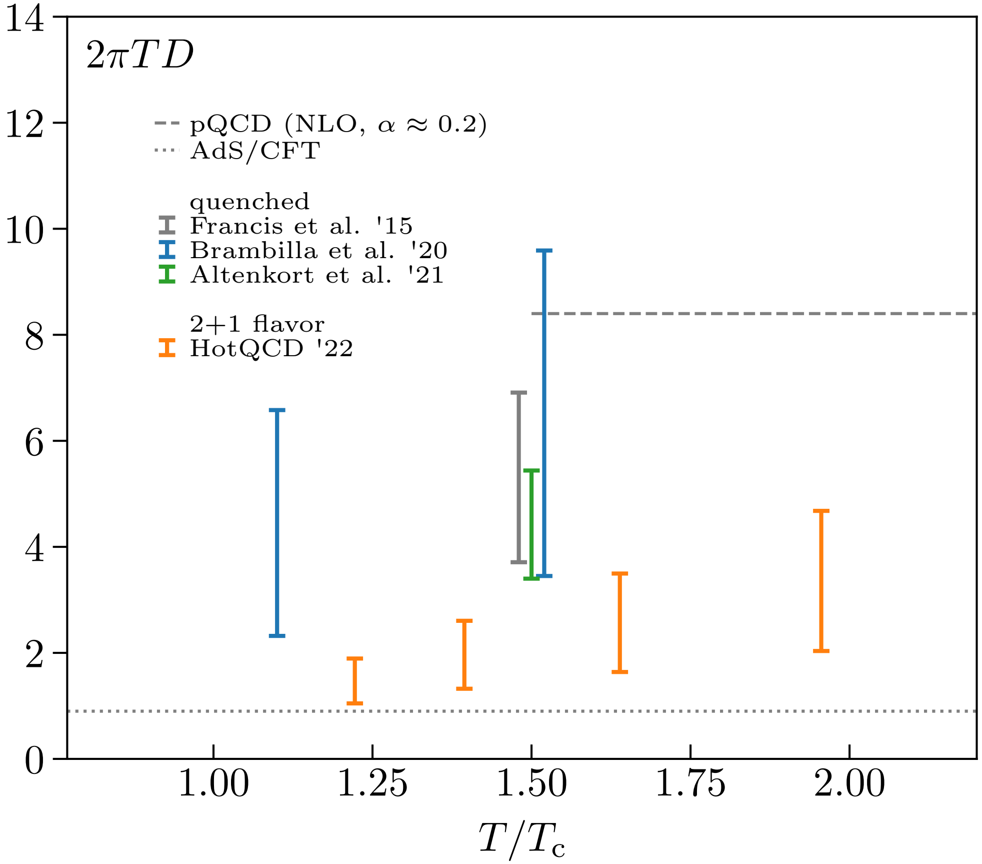


⇒ use known large and small energy behavior of the spectral

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

Heavy quark diffusion constant in QCD and *1/M* correction

2+1 flavor QCD with $m_\pi = 300$ MeV, $96^3 \times N_\tau$ lattice; Gradient flow for noise reduction



κ/T^3 is significantly larger in 2+1 flavor QCD than in quenched QCD and is close to the AdS/CFT limit

1/M correction: $1.5T_c : \kappa_B = (1.23 - 2.54)T^3$, $\kappa_B = (1.0 - 2.1)T^3$

Brambilla et al, arXiv:2206.02861 Banerjee et al, arXiv:2204.14075

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

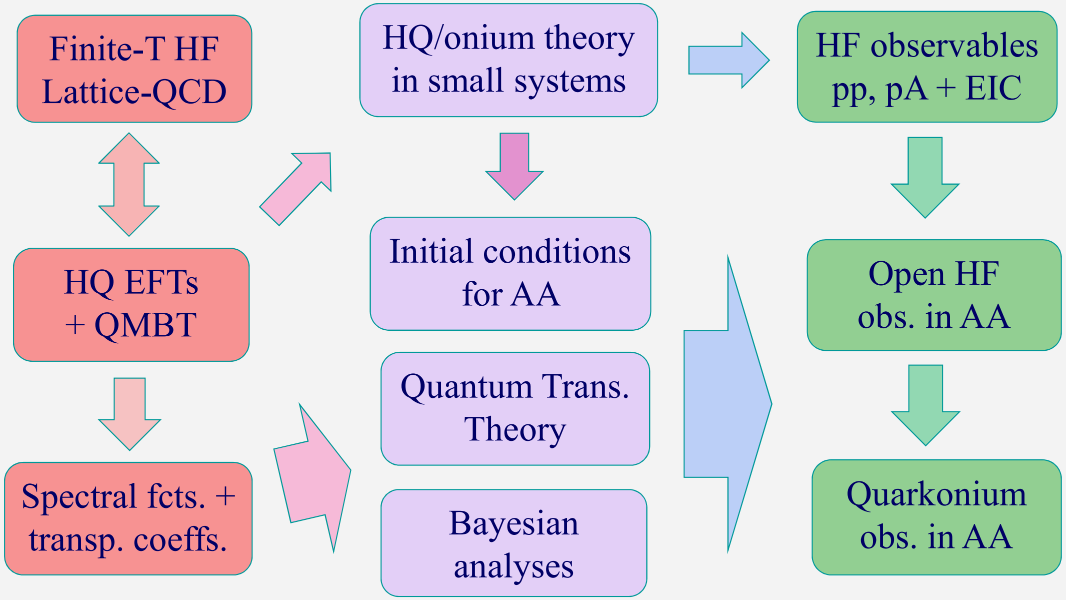
Lattice QCD and phenomenology of heavy flavor probes

New proposal for topical collaboration

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

See talk by I. Vitev

HEavy Flavor TheorY in QCD Matter


Finite-T HF Lattice-QCD

HQ EFTs + QMBT

Spectral fcts. + transp. coeffs.

HQ/onium theory in small systems

Initial conditions for AA

Quantum Trans. Theory

Bayesian analyses

HF observables pp, pA + EIC

Open HF obs. in AA

Quarkonium obs. in AA

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

Computational needs

Progress described above in lattice QCD calculations would not have been possible without SciDAC program and computational sources provided by USQCD clusters, NERSC, ALCC and INCITE programs

Need to increase the lattice extent and go to physical quark masses

$$\text{Currently } N_\tau = 12 \text{ or } m_\pi = 300 \text{ MeV}$$

Continue and increase investments in nuclear physics computing

Computational Nuclear Physics and AI/ML Workshop

- Organized by:
  - Alessandro Lovato (ANL)
  - Joe Carlson (LANL)
  - Phiala Shanahan (MIT)
  - Bronson Messer (ORNL)
  - Witold Nazarewicz (FRIB/MSU)
  - Amber Boehnlein (JLab)
  - Peter Petreczky (BNL)
  - Robert Edwards (JLab)
  - David Dean (JLab)
- 6-7 September 2022 at SURA in Washington, DC
- 60 registered participants (40 in person, 20 on-line), i
- https://indico.jlab.org/event/581/
  - All talks archived
  - Short white paper being prepared for the LRP

Computational Nuclear Physics and AI/ML Workshop

6-7 September, 2022 / SURA headquarters

Organized by:
Alessandro Lovato – Joe Carlson (LANL), Phiala Shanahan (MIT), Bronson Messer (ORNL)
Witold Nazarewicz (FRIB/MSU), Amber Boehnlein (JLab), Peter Petreczky (BNL)
Robert Edwards (JLab), David Dean (JLab)

Admin support: Jae Cho jcho@jlab.org Tea Jojua tjojua@sura.org Sherry Thomas sthomas@jlab.org

Schedule
Registration, schedule, and other information can be found at: https://indico.jlab.org/event/581/

Tuesday, 6 September

1:00 – 1:05	Welcome, David Dean and Sean Hearne
1:05 – 1:20	DOE remarks, Tim Hallman
1:20 – 2:00	QCD, William Detmold (JLab) and Swagato Mukherjee (BNL)
2:00 – 2:40	Quantum many-body problems, Thomas Papenbrock (UT/ORNL)
2:40 – 3:00	BREAK
3:00 – 3:40	Fundamental Symmetries,Emanuele Mereghetti (LANL)
3:40 – 4:20	Astrophysics, George Fuller (UCSD)
4:20 – 5:00	AI/ML, Amber Boehnlein (JLab)
5:00 – 5:40	Preliminary list of recommendations discussion (Peter Petreczky, lead)
5:40 – 7:30	Reception

Wednesday, 7 September

7:45 – 8:30	Continental Breakfast
8:30 – 10:00	Breakout Sessions 1. QCD (Phiala Shanahan, lead) 2. Nuclear Structure and fundamental symmetries (Alessandro Lovato, lead) 3. Astrophysics (Bronson Messer, lead)
10:00 – 10:30	Break
10:30 – 12:00	Breakout reports
12:00 – 1:00	Lunch
1:00 – 2:30	Recommendations discussion and next steps

Jefferson Lab
Thomas Jefferson National Accelerator Facility

SURA

Workshop Resolution

High-performance computing is essential to advance nuclear physics on the experimental and theory frontiers. Increased investments in computational nuclear physics will facilitate discoveries and capitalize on previous progress. Thus, we recommend a targeted program to ensure the utilization of ever-evolving HPC hardware via software and algorithmic development, which includes taking advantage of novel capabilities offered by AI/ML.

The key elements of this program are to:

1) Strengthen and expand programs and partnerships to support immediate needs in HPC and AI/ML, and also to target development of emerging technologies, such as quantum computing, and other opportunities.
2) Take full advantage of exciting possibilities offered by new hardware and software and AI/ML within the nuclear physics community through educational and training activities.
3) Establish programs to support cutting-edge developments of a multi-disciplinary workforce and cross-disciplinary collaborations in high-performance computing and AI/ML.
4) Expand access to computational hardware through dedicated and high-performance computing resources.

Similar computational nuclear physics workshop was organized for the 2015 Long Range Plan and its recommendation have been adopted as one of the initiatives in 2015 !

Summary

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

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

  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 ⇒ 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

- Need to interface lattice QCD and phenomenology ⇒ Theory Topical Collaboration

- Increased investments in computational nuclear physics are needed