A new method for numerical analytic continuation

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based on:
PRL 111 (2013) 18, 182003

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Motivation

- **Relativistic Heavy-Ion Collisions:** Investigation of the properties of the produced Quark-Gluon Plasma requires a thorough understanding of inherently dynamical processes:
  - Global bulk evolution characterized **by shear and bulk viscosities**
  - Broadening of high-energy jets described via the **jet quenching parameter qhat**
  - Energy loss of individual heavy quarks characterized via a **diffusion coefficient**
  - The melting of heavy quarkonium bound states via a **complex heavy quark potential**
- **Non-perturbative quantities:** Not accessible from usual perturbation theory.
- **Common challenge:** Real-time quantities are not directly accessible in non-perturbative simulations such as Lattice QCD Monte Carlo and require analytic continuation.
- **Spectral functions:** A bridge between the Euclidean and Minkowski time domain

$$D(\tau)=\int d\omega\, K(\tau,\omega)\,\rho(\omega) \quad\Rightarrow\quad D(t)=\int d\omega\, K(it,\omega)\,\rho(\omega)$$

  - Time dependence separated into integral kernel, real- and imaginary time observable from same ρ
  - **In practice** one faces the **ill defined problem** to extract from N_τ **noisy** correlator **estimates** $D(\tau_i)=D_i$ the positive and smooth function ρ(ω), **discretized at $N_\omega >> N_\tau$ points**. I.e. one attempts to invert the following convolution over a known Kernel function K(τ,ω):

$$D(\tau)=\int_{\omega_{min}}^{\omega_{max}} d\omega\, K(\tau,\omega)\rho(\omega) \xrightarrow{\text{discretization}} D_i=\sum_{l=1}^{N_\omega}\Delta\omega_l K_{il}\rho_l$$

  - Fortunately the **complete spectral function** from Euclidean time usually **not required**:

$$V=\lim_{t\to\infty}\frac{\int d\omega\,\omega e^{i\omega t}\rho(\omega)}{\int d\omega e^{i\omega t}\rho(\omega)} \qquad \xi=\lim_{\omega\to 0}\frac{\rho(\omega)}{\omega}$$

Heavy quark potential from position and width of lowest lying peak — Transport coefficients from slope at origin

- **Technical challenge:** The most prevalent method to date, the Maximum Entropy Method is based on Bayesian inference. Nevertheless even after more than a decade of application its reliability is still under discussion. Questions arise in regard to: M. Asakawa, T. Hatsuda and Y. Nakahara, Prog. Part. Nucl. Phys. 46, 459 (2001)
  - The standard implementation by Bryan artificially restricts the space of possible solutions.
  - Convergence is very slow due to flat directions in the Shannon Jaynes Entropy
  - Extending the search space significantly improves the reconstruction quality but also increases computational cost. Nevertheless peaks appear Gaussian even if Lorentzian shape is encoded in the the data. A. Rothkopf, J. Comput. Phys. 238 (2013) 106
  - Gaussian approximations enter the hyper-parameter α estimation. In addition the integration over ρ is extended beyond [0,∞]. J.Skilling, S.F.Gull, Lecture Notes-Monograph Series 20, 341 (1991) M.Jarrell and J.E.Gubernatis, Physics Reports, 269, 133-195, (1996)

New Bayesian Spectral Reconstruction

- Here we elaborate on a novel approach to spectral function reconstruction that avoids the above problems. Improvements are related to: the axiomatic construction of a **scale independent prior distribution**, explicit **integration of hyperparameters.**
- A naïve likelihood L fit (N_τ datapoint D_i vs N_ω parameters ρ_l) leads to degenerate solutions

$$D_i^\rho=\sum_{l=1}^{N_\omega}\Delta\omega_l e^{-\omega_l\tau_i}\rho_l \qquad L=\frac{1}{2}\sum_{i,j}\left(D_i-D_i^\rho\right)C_{ij}^{-1}\left(D_j-D_j^\rho\right)$$

C_{ij} covariance matrix

- **The Bayesian strategy**: Incorporation of **prior information (I)** allows regularization of an otherwise underdetermined χ^2 fit. see e.g.: C.M. Bishop, Pattern Recognition and Machine Learning, Springer, 2nd ed. (2007)

$$P[\rho|D,I]\propto P[D|\rho,I]\,P[\rho|I] \qquad P[D|\rho,I]=\exp[-L-\gamma(L-N_\tau)^2]$$

  - If L/N_τ>>1, ρ does not reproduce the datapoints within their errorbars, while if L/N_τ<<1 the spectrum will contain many unnatural structures arising from overfitting the noise in the data. Hence the most neutral reconstruction will satisfy L/N_τ= 1, which we impose as constraint arising from prior knowledge.
- **Improved prior functional:** enforces (1) positive definiteness of ρ (2) independence of the result from dimension of ρ (3) smoothness of ρ, where data does not imprint peaks
  - In general ρ(ω) does not have to be a probability distribution. Indeed, depending on the observable the spectrum is associated with, its scaling can differ from 1/ω. We hence require that the dimension of ρ and hence m shall not change the result of the reconstruction. I.e. we must construct our prior probability using ρ/m only.
  - ρ is a positive definite and smooth function. The prior functional shall impose these traits on the reconstructed spectrum even if no further prior information is known. I.e. in the case of $m(\omega)=m_0$, a smooth spectrum shall be chosen independently of m_0. Hence we penalize spectra which deviate between two adjacent frequencies ω_1 and ω_2.

$$P[\rho|I]=e^S \qquad S=\alpha\sum_{l=1}^{N_\omega}\Delta\omega_l\left(1-\frac{\rho_l}{m_l}+\log\left[\frac{\rho_l}{m_l}\right]\right)$$

m_l **default model**: correct spectrum in the absence of data. Y.Burnier, A. Rothkopf Phys.Rev.Lett. 111 (2013) 18, 182003

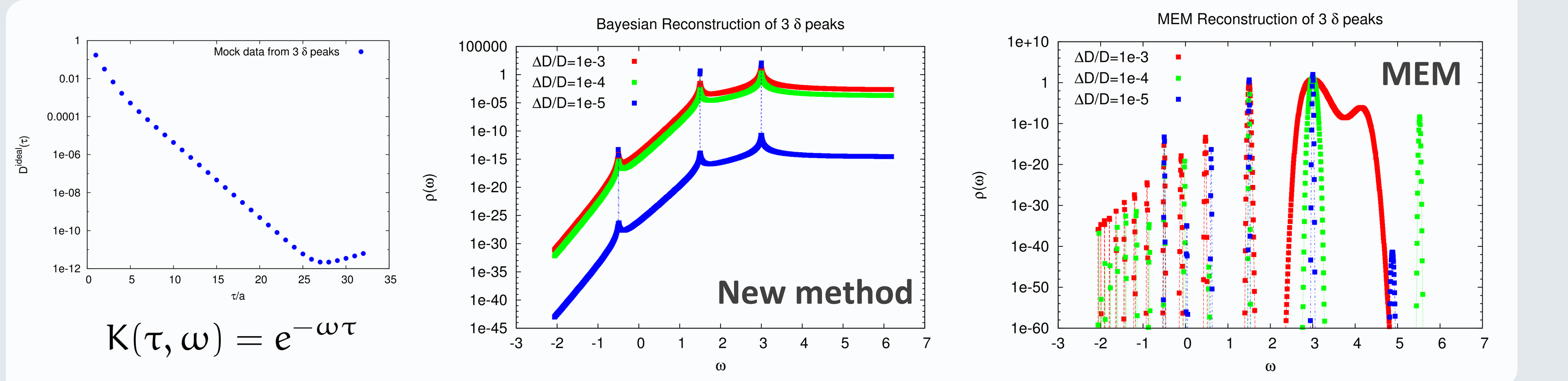
  - This new prior distribution is **strictly concave** and exhibits the same **quadratic behavior around the maximum** ρ=m as the Shanon-Jaynes entropy S_{SJ}. Hence the **uniqueness of its maximum** can be established analogously to the MEM. In the case where $\rho_l,m_l << 1/\alpha$ or $\rho_l << m_l$, their contribution to S and to the variation δS/δρ is not suppressed, thus we avoid the asymptotic flatness inherent in S_{SJ}. Proof of uniqueness for S_{SJ} in: M. Asakawa, T. Hatsuda and Y. Nakahara, Prog. Part. Nucl. Phys. 46, 459 (2001);
- **Hyperparameter α** is **integrated out** explicitly using no additional prior knowledge: P[α]=1

$$P[\rho|D,I]\propto P[D|\rho,I]\int_0^\infty d\alpha\, P[\rho|I,\alpha] \qquad \frac{\delta}{\delta\rho}P[\rho|D,I]\Big|_{\rho=\rho^{BR}}=0$$

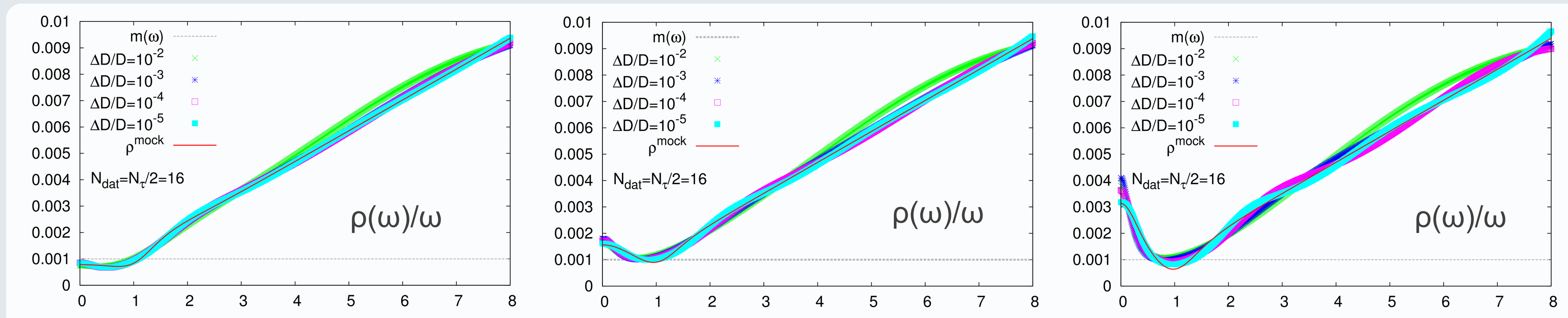
- **Bayesian solution**: Maximum of the α independent posterior (point estimate)
  - In practice we deploy the quasi-newton **LBFGS algorithm**, which allows us to **approach δP[ρ|D,m]/δρ=0** by varying each of the N_ω~1000 parameters ρ_l individually. Note that in contrast to the MEM with S_{SJ}, now without flat directions, we successfully **locate the global extremum of P[ρ|D,m]** and do not need to stop the algorithm at an artificial cutoff in step size.

Tests and Applications

- **Resolution test: Delta-peak spectral functions from mock data**
  - Spectral peaks encode vital information on physical observables, be it particle masses and their decay widths or more abstract quantities, such as the real- and imaginary part of the heavy quark potential. Here we test our reconstruction method on a simple spectrum of three delta peaks and compare to MEM.



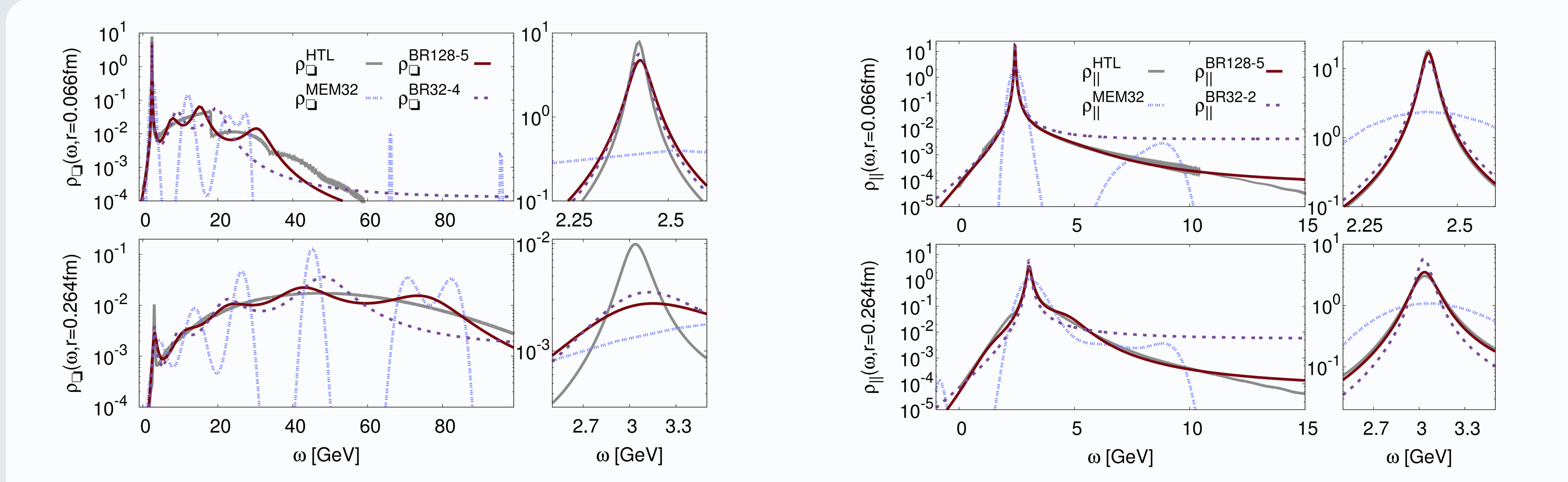
  - Both methods are supplied N_τ=32 ideal datapoints perturbed by Gaussian noise, corresponding to errors of $\Delta D/D=10^{-3}$ (red) 10^{-4} (green) 10^{-5} (blue). Note the absence of artificial peaks with the new method.
- **Transport coefficients:** Extract the peak at zero frequency in the normalized spectrum



  - Based on the modified T>0 Kernel: $K(\tau,\omega)=\omega\frac{\beta}{2}\frac{\cosh[\omega(\tau-\frac{1}{2}\beta)]}{\sinh[\omega\frac{\beta}{2}]}$ 15% deviation @ $\Delta D/D=10^{-4}$, <5% deviation @ $\Delta D/D=10^{-5}$
- **The heavy quark potential from HTL Euclidean correlators**
  - **Challenging** for spectral reconstruction since functional form of spectral peak needs to be faithfully reconstructed, i.e. not only **position** but **also width** of a **skewed Loretzian** is required. Y. Burnier and A. Rothkopf, Phys. Rev. D 86 (2012) 051503

$$\rho(r,\omega)\propto\frac{|\mathrm{Im}V(r)|\cos[\mathrm{Re}\sigma_\infty(r)]-(\mathrm{Re}V(r)-\omega)\sin[\mathrm{Re}\sigma_\infty(r)]}{\mathrm{Im}V(r)^2+(\mathrm{Re}V(r)-\omega)^2}+c_0(r)+c_1(r)(\mathrm{Re}V(r)-\omega)+\cdots$$

  - Test of the potential extraction via spectral reconstruction using leading order hard thermal loop perturbation theory, where the potential, the spectral function, as well as the Euclidean Wilson loops/ Wilson line correlators are known:

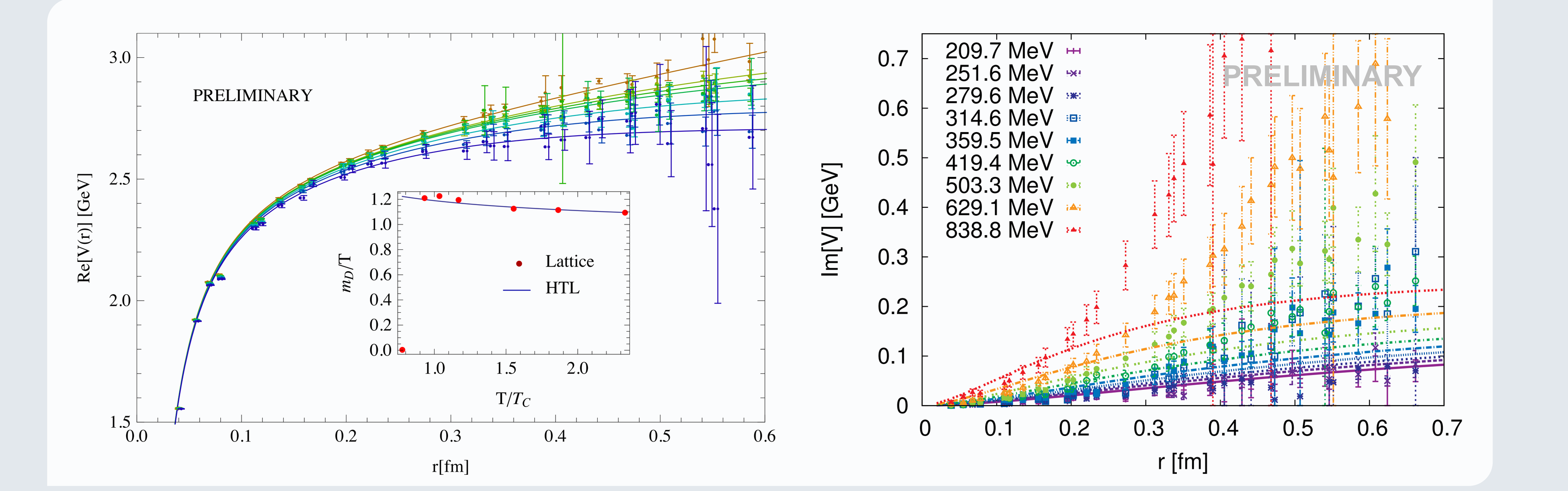


  - Comparison of the spectra: exact HTL result (gray), MEM reconstruction from 32 points (no noise added), our new method (BR) from 32 and 128 points with Gaussian noise added. Shown are two distances, r=0.06fm and r=0.26fm (top/bottom) and two observables: Wilson loop (left) Wilson lines (right)
- **Reconstruction of the HTL (T=2.33T_C) potential** based on the Euclidean HTL line correlator $V_{||}$: Re[V](r) requires 10^{-2}, Im[V](R) requires 10^{-5} errors for a reliable determination.
- **State of the art application: The heavy quark potential from lattice QCD simulations** Y. Burnier, A. Rothkopf, in preparation
  - Quenched lattice QCD: anisotropic lattices with naïve Wilson action $32^3 x N_\tau$
  - Fixed scale approach: β=7.0 $\xi=a_s/a_\tau=4$ a_s=0.039fm

N_τ	24	32	40	48	56	64	72	80	96
T/T_C	3.11	2.33	1.86	1.55	1.33	1.17	1.04	0.93	0.78
N_{meas}	2750	1570	1680	1110	760	1110	700	940	690

see also talk by A. Rothkopf Thu 17th parallels 16:20h

  - Spectra based on Wilson Line correlators in Coulomb gauge to avoid cusp divergences in the Wilson loop



Conclusion

- We presented a new approach to the reconstruction of spectral functions that contains three key differences compared to the standard MEM. A novel scale independent **prior functional S** as well as **explicit integration** of the **hyperparameter α** are combined with the **LBFGS algorithm** to access the full N_ω dimensional search space.
- Using mock data analyses based on leading order hard thermal loop resummed perturbation theory we showed that the extraction of the in-medium heavy quark potential from spectral functions of Wilson Loops or Wilson Line correlators is viable. The determination of the imaginary part, i.e. spectral widths, requires however high precision data and a relatively large number of datapoints. Current estimates for Re[V] and Im[V] from actual quenched lattice QCD simulations were presented.
- Y.B. is supported by SNF grant PZ00P2-142524 and A.R. acknowledges funding from the DFG

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