Sparse modeling approach to extract spectral functions with covariance of Euclidean-time correlators of lattice QCD

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Background & Motivation

- Spectral functions are needed to study the properties of the hot and dense medium in relativistic heavy-ion collisions.
  - ✓ differential cross section for thermal dilepton production $\frac{dW}{d\omega d^3p} \propto \frac{\rho_V(\omega, \vec{p}, T)}{\omega^2(e^{\omega/T} - 1)}$
    - ⟹ Probes of Quark-Gluon Plasma
  - ✓ heavy quark diffusion coefficient $D = \frac{1}{6\chi_s} \lim_{\omega \to 0} \sum_{i=1}^{3} \frac{\rho_{ii}^V(\omega, \vec{0})}{\omega}$
    - ⟹ Transport properties
  - ✓ …

Spectral function extracted from lattice QCD data

- Observables in LQCD:

Euclidean (imaginary time) meson correlation function

$$G(\tau,\vec{p}) = \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle J_H(\tau,\vec{x}) J_H(0,\vec{0}) \rangle$$

$$= \int_0^\infty d\omega K(\omega,\tau) \underline{\rho_H(\omega,\vec{p})}$$

Spectral function

$J_H(\tau,\vec{x}) \equiv \bar{\psi}(\tau,\vec{x})\gamma_H\psi(\tau,\vec{x})$: local meson operator

$$K(\omega,\tau) \equiv \frac{\cosh\left[\omega\left(\tau - \frac{1}{2T}\right)\right]}{\sinh\left(\frac{\omega}{2T}\right)} \xrightarrow[T\to 0]{} e^{-\omega\tau}$$

Discretized
& schematically

$$\underbrace{\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_M \end{pmatrix}}_{M \sim O(10)} = \begin{pmatrix} K_{11} & K_{12} & \cdots & \cdots & \cdots & K_{1N} \\ K_{21} & K_{22} & \cdots & \cdots & \cdots & K_{2N} \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ K_{M1} & \cdots & \cdots & \cdots & \cdots & K_{MN} \end{pmatrix} \underbrace{\begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \vdots \\ \vdots \\ \rho_N \end{pmatrix}}_{N \sim O(1000)}$$

➡ Extracting spectral functions is an ill-posed inverse problem.

Spectral function extracted from lattice QCD data

- Previous works (not inclusive)
  - ✓ Maximum entropy method

    [M. Asakawa, T. Hatsuda and Y. Nakahara, Prog. Part. Nucl. Phys. 46 (2001) 459-508]
  - ✓ Stochastic method

    [H.-T. Ding, et al., Phys. Rev. D 97, 094503 (2018)]
  - ✓ Backus Gilbert method

    [B. B. Brandt, A. Francis, H. B. Meyer, and D. Robaina, Phys. Rev. D 92, 094510 (2015)]
  - ✓ Sparse modeling

    [E. Itou, Y. Nagai, J. High Energ. Phys. 2020, 7 (2020)]

Various methods have been developed and used to calculate spectral functions, and it is important to check the spectral function with each other in various ways and to properly estimate the systematic error.

Sparse modeling

- Extracting spectral functions by using sparse modeling has been proposed in condensed matter physics. [H. Shinaoka, J. Otsuki, M. Ohzeki, K. Yoshimi, Phys. Rev. B 96 (2017) 035147] [J. Otsuki, M. Ohzeki, H. Shinaoka, K. Yoshimi, Phys. Rev. E 95 (2017) 061302]

  - Fitting with different regularization in MEM (we do not use default models)

  - The rank of the spectral function is reduced by dropping the contribution of small singular values.

    Singular value decomposition of kernel

    $$K = USV^{\mathrm{t}} \longrightarrow \boldsymbol{\rho}' \equiv V^{\mathrm{t}}\boldsymbol{\rho} \quad \boldsymbol{G}' \equiv U^{\mathrm{t}}\boldsymbol{G}$$

  - L1 regularization term is added to cost function. (LASSO form problem)

    $$F(\boldsymbol{\rho}') = \frac{1}{2}(\boldsymbol{G}' - S\boldsymbol{\rho}')^2 + \lambda||\boldsymbol{\rho}'||_1$$

    L1 norm: $||\boldsymbol{\rho}'||_1 \equiv \sum_l |\rho'_l|$

    λ is a positive hyperparameter.

  - This optimization problem is solved by alternating direction method of multipliers(ADMM).

    [S. Boyd, et al., Foundations and Trends R in Machine Learning 3, 1 (2011)]

Update from previous work

- Update from E. Itou's work:
  - ✓ Covariance matrix is taken account.

$$F(\boldsymbol{\rho}') = \frac{1}{2}(\boldsymbol{G} - US\boldsymbol{\rho}')^{\mathrm{t}}\underline{C}^{-1}(\boldsymbol{G} - US\boldsymbol{\rho}') + \lambda||\boldsymbol{\rho}'||_1$$

Covariance matrix

G between different Euclidean times are correlated.

⟹ The covariance matrix is needed to be considered.

  - ✓ Apply to mock data for checking the applicability of the method.

Sparse modeling in our study

1. Carry out the singular value decomposition of the kernel matrix K(ω,τ):

   $K = USV^{\mathrm{t}}$ S is an M×N diagonal matrix. U and V are M×M and N×N orthogonal matrices, respectively. M and N are the # of points of G(τ) and ρ(ω), respectively.

2. Transform the basis of ρ by V^{t}: $\boldsymbol{\rho}' \equiv V^{\mathrm{t}}\boldsymbol{\rho}$
3. The components of ρ'_l corresponding to small singular values satisfied with $s_l/s_1 < 10^{-15}$ are dropped.

➡ At the same time, the sizes of U, S and V are reduced.

S : M×N → L×L
U : M×M → M×L
V : N×N → N×L

L is the number of components of singular values satisfied with $s_l/s_1 < 10^{-15}$.

Sparse modeling in our study

4. The cost function F(ρ') consists of the square error with covariance matrix and the L1 regularization term.

Covariance matrix In previous work, C is not considered.

$$F(\boldsymbol{\rho}') = \frac{1}{2}(\boldsymbol{G} - US\boldsymbol{\rho}')^{\mathrm{t}}\underline{C}^{-1}(\boldsymbol{G} - US\boldsymbol{\rho}') + \lambda||\boldsymbol{\rho}'||_1 \equiv \chi^2(\boldsymbol{\rho}') + \lambda||\boldsymbol{\rho}'||_1$$

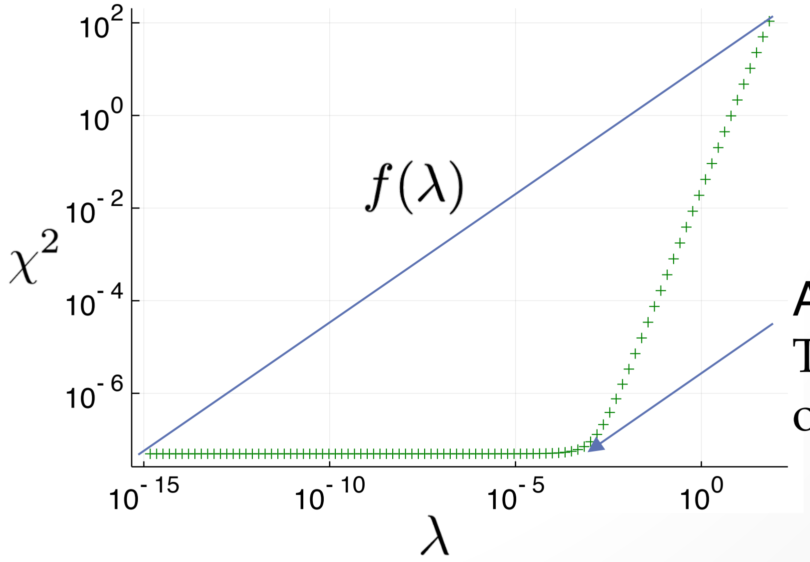
5. Estimate the optimal value of λ, λ_{opt} same as the previous study.

[E. Itou, Y. Nagai, J. High Energ. Phys. 2020, 7 (2020)]

6. Find the most likely spectral function ρ by using ADMM algorithm.

✓ Minimize the cost function F(**ρ**') subject to the positivity constraint of $\rho_j \geq 0$.

The components of the vector **ρ**



$f(\lambda)$: a line in log-log scale

An optimal value λ_{opt}: The value of λ at the position of the kink in χ^2.

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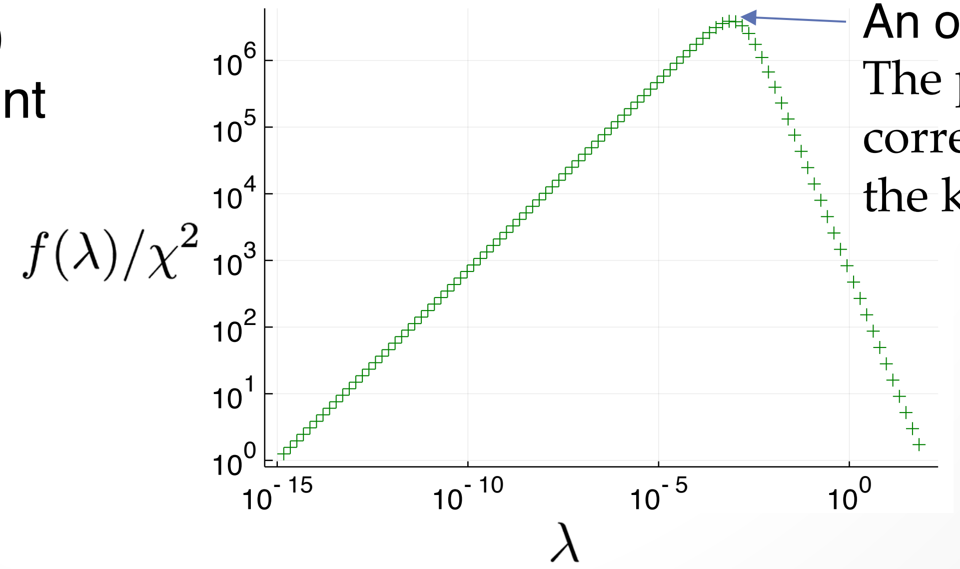


An optimal value λ_{opt}:
The peak in the ratio $f(\lambda)/\chi^2$ corresponds to the position of the kink in χ^2.

Mock data test

- Mock data: vector channel of e^+e^- annihilation [T. Yamazaki, et al.(CP-PACS Collaboration), Phys.Rev.D65:014501,2002]

Spectral function $$\rho_{in}(\omega) = \frac{2\omega^2}{\pi}\left[\underbrace{F_\rho^2 \frac{\Gamma_\rho(\omega) m_\rho}{(\omega^2 - m_\rho^2)^2 + \Gamma_\rho^2(\omega) m_\rho^2}}_{\text{peak}} + \underbrace{\frac{1}{8\pi}\left(1 + \frac{\alpha_s}{\pi}\right)\frac{1}{1 + e^{(\omega_0 - \omega)/\delta}}}_{\text{continuum}}\right]$$

- $\langle 0|\bar{d}\gamma_\mu u|\rho\rangle = \sqrt{2} F_\rho m_\rho \epsilon_\mu = \sqrt{2} f_\rho m_\rho^2 \epsilon_\mu$

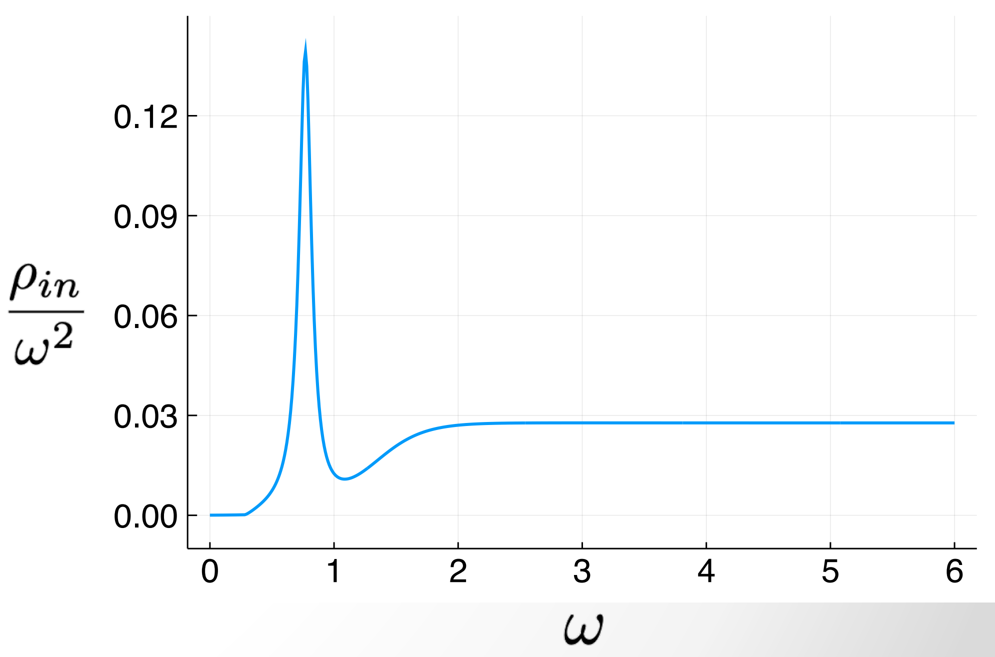
  defines the residue of ρ meson resonance F_ρ.

- $\Gamma_\rho(\omega) = \frac{1}{48\pi}\frac{m_\rho^3}{F_\rho^2}\left(1 - \frac{4m_\pi^2}{\omega^2}\right)^{3/2}\theta(\omega - 2m_\pi)$

  represents the threshold of $\rho \to \pi\,\pi$ decay.

- The values of parameters:

  $m_\rho = 0.77,\ m_\pi = 0.14,\ F_\rho = 0.142,\ \omega_0 = 1.3,\ \delta = 0.2,\ \alpha_s = 0.3$



Mock data test

- The central values of correlation function G(τ)

$$G(\tau) = \int d\omega \rho_{in}(\omega) K(\omega, \tau) \qquad K(\omega, \tau) = e^{-\omega\tau}$$

Δτ can be set from $\tau_{max} = \Delta\tau(N_\tau - 1)$.
We set Δτ=0.5.

- Errors of G(τ) are generated by gaussian random numbers with the variance

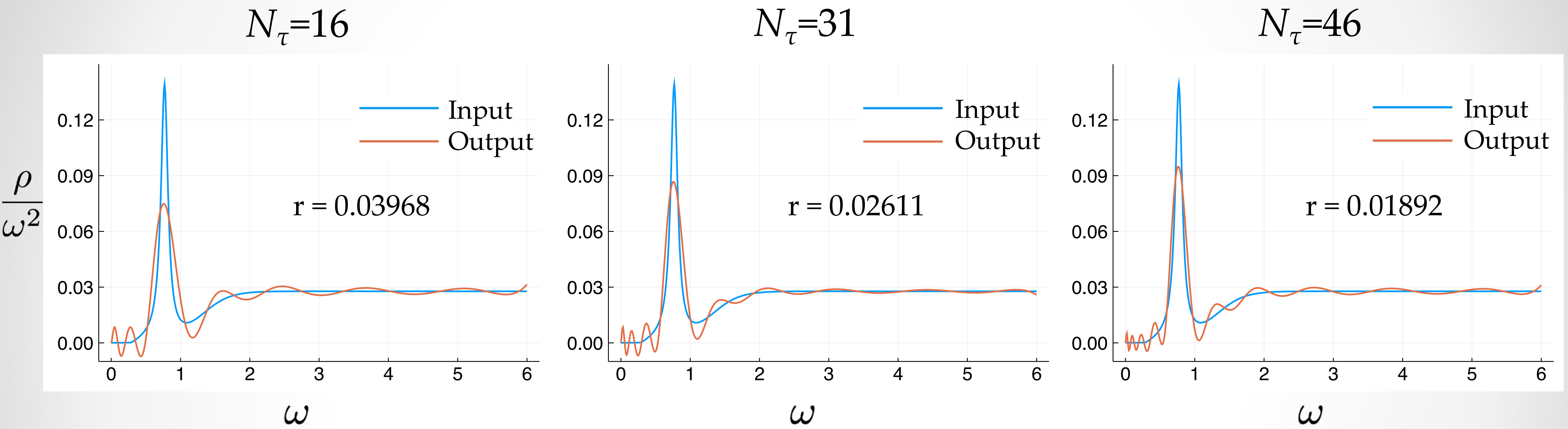
$$\sigma(\tau) = b \cdot e^{a\tau} G(\tau) \qquad a = 0.1 \qquad b = 10^{-10}$$

- In this test, no correlation between different τ is considered.

→ The covariance matrix C is set to diagonal.

- The range of ω: $0 \leq \omega \leq 6$, # of ω points: N_ω=601
- We performed tests on three types of N_τ: $N_\tau = 16,\ 31,\ 46$
- Reconstruction error: $r = \sum_{j=1}^{N_\omega} ((\rho_{in}(\omega_j) - \rho_{out}(\omega_j))/\omega^2)^2$

Results of mock data test

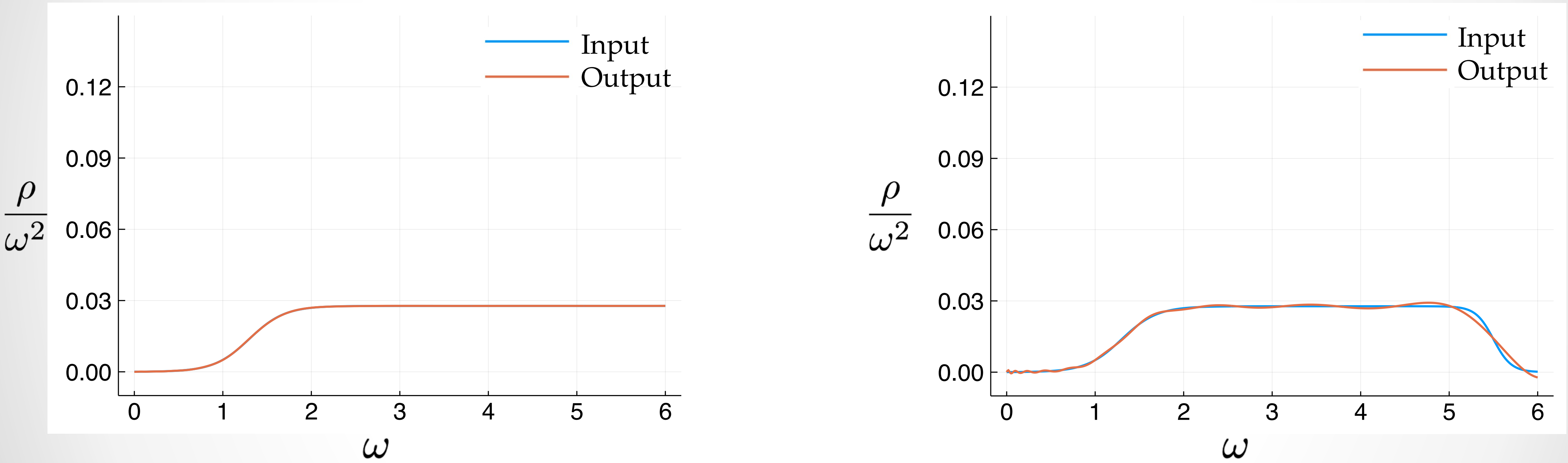


- Reconstruction error becomes smaller as N_τ becomes longer.
- Positivity condition is not satisfied in the low-ω region.

Results of mock data test

- Mock data (N_τ=46)

Only continuum ρ_{in} | Continuum and dumped ρ_{in}

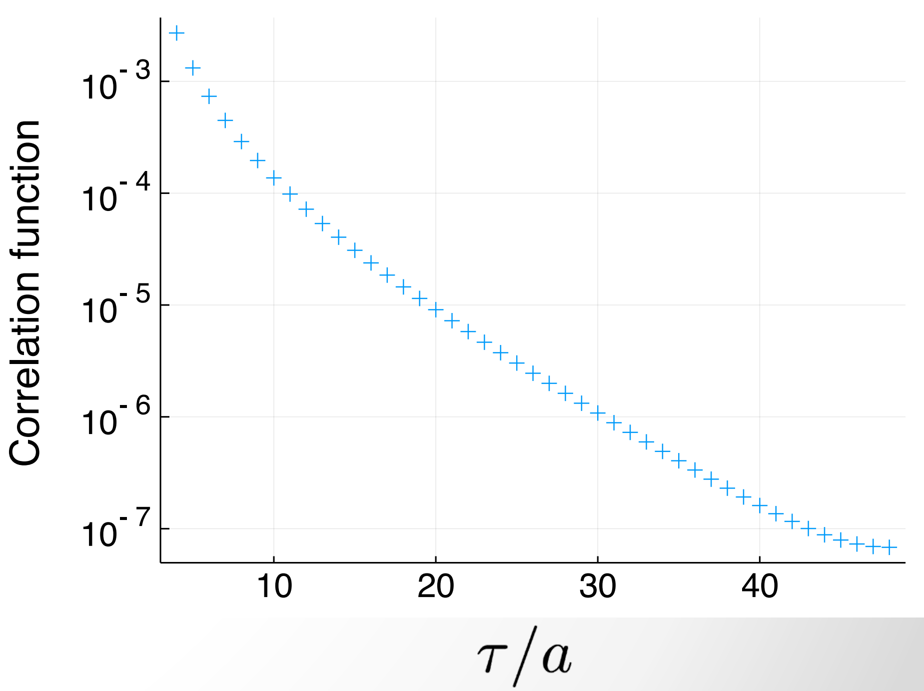


- Positivity condition is almost satisfied.
  - ➢ The oscillations of ρ_{out} are weak when there is no peak in ρ_{in}.

Lattice QCD data

- Standard plaquette gauge + O(a)-improved Wilson quark action
- In the quenched approximation
- Lattice spacing: $a = 0.010\,\mathrm{fm},\ a^{-1} \simeq 18.97\,\mathrm{GeV}$
- Spatial and temporal extents: $N_\sigma = 128,\ N_\tau = 96$
- Vector channel
- # of conf.: 234

[H.-T. Ding, A. Francis, O. Kaczmarek, F. Karsch, H. Satz, W. Soeldner, Phys. Rev. D 86, 014509 (2012)]



Normalization

- Kernel

$$K(\omega,\tau) \equiv \frac{\cosh\left[\omega\left(\tau - \frac{1}{2T}\right)\right]}{\sinh\left(\frac{\omega}{2T}\right)}$$

Diverges at $\omega = 0$.

- Correlation function has lattice cutoff effects at small distances.

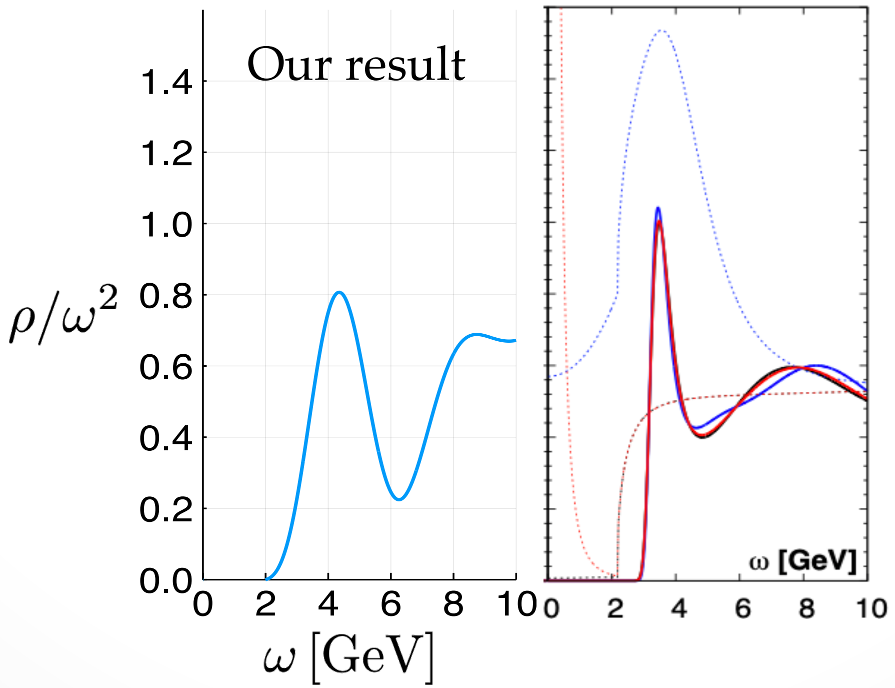
$$\tilde{K}(\omega,\tau;\tau_0) \equiv \frac{K(\omega,\tau)}{K(\omega,\tau_0)} = \frac{\cosh\left[\omega\left(\tau - \frac{1}{2T}\right)\right]}{\cosh\left[\omega\left(\tau_0 - \frac{1}{2T}\right)\right]}$$

$$\tilde{\rho}(\omega;\tau_0) = \rho(\omega)K(\omega,\tau_0)$$

We used the correlation function data from τ_0/a to $N_\tau/2$ in our analysis.
We chose $\tau_0/a = 4$ to reduce the cutoff effects.

Results from lattice QCD data

- The value of the spectral function increases around 2 GeV.
- Broad peak around 4 GeV.
  - ➢ A bit larger compared to the results of MEM（3.48 GeV）and the J/ψ mass on this lattice（3.472 GeV）.



[H.-T. Ding, A. Francis, O. Kaczmarek, F. Karsch, H. Satz, W. Soeldner, Phys. Rev. D 86, 014509 (2012)]

Summary

- We applied sparse modeling(SpM) for extracting spectral functions from Euclidean-time correlation functions.
- We took account of covariance between different Euclidean times of the correlation function for SpM.
- We tested SpM with mock data and checked applicability of SpM.
- We tried to extract spectral functions from vector charmonium correlation functions obtained from lattice QCD.

Outlook

- We should check the following points systematically.
  - ✓ Positivity of spectral functions
  - ✓ Optimal value of λ
  - ✓ Convergence of ADMM iterations
  - ✓ …
- Whether transport peaks appear at higher temperature.

Searching λ_{opt}

1. Fix a range of λ, $[\lambda_{min}, \lambda_{max}]$
2. Calculate $\chi^2(\rho')$ for each λ by using ADMM iterations
   - ✓ # of iterations: 10000
3. Obtain a function f(λ) in log-log scale by connecting $f(\lambda_{min})$ with $f(\lambda_{max})$
4. Calculate the ratio $f(\lambda)/\chi^2$

   The λ located at the peak position of $f(\lambda)/\chi^2$ corresponds to λ_{opt}.