

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

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We present our sparse modeling study to extract spectral functions from Euclidean-time correlation functions. In this study covariance between different Euclidean times of the correlation function is taken into account, which was not done in previous studies. In order to check applicability of the method, we firstly test it with mock data which imitate possible charmonium spectral functions. Then, we extract spectral functions from correlation functions obtained from lattice QCD at finite temperature.

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1. Introduction

Meson spectral functions play a crucial role to study properties of the hot and dense medium formed in relativistic heavy ion collisions since they carry important theoretical information on probes of the Quark-Gluon Plasma such as the thermal dilepton rate [1–3] and quarkonia [4]. Especially, the low frequency part of the spectral function is associated with transport coefficients (e.g., the heavy quark diffusion coefficient [5]), which are important inputs for explaining transport phenomena in the experiments.

Lattice QCD calculations, however, cannot obtain the spectral function directly but it is accessible from the meson correlation function G of Euclidean time τ through the following relation:

$$G(\tau) = \int d^3x \langle J_H(\tau, \vec{x}) J_H(0, \vec{0}) \rangle = \int_0^\infty d\omega K(\omega, \tau) \rho_H(\omega), \quad (1)$$

where J_H represents the local meson operator of a channel H and K is the integration kernel defined by

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

in the Euclidean time range $0 \leq \tau \leq 1/T$ with temperature T .

When the frequency ω is discretized, eq. (1) can be simply written as a linear equation

$$\vec{G} = K \vec{\rho}, \quad (3)$$

where \vec{G} and $\vec{\rho}$ are M and N dimensional vectors, respectively, and K is an $M \times N$ matrix. For typical lattice QCD calculations the temporal lattice size, i.e., M is of $O(10)$ while N must be of $O(1000)$ for sufficiently good resolution of the spectral function. Therefore, solving eq. (3) to extract the spectral function is an ill-posed inverse problem.

There are lots of previous studies on extracting spectral functions from lattice QCD data, using various techniques based on different ideas [6–8]. Sparse modeling is one of such techniques, which was applied recently for the first time to lattice QCD data to obtain spectral functions of the energy-momentum tensor and the shear viscosity [9]. In this study we conduct a more comprehensive investigation into the applicability of sparse modeling. Moreover, we also compare our results with those of one of the previous studies to properly estimate the systematic uncertainty.

2. Sparse modeling

Extracting spectral functions by using sparse modeling has been proposed in condensed matter physics [10, 11]. The following is a brief summary of the sparse modeling procedures in this study.

1. Perform a singular value decomposition of the kernel K :

$$K = USV^t, \quad (4)$$

where S is a diagonal matrix composed of singular values, and U and V are $M \times M$ and $N \times N$ orthogonal matrices, respectively.

2. Transform the basis of the correlation function \vec{G} and the spectral function $\vec{\rho}$ by U^t and V^t , respectively:

$$\vec{G}' \equiv U^t \vec{G}, \quad \vec{\rho}' \equiv V^t \vec{\rho}. \quad (5)$$

3. Choose up to L -th largest singular values satisfied with the condition $s_l/s_1 \geq 10^{-15}$, where s_l is the l -th largest singular value, and drop the components of $\vec{\rho}'$ and \vec{G}' corresponding to the other small singular values, which reduces the size of U , V and S to $M \times L$, $N \times L$ and $L \times L$, respectively.

4. Construct the cost function $F(\vec{\rho}')$ from the square error and the L_1 regularization term:

$$F(\vec{\rho}') = \frac{1}{2} (\vec{G}' - S\vec{\rho}')^t U^t C^{-1} U (\vec{G}' - S\vec{\rho}') + \lambda \|\vec{\rho}'\|_1 \equiv \chi^2(\vec{\rho}') + \lambda \|\vec{\rho}'\|_1. \quad (6)$$

Here, C in the first term is the covariance matrix defined by

$$C_{ij} = \frac{1}{N_{\text{conf}}(N_{\text{conf}} - 1)} \sum_{n=1}^{N_{\text{conf}}} \left(G(\tau_i) - G^{(n)}(\tau_i) \right) \left(G(\tau_j) - G^{(n)}(\tau_j) \right), \quad (7)$$

$$G(\tau_i) = \frac{1}{N_{\text{conf}}} \sum_{n=1}^{N_{\text{conf}}} G^{(n)}(\tau_i), \quad (8)$$

where N_{conf} is the total number of gauge configurations and $G^{(n)}(\tau)$ is the value of the correlation function measured on the n -th gauge configuration. In the second term $\|\cdot\|_1$ stands for the L_1 norm defined by $\|\vec{\rho}'\|_1 \equiv \sum_{i=1}^L |\rho'_i|$ and λ is a positive hyperparameter which controls the contribution of the L_1 regularization relative to the square error. Note that the commonly-used maximum entropy method has a different regularization term proportional to the Shannon-Jaynes entropy, which measures difference between an output spectral function and a default model which contains prior information.

5. Estimate the optimal value of λ , λ_{opt} , in the same way as the previous study [9], i.e., we vary $\chi^2(\vec{\rho}')$ as a function of λ and search for a kink (see fig. 1).
6. Find the most likely spectral function by minimizing the cost function $F(\vec{\rho}')$ using the ADMM algorithm [12] with the positivity constraint $\rho_i \geq 0$.

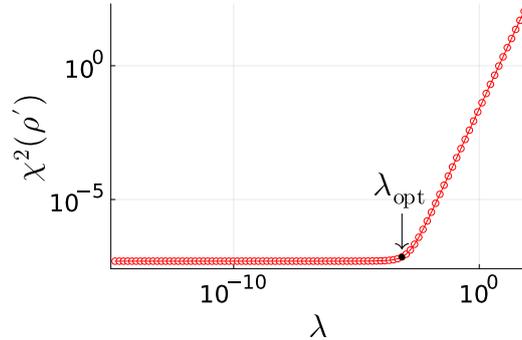


Figure 1: $\chi^2(\vec{\rho}')$ in eq. (6) as a function of λ in the mock data test with $N_\tau = 16$ mentioned later. The black filled circle represents the optimal value of λ , λ_{opt} .

m_ρ	m_π	F_ρ	ω_0	δ	α_s
0.77	0.14	0.142	1.3	0.2	0.3

Table 1: The values of parameters in $\rho_{\text{in}}(\omega)$. The lattice spacing a is set to 1 GeV^{-1} .

What differs from the previous study [9] is that the covariance matrix is considered in $\chi^2(\vec{\rho}')$ of the cost function so that correlation of G between different imaginary times is taken into account.

3. Mock data tests

Before we analyze the actual lattice QCD data by using sparse modeling, we test it with mock data which imitate possible charmonium spectral functions.

We used the same mock data to those defined in ref. [13]. The input spectral function $\rho_{\text{in}}(\omega)$ was set to that in the vector channel of electron-positron pair annihilation, which is given by

$$\rho_{\text{in}}(\omega) = \frac{2\omega^2}{\pi} \left[F_\rho^2 \frac{\Gamma_\rho(\omega)m_\rho}{(\omega^2 - m_\rho^2)^2 + \Gamma_\rho^2(\omega)m_\rho^2} + \frac{1}{8\pi} \left(1 + \frac{\alpha_s}{\pi} \right) \frac{1}{1 + e^{(\omega_0 - \omega)/\delta}} \right], \quad (9)$$

where F_ρ is the residue of ρ meson resonance defined by

$$\langle 0 | \bar{d} \gamma_\mu u | \rho \rangle = \sqrt{2} F_\rho m_\rho \epsilon_\mu = \sqrt{2} f_\rho m_\rho^2 \epsilon_\mu, \quad (10)$$

with the polarization vector ϵ_μ , and the function $\Gamma_\rho(\omega)$ represents the threshold of decay from a ρ meson to two π mesons as

$$\Gamma_\rho(\omega) = \frac{1}{48\pi} \frac{m_\rho^3}{F_\rho^2} \left(1 - \frac{4m_\pi^2}{\omega^2} \right)^{3/2} \theta(\omega - 2m_\pi), \quad (11)$$

with the ρ meson mass m_ρ and the pion mass m_π . We set the lattice spacing a to 1 GeV^{-1} . The values of the parameter such as m_ρ and m_π are listed in table 1.

The central values of correlation function $G(\tau)$ were given by integrating $\rho_{\text{in}} K$, where $K = e^{-\omega\tau}$, over ω . Since this kernel is only an exponentially damped function, the imaginary time resolution $\Delta\tau$ was set from $\tau_{\text{max}} = \Delta\tau(N_\tau - 1)$, where τ_{max} and N_τ represent the maximum imaginary time length and the temporal lattice size, respectively. In this study, we fixed $\Delta\tau$ to 0.5. Errors of $G(\tau)$ were generated by gaussian random numbers with the variance $\sigma(\tau) = b \cdot e^{a\tau} G(\tau)$ in order to incorporate the fact that the error of lattice correlation functions increases as τ increases. We used $a = 0.1$ and $b = 10^{-10}$, respectively. In this test, no correlation of $G(\tau)$ between different τ was considered, i.e., C is diagonal.

In this study, we consider that the range of ω is from 0 to 6 and the number of points in ω -space is $N_\omega = 601$. We performed tests on three different N_τ which were set to 16, 31 and 46. In order to measure the difference between the input data of the spectral function ρ_{in} and the corresponding output result ρ_{out} , the reconstruction error r is defined by $r = \sum_{j=1}^{N_\omega} ((\rho_{\text{in}}(\omega_j) - \rho_{\text{out}}(\omega_j))/\omega^2)^2$.

Figures 2(a)-(c) show the spectral function as a function of ω for $N_\tau = 16, 31$ and 46, respectively. The blue dashed lines and red solid lines represent ρ_{in} and ρ_{out} , respectively. The values of the reconstruction error r for each N_τ are shown in each figure. The reconstruction error

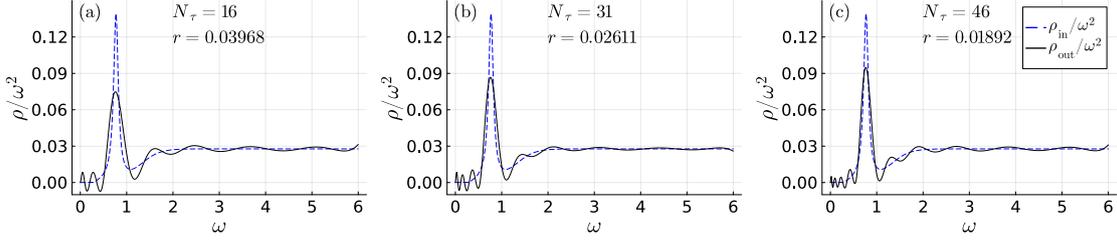


Figure 2: Spectral functions calculated by using sparse modeling in the mock data tests with (a) $N_\tau = 16$, (b) $N_\tau = 31$ and (c) $N_\tau = 46$. The blue dashed lines and red solid lines represent the input mock data ρ_{in} and the output result ρ_{out} .

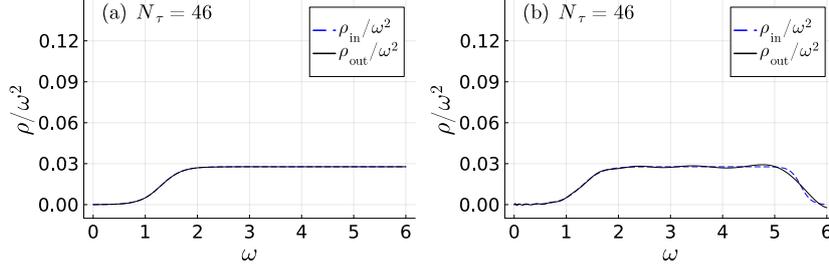


Figure 3: The same as fig. 2 but for the mock data with no peak. In figure (b), we further dumped ρ_{in} in the high- ω region. In figure (a), the two lines overlap each other almost perfectly.

r becomes smaller as N_τ becomes larger. Unfortunately, even though the positivity condition is imposed in our analysis, it is not satisfied in the low- ω region.

We also tested the case where we intentionally removed the peak from ρ_{in} . Figures 3(a) and (b) show the resulting spectral functions as a function of ω with $N_\tau = 46$. In fig. 3(b), we further dumped ρ_{in} in the high- ω region. In both cases, the oscillations of ρ_{out} are weaker than those in the case of ρ_{in} with a peak, and the positivity condition is almost satisfied.

4. Results from lattice data

Next, we extracted the spectral function from actual lattice QCD data.

The lattice data used in this study were given in ref. [14], where the correlation functions were measured with the $O(a)$ -improved Wilson quark action on quenched gauge configurations generated by using the standard plaquette gauge action. The lattice spacing $a = 0.010$ fm and the corresponding a^{-1} is about 18.97 GeV. The spatial extent N_σ and the temporal extent N_τ are 128 and 96, respectively. This setup corresponds to temperature $T \simeq 0.73T_c$. We utilized meson correlation functions in the vector channel. The number of gauge configurations is 234.

The integration kernel is given in eq. (2), which diverges at $\omega = 0$. Moreover, the correlation function is influenced by lattice cutoff effects at small τ distances. To address these issues, we used a modified kernel and a modified spectral function defined by

$$\tilde{K}(\omega, \tau; \tau_0) \equiv \omega^2 \frac{K(\omega, \tau)}{K(\omega, \tau_0)} = \omega^2 \frac{\cosh \left[\omega \left(\tau - \frac{1}{2T} \right) \right]}{\cosh \left[\omega \left(\tau_0 - \frac{1}{2T} \right) \right]}, \quad \tilde{\rho}(\omega; \tau_0) = \frac{\rho(\omega)}{\omega^2} K(\omega, \tau_0), \quad (12)$$

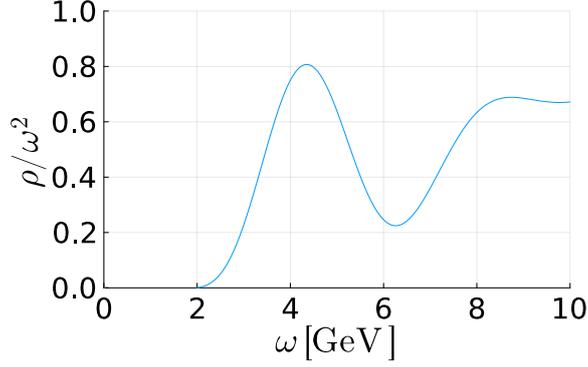


Figure 4: Spectral function obtained from the actual lattice QCD data.

and we used the correlation function data from τ_0/a to $N_\tau/2$, where τ_0/a was set to 4.

Figure 4 shows our result of the spectral function. The spectral function starts increasing around 2 GeV and has a broad peak around 4 GeV. The locations of the first peaks obtained from MEM is about 3.48 GeV and the J/ψ mass given by a single exponential fitting to the spatial correlation function is about 3.47 GeV [14]. Our result is a bit larger compared to these results.

5. Summary and outlook

We applied sparse modeling for extracting the spectral function from the Euclidean-time meson correlation function. Since the correlation function at different imaginary times correlate with each other, in the cost function we introduced the square error term with the covariance matrix so that covariance of the correlation function between different Euclidean times were taken into account.

First, we tested sparse modeling with mock data of the spectral function in the vector channel of electron-positron pair annihilation and checked applicability of sparse modeling. This test confirmed that reconstruction error becomes smaller as the number of data points of the correlation function becomes longer. We also found that spectral functions with a peak violate the positivity condition, while those with no peak are almost positive. Then, we tried to extract the spectral function from the vector charmonium correlation function obtained from lattice QCD. Then, We got a spectral function with a broad peak around 4 GeV, which is a bit larger compared to the results in the previous study.

Base on this study, it is necessary to further investigate how to keep positivity of spectral functions, how to find the optimal λ and convergence of ADMM iterations. Investigating whether transport peaks appear in the spectral functions at higher temperature is also our future work.

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