Sparse modeling study to extract spectral functions from lattice QCD data

Junichi Takahashi

Meteorological College, Japan Meteorological Agency

Hiroshi Ohno (University of Tsukuba), Akio Tomiya (TWCU)

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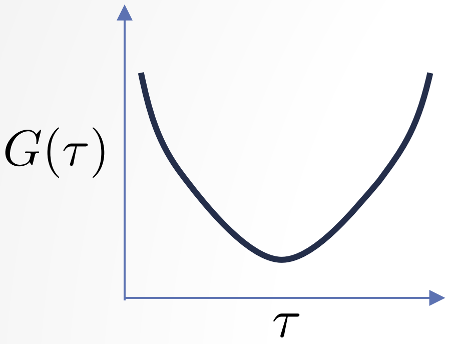
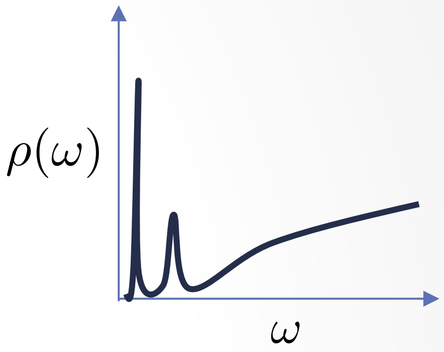
Imaginary time correlation function and spectral function

Imaginary time correlation function



Spectral function



Analytical continuation

$$G(\tau) = \int_0^\infty d\omega K(\tau,\omega)\rho(\omega)$$

Discretized & schematically

$$N_\tau \sim O(10) \left\{ \begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_{N_\tau} \end{pmatrix} \right. = \begin{pmatrix} K_{11} & K_{12} & \cdots & \cdots & K_{1N_\omega} \\ K_{21} & K_{22} & \cdots & \cdots & K_{2N_\omega} \\ \vdots & \vdots & \cdots & \cdots & \vdots \\ K_{N_\tau 1} & \cdots & \cdots & \cdots & K_{N_\tau N_\omega} \end{pmatrix} \left. \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \vdots \\ \rho_{N_\omega} \end{pmatrix} \right\} N_\omega \sim O(1000)$$

Extracting spectral functions is an ill-posed inverse problem.

Spectral function extracted from lattice QCD data

- Previous works (not inclusive)
  - ✓ Maximum entropy method (MEM)
    [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 (SpM)
    [E. Itou, Y. Nagai, J. High Energ. Phys. 2020, 7 (2020)]

> It is important to check the spectral function with each other in various ways and to properly estimate the systematic error.

- Our presentation @ Lattice2023
  - ➢ We checked the applicability of SpM by performing mock data tests, which had never been done before for the calculation of spectral functions using SpM.
  - ➢ We tried to extract spectral functions from mean values of charmonium correlation functions in the vector channel obtained from lattice QCD.

Update from our previous study

- Mock data test
  - ➢ Using correlation functions reconstructed from mock charmonium spectral functions.
  - ➢ Manually adding noises corresponding to the errors to the correlation functions and preparing several of them.

    ⇧

    The mean value and covariance matrix of the correlation functions can be considered as in actual lattice calculations.

- Spectral function from lattice QCD data
  - ➢ Extracting the spectral functions in the pseudoscalar channel in addition to the vector channel.
  - ➢ Estimating errors of the spectral functions by Jackknife analyses.

Sparse modeling

- Extracting spectral functions by using SpM 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.)

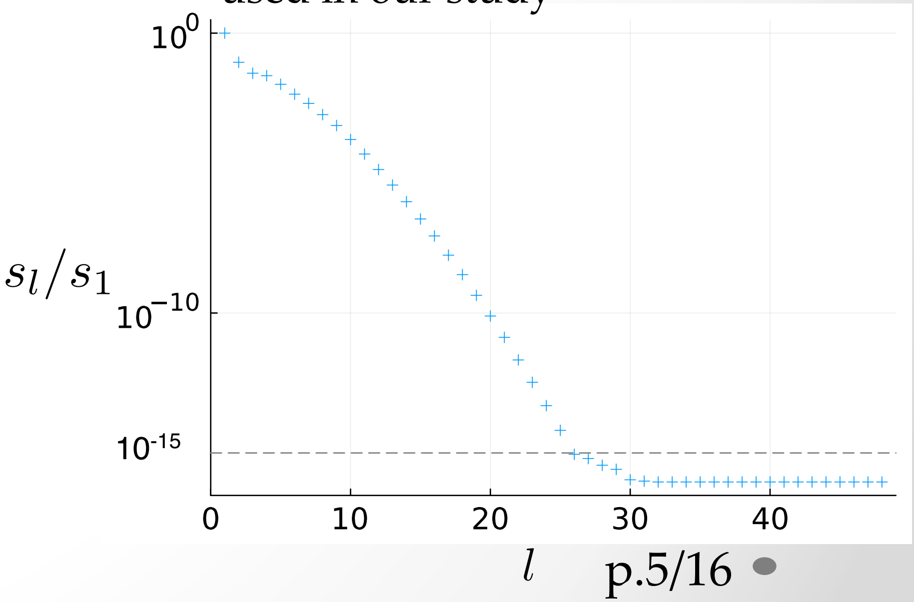
- The ranks of the spectral function and the correlation function are reduced by dropping the contribution of small singular values s_l.

Singular value decomposition of kernel

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

➢ In our study, the components of **ρ**' and **G**' corresponding to small singular values satisfied with $s_l/s_1 < 10^{-15}$ dropped.

✓ An example of singular values of K used in our study



Sparse modeling

- Cost function: χ^2 term + L1 regularization term (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 iteratively by alternating direction method of multipliers (ADMM). [S. Boyd, et al., Foundations and Trends R in Machine Learning 3, 1 (2011)]
  - The problem is solved at various λ and the most likely spectral function ρ can be found at the optimal λ.
  - In our study, estimation of the optimal λ is same as the previous study.

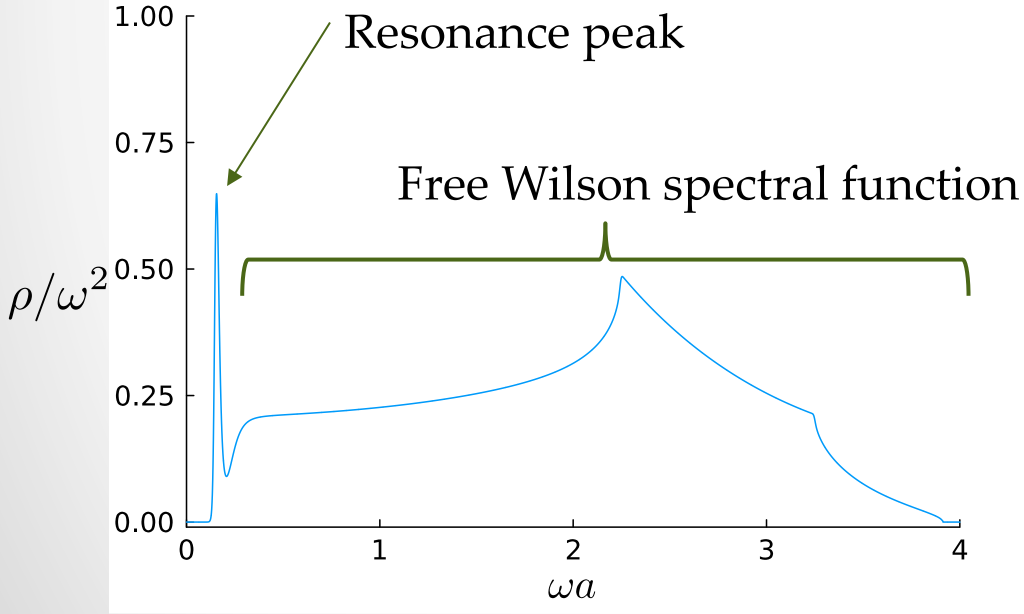
[E. Itou, Y. Nagai, J. High Energ. Phys. 2020, 7 (2020)]

See backup slides for detail.

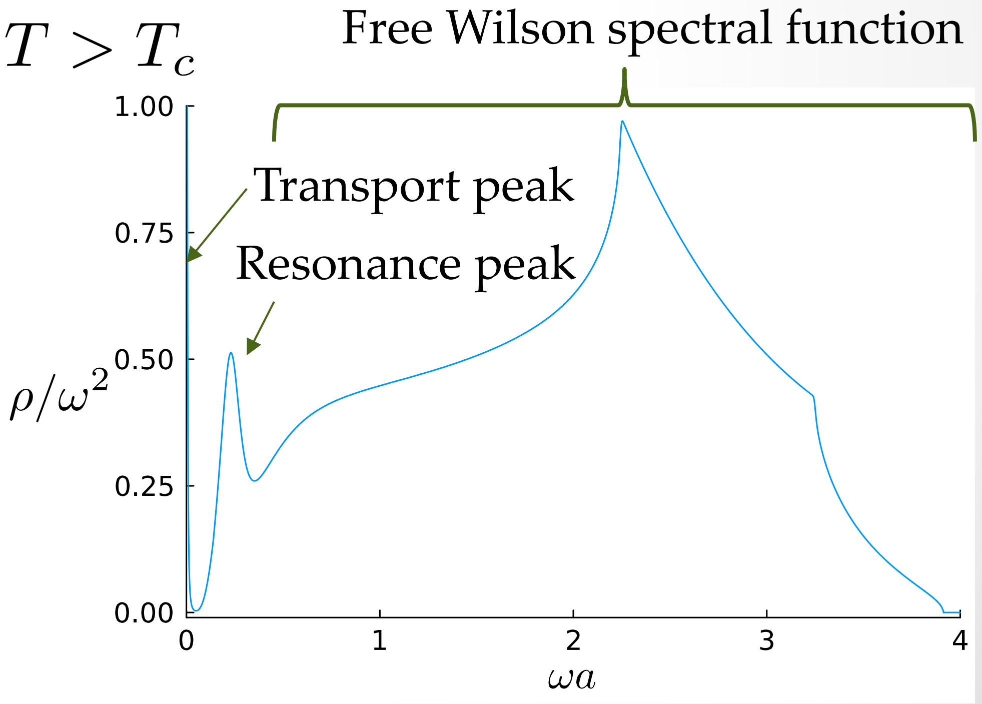
Mock data test

- Mock spectral functions: [H.-T. Ding, et al., Phys. Rev. D 97, 094503 (2018)]
  - ➢ $T < T_c$: resonance peak (J/ψ meson mass) + free Wilson spectral function
  - ➢ $T > T_c$: transport peak + broader resonance peak + free Wilson spectral function
- The range of ω: $0 \leq \omega a \leq 4$ (a: lattice spacing), # of ω points: N_ω=8001

$T < T_c$



$T > T_c$



Mock data test

- The central values of correlation function G(τ)

$$G(\tau) = \int d\omega \rho(\omega) K(\omega, \tau)$$

  - # of τ points: $N_\tau = 48,\ 64,\ 96$

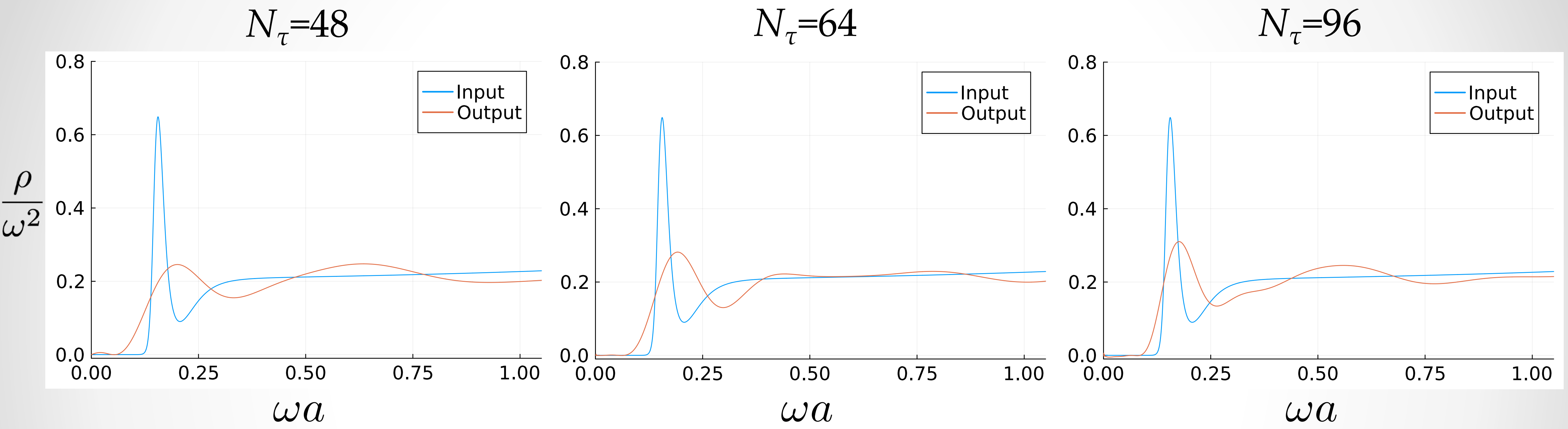
- Errors of G(τ) are generated by gaussian random numbers
  - Variance: $\sigma(\tau) = \epsilon \cdot \tau \cdot G(\tau)$
  - Consider three types of noise level: $\epsilon = 10^{-2},\ 5 \times 10^{-3},\ 10^{-5}$
  - Prepare G(τ) with errors ($N_{\rm conf}$=300)

    ⇨ calculate covariance matrix

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

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

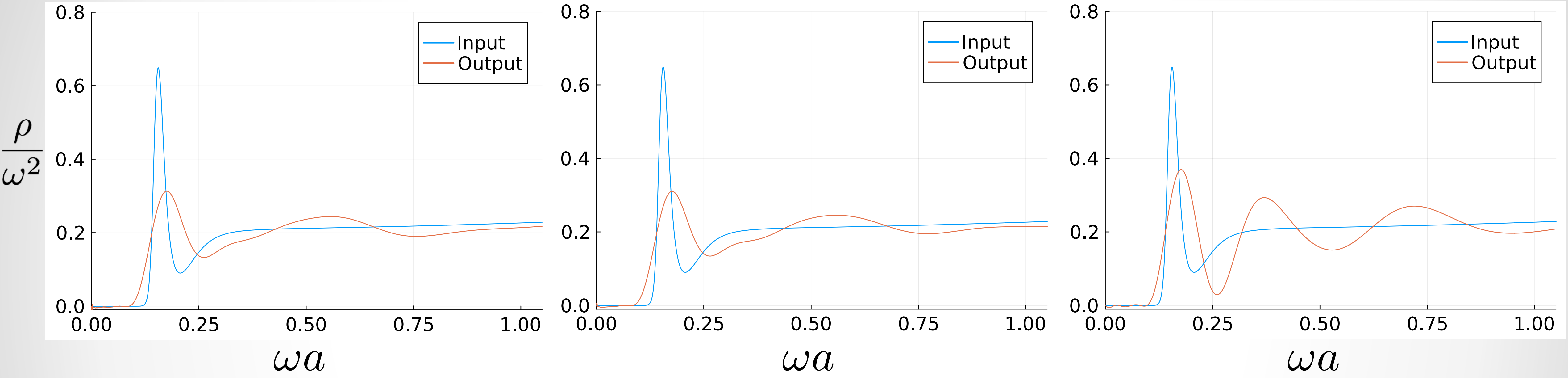
Results of mock data test (T<T$_c$, noise level $\varepsilon=5\times10^{-3}$)



- The resonance peak becomes sharper as N_τ increases.
- Similar results are obtained for other noise levels.

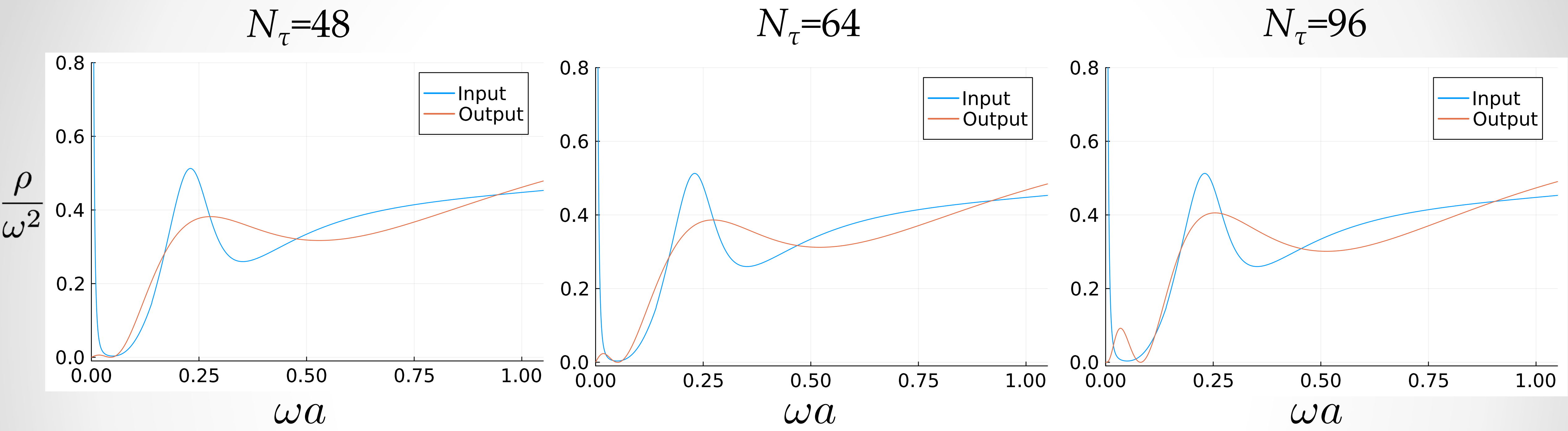
Results of mock data test (T<T$_c$, N_τ=96)

Noise level $\varepsilon = 10^{-2}$ $\varepsilon = 5\times10^{-3}$ $\varepsilon = 10^{-5}$



- The resonance peak becomes sharper as noise level ε decreases.
- Similar results are obtained for other N_τ.

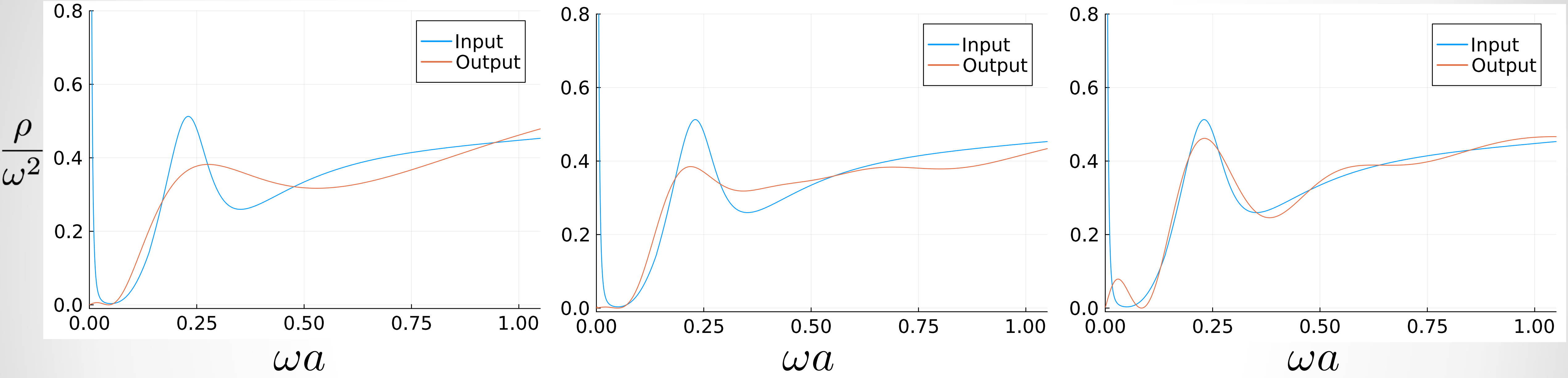
Results of mock data test (T>T$_c$, noise level ε=10^{-2})



- The resonance peak becomes sharper as N_τ increases.
- The transport peaks are not reproduced.
- Similar results are obtained for other noise levels.

Results of mock data test (T>T_c, N_τ=48)

Noise level $\varepsilon=10^{-2}$ $\quad$ $\varepsilon=5\times10^{-3}$ $\quad$ $\varepsilon=10^{-5}$



- The resonance peak becomes sharper as noise level ε decreases.
- Similar results are obtained for other N_τ.

Lattice QCD data

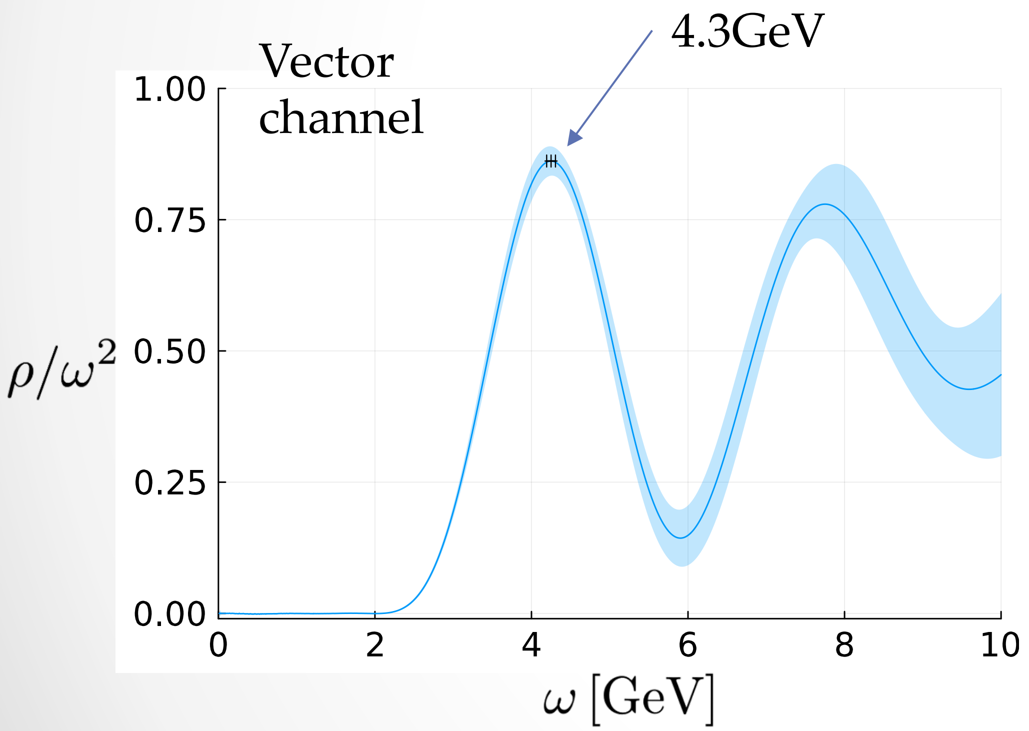
- Standard plaquette gauge + O(a)-improved Wilson quark action
- In the quenched approximation
- Lattice spacing: $a = 0.010\,\mathrm{fm},\ a^{-1} \simeq 18.97\,\mathrm{GeV}$
- Spatial and temporal extents: $N_\sigma = 128,\ N_\tau = 96,\ 48$ for $T/T_c = 0.73,\ 1.46$
- Charmonium correlation functions in pseudoscalar channel and vector channel
- # of conf.: 234 $(N_\tau = 96)$, 461 $(N_\tau = 48)$

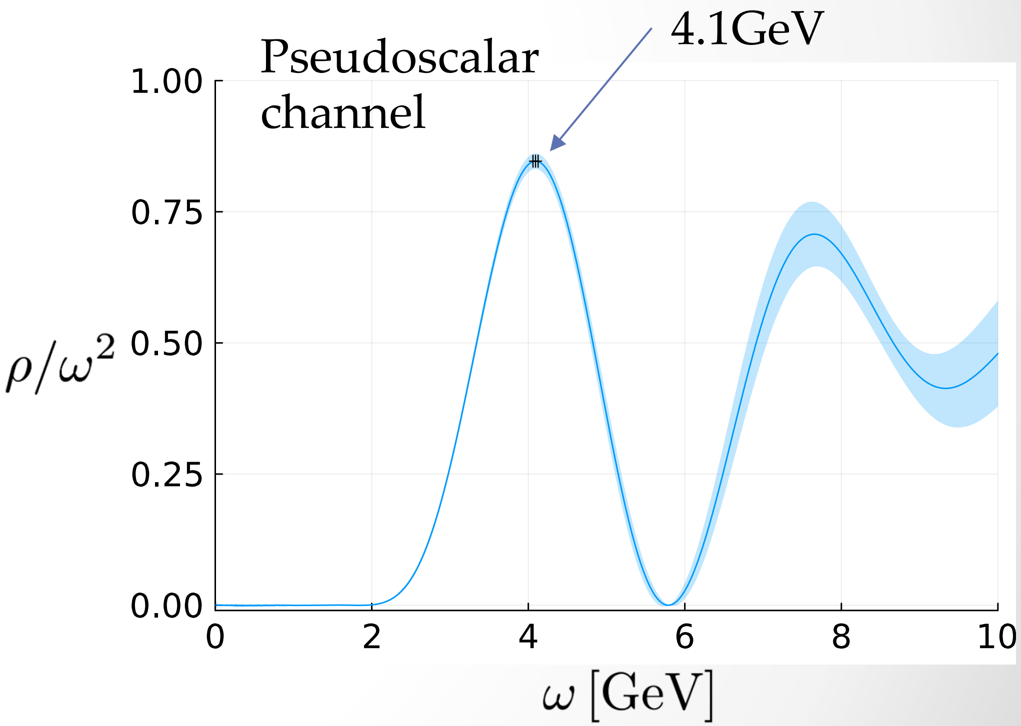
  [H.-T. Ding, A. Francis, O. Kaczmarek, F. Karsch, H. Satz, W. Soeldner, Phys. Rev. D 86, 014509 (2012)]

- Statistical errors: Jackknife analyses

Results from lattice QCD data ($T=0.73T_c$)

- Broad peak about 4GeV.
  - ➢ Results of MEM: 3.48GeV (vector), 3.31GeV (pseudoscalar) [H.-T. Ding, A. Francis, O. Kaczmarek, F. Karsch, H. Satz, W. Soeldner, Phys. Rev. D 86, 014509 (2012)]





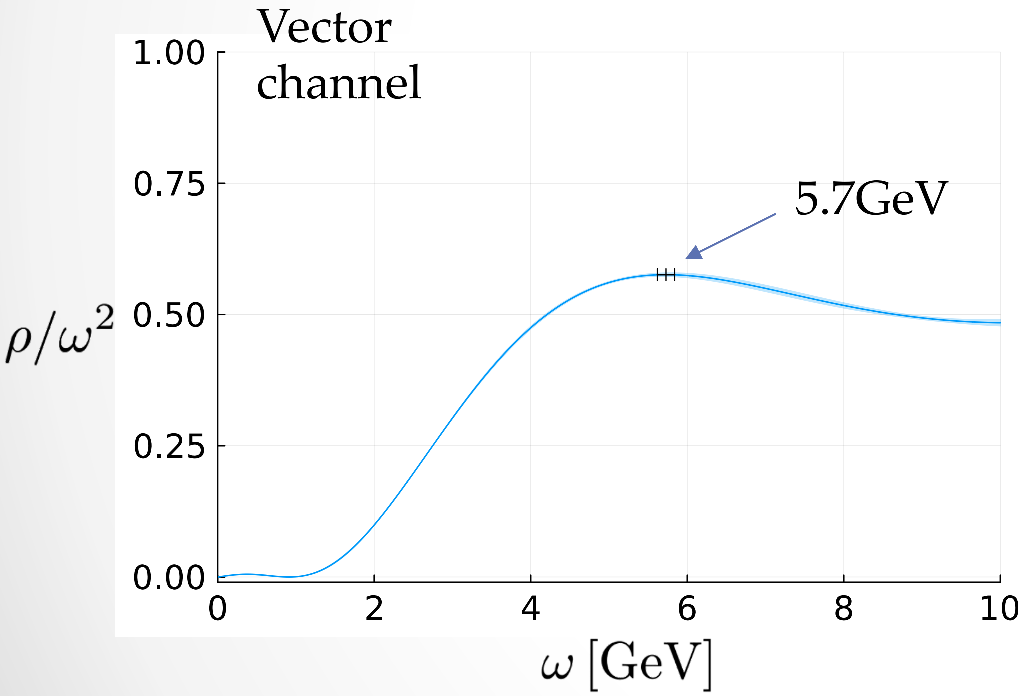
Shaded areas: statistical errors, solid lines: mean values,
horizontal error bars: statistical uncertainties of the peak location

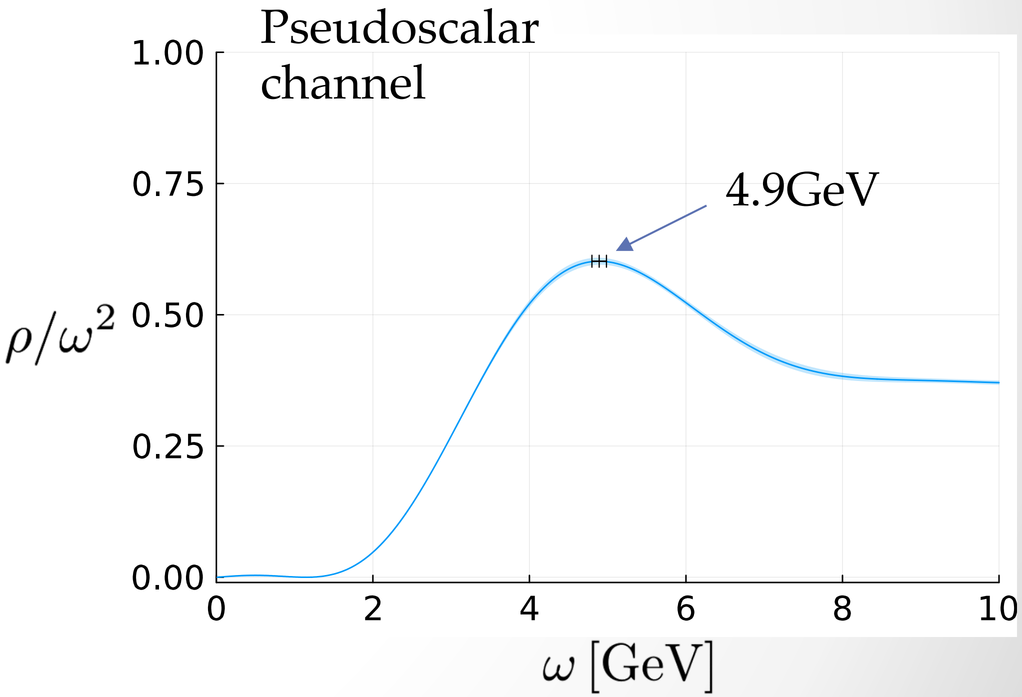
Results from lattice QCD data ($T=1.46T_c$)

- The resonance peaks become much broader and are shifted higher energy (~5GeV).
  - ➢ Results of MEM: 4.7GeV (vector), 4.1GeV (pseudoscalar)

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

- The transport peaks are not appeared.





Shaded areas: statistical errors, solid lines: mean values,
horizontal error bars: statistical uncertainties of the peak location

Summary

- Sparse modeling (SpM) is a useful method for obtaining a reasonable solution to an ill-posed inverse problem such as the extraction of spectral functions.
- We applied SpM to extract spectral functions from charmonium correlation functions.
- Mock data test:
  - ➢ The longer N_τ or the smaller the noise level ε, the better the spectral function can be reproduced.
- Results from lattice QCD data:
  - ➢ Although the position and width of the peaks are not the same as the MEM results, the qualitative behavior is similar. ⇨ Reflecting model-independent properties.
- To estimate the transport peak, assumptions beyond SpM, such as the shape of the transport peak, might be needed.

Sparse modeling in our study

1. Calculate the covariance matrix C and carry out the Cholesky decomposition:

$$C^{-1} = W^{\mathrm{t}} W$$

2. Transform G and K by W: $\boldsymbol{G}_W = W\boldsymbol{G},\ K_W = WK$

3. Carry out the singular value decomposition of K_W: $K_W = USV^{\mathrm{t}}$

S is an Nτ×Nω diagonal matrix. U and V are Nτ×Nτ and Nω×Nω orthogonal matrices, respectively.

Nτ and Nω are the # of points of G(τ) and ρ(ω), respectively.

4. Transform the basis of G_W and ρ by U^t and V^t, respectively:

$$\boldsymbol{\rho}'_W = V^{\mathrm{t}}\boldsymbol{\rho},\ \boldsymbol{G}'_W = U^{\mathrm{t}}\boldsymbol{G}_W$$

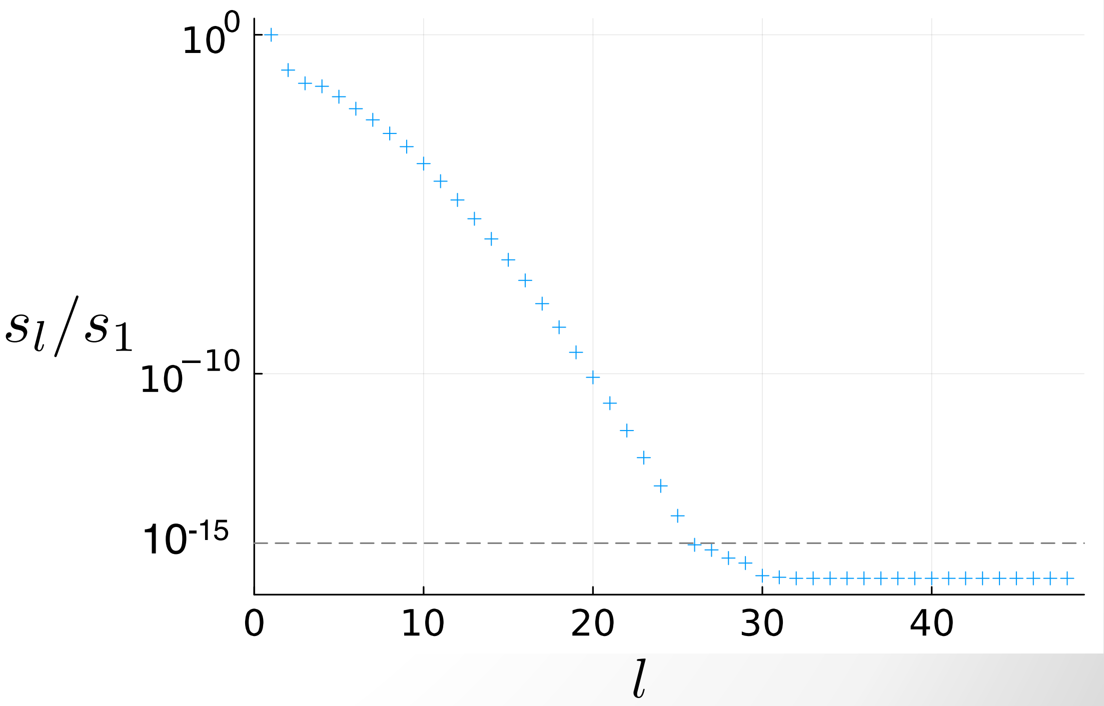
Sparse modeling in our study

5. The components of $\boldsymbol{\rho}_W$' and $\mathbf{G}_W$' 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.

$$\begin{cases} S : N_\tau \times N_\omega \rightarrow L \times L, \\ U : N_\tau \times N_\tau \rightarrow N_\tau \times L, \\ V : N_\omega \times N_\omega \rightarrow N_\omega \times L \end{cases}$$

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

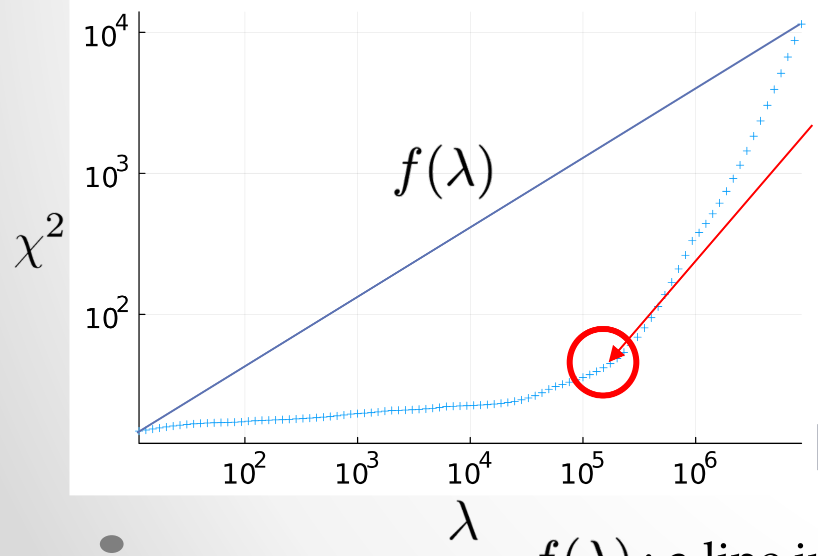


Sparse modeling in our study

6. The cost function F(ρ’) consists of the square error and the L1 regularization term.

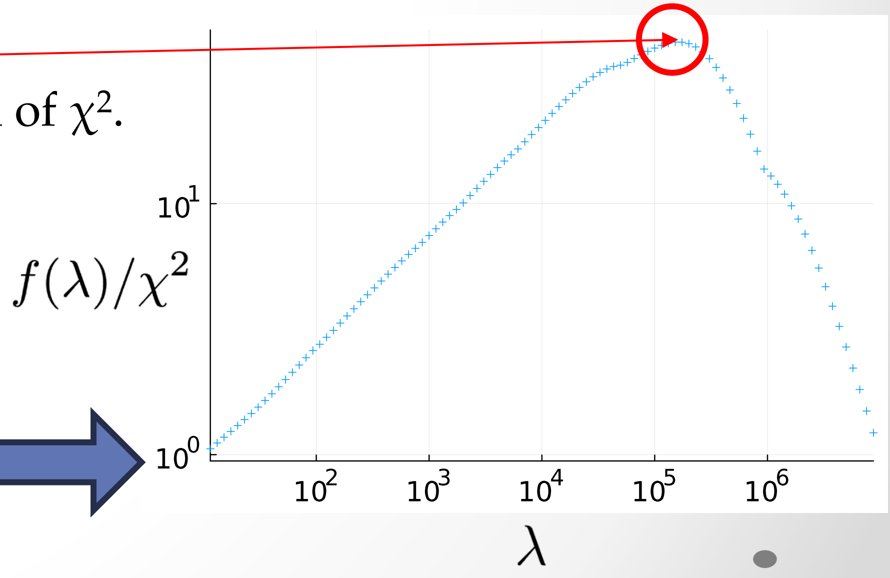
$$F(\boldsymbol{\rho}'_W) = \frac{1}{2}(\boldsymbol{G}'_W - S\boldsymbol{\rho}'_W)^2 + \lambda||\boldsymbol{\rho}'_W||_1 \equiv \chi^2(\boldsymbol{\rho}'_W) + \lambda||\boldsymbol{\rho}'_W||_1$$

7. Solve the optimization problem at various λ by using ADMM and find the most likely spectral function **ρ**.



An optimal value λ_{opt}:
The value of λ at the kink position of χ^2.
(Estimation of λ_{opt} is same as the previous study.)

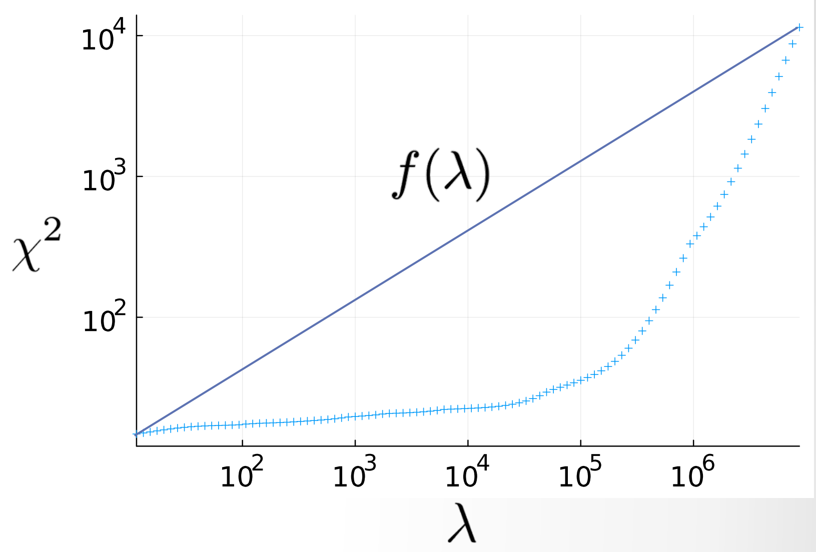
[E. Itou, Y. Nagai, J. High Energ. Phys. 2020, 7 (2020)]

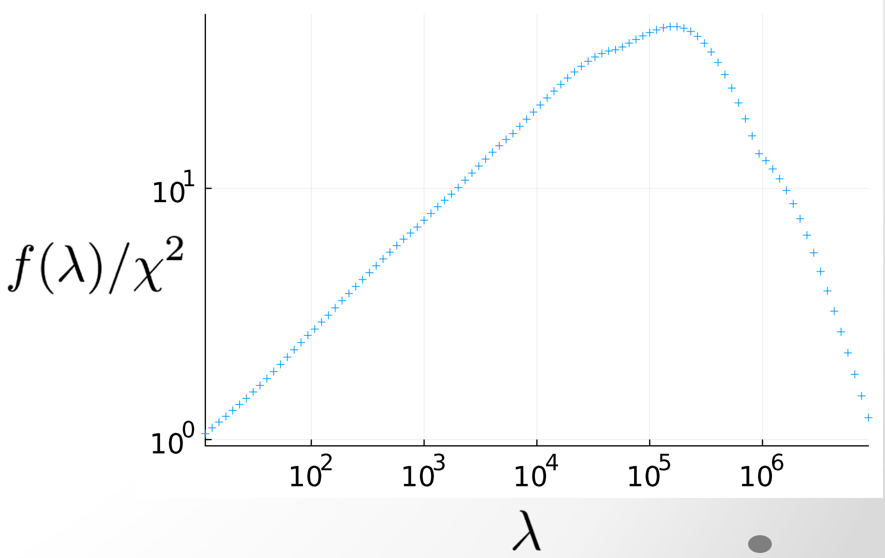


$f(\lambda)$: a line in log-log scale

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}.





Mock spectral function

- $\mathrm{T < T_c}$: $\hat{\rho}_{T<T_c}(\hat{\omega}) = \tilde{\Theta}(\hat{\omega},\hat{\omega}_1,\Delta_1)(1-\tilde{\Theta}(\hat{\omega},\hat{\omega}_2,\Delta_2))\hat{\rho}_{res}(\hat{\omega}) + \tilde{\Theta}(\hat{\omega},\hat{\omega}_3,\Delta_3)\hat{\rho}_{Wilson}(\hat{\omega})$
- $\mathrm{T > T_c}$: $\hat{\rho}_{T>T_c}(\hat{\omega}) = \hat{\rho}_{trans}(\hat{\omega}) + \tilde{\Theta}(\hat{\omega},\hat{\omega}_4,\Delta_4)(1-\tilde{\Theta}(\hat{\omega},\hat{\omega}_5,\Delta_5))\hat{\rho}_{res}(\hat{\omega}) + \tilde{\Theta}(\hat{\omega},\hat{\omega}_6,\Delta_6)\hat{\rho}_{Wilson}(\hat{\omega})$

✓ Transport peak: $\hat{\rho}_{trans}(\hat{\omega}) = c_{trans}\dfrac{\hat{\omega}\eta}{\hat{\omega}^2+\eta^2}$ ✓ Resonance peak: $\hat{\rho}_{res}(\hat{\omega}) = c_{res}\dfrac{\Gamma M\hat{\omega}^2}{(\hat{\omega}^2-M^2)^2+M^2\Gamma^2}$

✓ Free Wilson spectral function:

$$\hat{\rho}_{Wilson}(\hat{\omega}) = c_{Wilson}\frac{4\pi N_c}{N_\sigma^3}\sum_{\vec{k}}\sinh\left(\frac{\hat{\omega}}{2\hat{T}}\right)\left[b^{(1)} - b^{(2)}\frac{\sum_{i=1}^3 \sin^2 k_i}{\sinh^2 E_{\vec{k}}(m)}\right]\frac{\delta(\hat{\omega}-2E_{\vec{k}}(m))}{2(1+M_{\vec{k}}(m))^2\cosh^2\left(\frac{E_{\vec{k}}(m)}{2\hat{T}}\right)}$$

$$\cosh E_{\vec{k}}(m) = 1 + \frac{K_{\vec{k}}^2 + M_{\vec{k}}^2(m)}{2(1+M_{\vec{k}}(m))}, \qquad K_{\vec{k}} = \sum_{i=1}^3 \gamma_i \sin k_i, \qquad M_{\vec{k}}(m) = \sum_{i=1}^3 (1-\cos k_i) + m$$

✓ Modified theta function: $\tilde{\Theta}(\hat{\omega},\hat{\omega}_i,\Delta_i) = \left(1+\exp\left(\dfrac{\hat{\omega}_i^2-\hat{\omega}^2}{\hat{\omega}\Delta_i}\right)\right)^{-1}$

$\hat{\omega} = \omega a,\ \hat{\rho} = \rho a^2$

Spectral function	Parameters
$\hat{\rho}_{res}$ for $T < T_c$	$c_{res} = 0.08/7,\ \Gamma = 0.05,\ M = 0.155$
$\hat{\rho}_{Wilson}$ for $T < T_c$	$c_{Wilson} = 0.5,\ b^{(1)} = 2,\ b^{(2)} = 1,\ m = 0.073,\ N_c = 3,\ N_\sigma = 4096$
$\hat{\rho}_{trans}$ for $T > T_c$	$c_{trans} = 5\times10^{-5},\ \eta = 0.006$
$\hat{\rho}_{res}$ for $T > T_c$	$c_{res} = 0.06,\ \Gamma = 0.15,\ M = 0.225$
$\hat{\rho}_{Wilson}$ for $T > T_c$	$c_{Wilson} = 1,\ b^{(1)} = 3,\ b^{(2)} = 1,\ m = 0.073,\ N_c = 3,\ N_\sigma = 4096$

$\hat{\omega}_1 = 0.145$	$\Delta_1 = 0.01$
$\hat{\omega}_2 = 0.155$	$\Delta_2 = 0.05$
$\hat{\omega}_3 = 0.225$	$\Delta_3 = 0.05$
$\hat{\omega}_4 = 0.225$	$\Delta_4 = 0.15$
$\hat{\omega}_5 = 0.225$	$\Delta_5 = 0.15$
$\hat{\omega}_6 = 0.350$	$\Delta_6 = 0.20$

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.

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

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

τ_0 : reference imaginary time

We used the correlation function data from τ_0/a to $N_\tau/2$ in our analysis.
We chose $\tau_0/a = 1$ in mock data tests and $\tau_0/a = 4$ for LQCD data.