Letter

Reconstructing spectral functions via automatic differentiation

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Reconstructing spectral functions from Euclidean Green's functions is an important inverse problem in many-body physics. However, the inversion is proved to be ill-posed in the realistic systems with noisy Green's functions. In this paper we propose an automatic differentiation (AD) framework as a generic tool for the spectral reconstruction from propagator observable. Exploiting the neural networks' regularization as a nonlocal smoothness regulator of the spectral function, we represent spectral functions by neural networks and use the propagator's reconstruction error to optimize the network parameters unsupervisedly. In the training process, except for the positive-definite form for the spectral function, there are no other explicit physical priors embedded into the neural networks. The reconstruction performance is assessed through relative entropy and mean square error for two different network representations. Compared to the maximum entropy method, the AD framework achieves better performance in the large-noise situation. It is noted that the freedom of introducing nonlocal regularization is an inherent advantage of the present framework and may lead to substantial improvements in solving inverse problems.

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I. INTRODUCTION

The numerical solution to inverse problems is a vital area of research in many domains of science. In physics, especially quantum many-body systems, it is necessary to perform an analytic continuation of function from finite observations which however is ill-posed [1,2]. It is encountered for example, in Euclidean quantum field theory (QFT) when one aims at rebuilding spectral functions based on some discrete data points along the Euclidean axis. More specifically, the inverse problem occurs when we take a nonperturbative Monte Carlo simulations (e.g., lattice QCD) and try to bridge the propagator data points with physical spectra [3]. The knowledge of spectral function will be further applied in transport process and nonequilibrium phenomena in heavy ion collisions [3,4].

In general, the problem set-up is from a Fredholm equation of the first kind, which takes the following form,

$$g(t) = K \circ f \coloneqq \int_a^b K(t,s) f(s) ds, \tag{1}$$

and the problem is to reconstruct the function $f(s)$ given the continuous kernel function $K(t,s)$ and the function $g(t)$. In realistic systems, $g(t)$ is often available in a discrete form numerically. When dealing with a finite set of data points with nonvanishing uncertainty, the inverse transform becomes ill-conditioned or degenerated [5,6]. Regarding the convolution kernel as a linear operator, it can be expanded by basis functions in a Hilbert space. McWhirter and Pike [7] and the authors of Ref. [8] respectively show that kernels of Laplace transformation, $[K(t,s) = e^{-st}]$, and Källen-Lehmann (KL) transformation, $[K(t,s) = s(s^2+t^2)^{-1}\pi^{-1}]$, have eigenvalues with arbitrarily small magnitude, and their corresponding eigenfunctions—referred to as null-modes—induce negligible changes in function $g(t)$. Meanwhile, the null-modes correspond to arbitrarily large eigenvalues of the inversion operator. Therefore, the inversion is numerically unstable when reconstructing $f(s)$ from a noisy $g(t)$. In Fig. 1, we show examples of different $f(s)$ functions (at the left-hand side) that correspond to $g(t)$ functions with negligible differences (at the right-hand side).

Many efforts have been made to break the degeneracy by adding regulator terms inside the inversion process, such as the Tikhonov regularization [6,9]. In past two decades, the most common approach in such reconstruction task is

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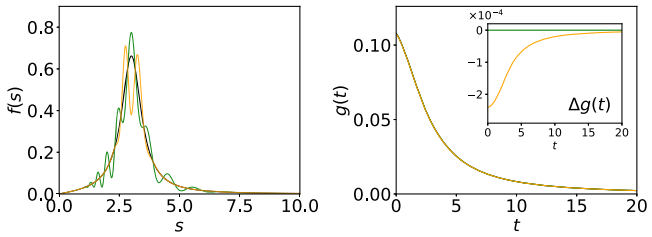

FIG. 1. Spectral functions differed by null-modes (left) and their corresponding Källen-Lehmann correlation functions (right). The insert figure shows the differences in propagator caused by null-modes.

statistical inference. It comprises prior knowledge from physical domains to regularize the inversion [3,10,11]. As one classical paradigm, introducing Shannon-Jaynes entropy regularizes the reconstruction to an unique solution with suppressing null-modes [12–14], that is the maximum entropy method (MEM) [1,3]. In general, the MEM addresses this problem by regularization of the least-squares fit with an entropy term $S[f] = -\int ds[f(s) - m(s) - f(s)\ln(f(s)/m(s))]$. Standard optimizations aim to maximize $Q[f] = \chi^2[f]/2 - \alpha S[f]$ through changing $f(s)$ guided by a prior model $m(s)$, where α is a positive parameter that weights the relative importance between the entropy and the error terms. Although both Tikhonov and Shannon-Jaynes regularization terms yield a unique solution of $f(s)$, it is not guaranteed that the reconstructed $f(s)$ is the physical one. Besides, there are some studies employing supervised approaches to train deep neural networks (DNNs) for learning the inverse mapping [15–19]. In these works, the prior knowledge is encoded in amounts of training data from specific physics insights, whereas one should be careful about the risk that biases might be introduced in training sets. Efforts have been made in unbiased reconstructions by designing physics-informed networks and using complete basis to prepare training data sets [19]. Besides, to alleviate the dependence on specific kinds of training data, there are also studies adopting the radial basis functions and Gaussian process [20,21] to perform the inversion directly.

In this paper we propose an unsupervised automatic differentiation (AD) approach to solve a spectral reconstruction task without training data preparation. Noting the oscillation caused by null-modes, it is natural to add smoothness condition to regularize the degeneracy. Therefore, we represent spectral functions by artificial neural networks (ANNs), in which the ANNs can preserve smoothness automatically [22]. Algorithms based on ANNs have been deployed to address various physics problems, e.g., determining the parton distribution function [25,26], reconstructing the spectral function [15,19,20], identifying phase transition [27–31], assisting lattice field theory calculation [32–35], evaluating centrality for heavy ion collisions [36–38], parameter estimation under detector effects [39,40], and speeding up hydrodynamics simulation [41]. Here we focus on the quality of the spectral function reconstructed from inverting the KL convolution [42],

$$D(p) = \int_0^\infty K(p,\omega)\rho(\omega)d\omega \equiv \int_0^\infty \frac{\omega\rho(\omega)}{\omega^2 + p^2}\frac{d\omega}{\pi}, \tag{2}$$

where $D(p)$ is a propagator derived from a given spectral function $\rho(\omega)$. It is related to a wide range of quantum many-body systems, yet proved to be difficult to solve satisfactorily [13,14]. It shall be worth noting that the framework discussed herein may be applied to other ill-conditioned kernels even extended to different tasks.

II. AUTOMATIC DIFFERENTIATION

Figure 2 shows the flow chart of the devised AD framework with network representations to reconstruct spectral from propagator observable. More details about the AD and related back-propagation algorithm can be found in the Supplemental Materials [43]. The output of network representations are $\vec{\rho} = [\rho_1, \rho_2, \ldots, \rho_{N_\omega}]$, from which we can calculate the propagator as $D(p) = \sum_i^{N_\omega} K(p,\omega_i)\rho_i\Delta\omega$. As Fig. 2 shows, after the forward process of the network and convolution, we can get the spectral $\vec{\rho}$ and further the correlators' reconstruction error as loss function,

$$\mathcal{L} = \sum_i^{N_p} w_i(\mathrm{D}_i - D(p_i))^2, \tag{3}$$

where D_i is observed data at p_i, and w_i denote extra weights of each observation. When taking the inverse variance as w_i, Eq. (3) becomes the standard χ^2 function. Meanwhile, one can directly extend it to multiple data points by making summation over them with calculating all variances. To optimize the parameters of network representations $\{\boldsymbol{\theta}\}$ with loss function, we implement gradient-based algorithms. It derives as

$$\nabla_{\boldsymbol{\theta}}\mathcal{L} = \sum_{j,k} K(p_j,\omega_k)\frac{\partial\mathcal{L}}{\partial D(p_j)}\nabla_{\boldsymbol{\theta}}\rho_k, \tag{4}$$

where $\nabla_{\boldsymbol{\theta}}\rho_k$ is computed by the standard backward propagation (BP) method in deep learning [23]. The reconstruction error will be transmitted to each layer of neural networks, combined with gradients derived from automatic differentiation [44], they are used to optimize the parameters of neural networks. In our case, the Adam optimizer is adopted in following computations [45].

III. NEURAL NETWORK REPRESENTATIONS

As Fig. 2 shown, we develop two representations with different levels of nonlocal correlations among $\rho(\omega_i)$'s to represent the spectral functions with ANNs. The first is demonstrated in Fig. 2(a) and named NN, in which we use

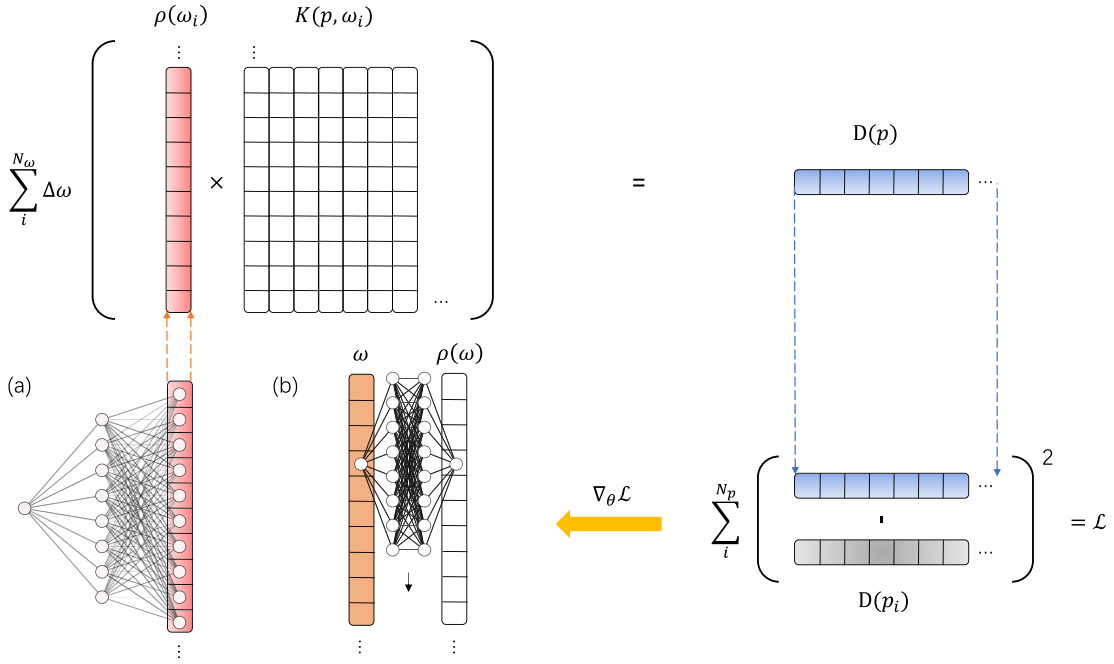

FIG. 2. Automatic differential framework to reconstruct spectral from observations: (a) NN. Neural networks have outputs as a list representation of spectrum $\rho_i(\omega_i)$ and (b) NN-P2P. Neural networks have input and output nodes as (ω_i, ρ_i) pairwise.

L-layers neural network to represent in list format the spectral function $\rho(\omega)$ with a constant input node $a^0 = C$ and multiple output nodes $a^L = [\rho_1, \rho_2, \ldots, \rho_{N_\omega}]$. The width of the lth layer inside the network is n_l, to which the associated weight parameters control the correlation among the discrete outputs in a concealed form. In a special case, a discrete list of ρ_i itself is equivalent to set $L = 1$ without any bias nodes; meanwhile, the differentiable variables are directly elements of $\vec{\rho}$ as network weights. If one approximates the integration over frequencies ω_i to be summation over N_ω points at fixed frequency interval $d\omega$, then it is suitable to the vectorized AD framework described above. The second representation with ANNs is shown in Fig. 2(b), where the input node is $a^0 = \omega$ and the output node is interpreted to be $a^L = \rho(\omega)$. It is termed as point-to-point neural networks (abbreviated as NN-P2P) and it consists of finite first-order differentiable modules, in which the continuity of function $\rho(\omega)$ is naturally preserved [24,47].

We adopt width $= 64$ and depth $= 3$ as default parameter setting in the whole paper, which is explained in the Supplemental Materials [43]. Besides, a pedagogical introduction of the machine learning background can also be found there. For the optimization of the neural network representations, we adopt the Adam optimizer [48] with L_2 regularization for NN, which is a summation over the L_2 norm of all differentiable weights of the network, $L_2 = \lambda \sum_i (\theta_{W,i})^2$ with $\lambda = 10^{-2}$ in the beginning of the warmup stage of training process. For speeding up the training process, we obey an annealing strategy to loosen the value of λ from the initial tight regularization repeatedly to small enough value (smaller than 10^{-8}) in first 40,000 epochs. We checked that end values of λ do not alter the reconstruction results once it is smaller than 10^{-8}. To converge fast, we also adopt a smoothness regulator here, which derives as $L_s = \lambda_s \sum_{i=1}^{N_\omega} (\rho_i - \rho_{i-1})^2$. The initial smoothness regulator is $\lambda_s = 10^{-3}$, then it decreases to 0 in the final step of the warm-up. After that, early stopping is applied for the training with the criterion to be when error between observed $\tilde{D}(p)$ and reconstructed $D(p)$ does not decrease, or the whole training exceeds 250,000 epochs. The learning rate is 10^{-3} for all cases, and there is no any explicit regulators for NN-P2P only implicit nonlocal correlations. Besides, the physical prior we embedded into these representations is the positive-definiteness of fermionic spectral functions (in the lattice QCD case, they are hadronic spectra), which is introduced by applying the softplus activation function at output layer as $\sigma(x) = \ln(1 + e^x)$.

IV. RECONSTRUCTION PERFORMANCE

In this section we demonstrate the performance of our framework by testing their quality in reverting the Green's functions of known spectral functions (also known as mock data). We start with a superposed collection of Breit-Wigner peaks, which is based on a parametrization obtained directly from one-loop perturbative quantum field theory [15,49]. Each individual Breit-Wigner spectral function is given by

$$\rho^{(\mathrm{BW})}(\omega) = \frac{4A\Gamma\omega}{(M^2 + \Gamma^2 - \omega^2)^2 + 4\Gamma^2\omega^2}. \tag{5}$$

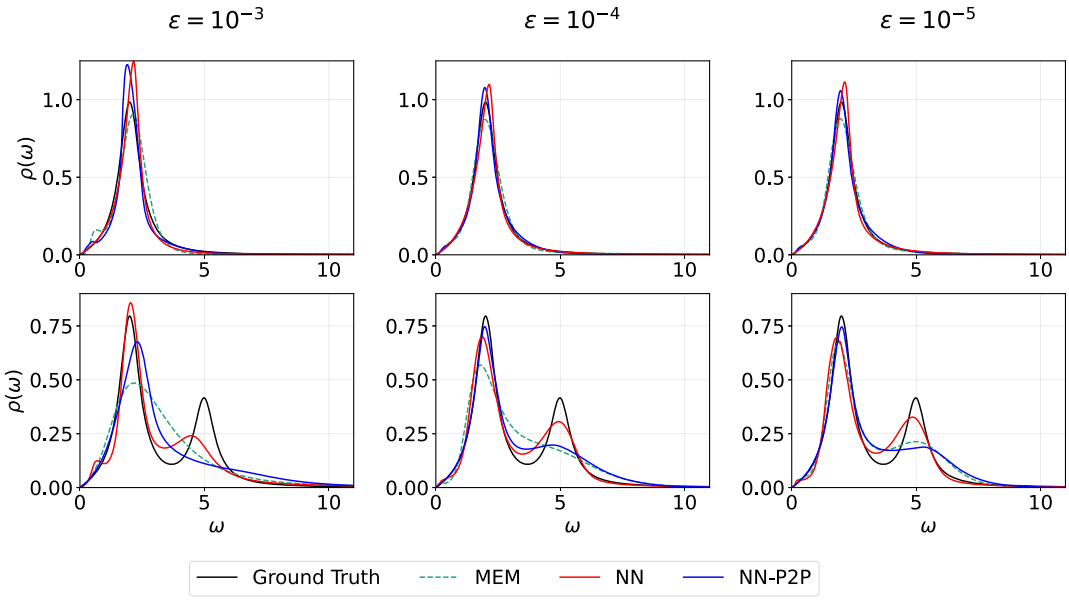

FIG. 3. The predicted spectral functions from MEM, NN, and NN-P2P. From left to right panels, different Gaussian noises are added to the propagator data with $\varepsilon = 10^{-3}, 10^{-4}$, and 10^{-5} in the case of $N_p = 25$ and $N_\omega = 500$ for the spectral. Note that MEM with fixed small α by hand might get improvement, as shown in the Supplemental Material [43] with comparison to AD.

Here M denotes the mass of the corresponding state, Γ is its width and A amounts to a positive normalization constant. The multipeak structure is built by combining different single-peak modules together.

Two profiles of spectral functions from Eq. (5) are set as ground truths. In Fig. 3, the upper is from a single-peak spectrum with $A = 1.0, \Gamma = 0.5, M = 2.0$ (hereafter in paper we omit the energy unit of mass M, width Γ, frequency ω, and momentum p) and the below one is from double-peak profile with $A_1 = 0.8, A_2 = 1.0, \Gamma_1 = \Gamma_2 = 0.5, M_1 = 2.0, M_2 = 5.0$. To imitate the realistic observable data, we follow Ref. [3] and add noise to the mock data with $\tilde{D}_i = \mathrm{D}(p_i) + n_{i,\varepsilon}$, where the noise term follows normal distribution with variance $\sigma^2_{i,\varepsilon} = (\varepsilon \mathrm{D}(p_i) p_i / \Delta p_i)^2$, $P(n_{i,\varepsilon}) = \mathcal{N}(0, \sigma^2_{i,\varepsilon})$. In Fig. 3, we compare the reconstruction results with $\varepsilon = 10^{-3}$, 10^{-4}, 10^{-5}, respectively. The two network representations are marked by blue and red lines. They all show remarkable reconstruction performances for a single peak at each noise level. As a comparison, results from MEM are also shown as green lines. We see that MEM show oscillations around zero-point under different noise backgrounds. The rebuilding spectral function from NN-P2P do not oscillate. This is especially important for such a task of extracting the transport coefficients from real-world lattice calculation data [3,15].

For mock data with two peaks, we observe that the nonlocal smoothness condition of NN-P2P slightly suppress the bimodal structure, whereas NN successfully unfolds the two-peaks information from Green's functions even with noise $\varepsilon = 10^{-3}$. Although NN-P2P misses the second peak which may appear in the case of bimodal as MEM, the calculations of different order momentum from spectral function will not be disturbed. Another advantage of the NN-P2P architecture is its stable performance of the spectral function at small ω limit, which is important for the measurement of conductivity $\sigma \propto \lim_{\omega\to 0} \rho(\omega)/\omega$ [50,51]. The smoothness condition automatically encoded in the network setup suppresses the oscillating null-modes especially at small frequency region, and therefore allows the reliable extraction of conductivity in NN-P2P.

In order to examine the robustness of our method against forms of spectral function, we further apply the framework to mock data prepared by Gaussian form $\rho_G(\omega) = (2\pi\Gamma^2)^{-1} \exp -((\omega - M)^2/2\Gamma^2)$ (A single peak spectrum with $\Gamma = 0.4, M = 2.5$, and the double peak profile is setting as $\Gamma_1 = \Gamma_2 = 0.4, M_1 = 2.0, M_2 = 6.0$), and Lorentzian form $\rho_L(\omega) = \Gamma^2[\pi\Gamma((\omega - M)^2 + \Gamma^2)]^{-1}$ with $\Gamma = 0.3, M = 4.0$. The results are shown in Fig. 4, and it indicates that neural network representations, NN-P2P and NN, can be generalized to other cases, and can reach at least comparable performances to the MEM method.

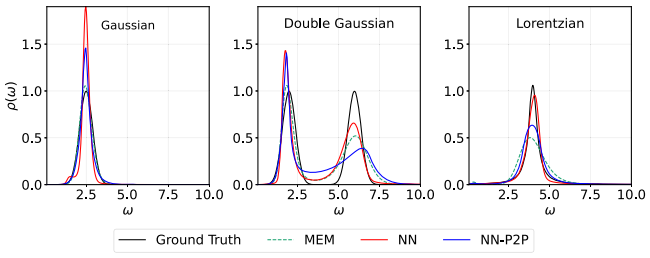

FIG. 4. Reconstructed spectra with MEM, NN, and NN-P2P from the correlators at noise level $\epsilon = 10^{-4}$ with $N_p = 25$ points.

V. EXTENSIONS

In addition to the above reconstructions, we also validate the framework in another two physics motivated cases. The first is to rebuild nonpositive-definite spectral functions—where classical MEM approaches are normally not applicable, unless adopting suitable representations within Bayesian inference perspective [10,21,52,53]. The reason for choosing such a setup is that there are many circumstances the spectra would display positivity violation, which can be related to confined particles e.g., gluons and ghosts, or thermal excitations with long-range correlation in strongly coupled system [21,53,54]. In Fig. 5, we test our NN representation using the correlators generated from the double peak profile, with the first peak turning negative, $A_1 = -0.3$, $A_2 = 1.0, \Gamma_1 = \Gamma_2 = 0.5, M_1 = 2.0, M_2 = 3.5$ (Parameter set I) and $A_1 = 0.3, A_2 = -1.0, \Gamma_1 = \Gamma_2 = 0.5, M_1 = 2.0, M_2 = 3.5$ (Parameter set II). The errors added to correlators obey the same form explained before. The hierarchical architecture of NN representation is unchanged, but the positive activation function of output layer is removed to loosen the positive-definite condition, accordingly the multiplier factor is replaced by $\omega e^{-\omega}$ to suit the low- and large-ω limits. The reconstructions indicate that our NN works consistently well in constructing such spectral functions with nonpositive parts at the location and width of peaks.

The other demonstration case we did is in a more realistic scenario. The hadron spectral function $\rho(\omega, T)$ is encoded in a thermal correlator $G(\tau, T)$ at temperature T [49]. The temperature dependent correlator can be calculated along the imaginary time τ-axis. The physics motivated spectral functions proposed in Ref. [19] are used to test our framework. The correlators are generated with lattice QCD noise-level noises. The spectral function has two parts, a resonance peak and a continuum function. Details can be found in our Supplemental Materials [43]. We test the NN representation using two parameter sets $C_{\text{res}} = 2.0, C_{\text{cont}} = 2.1, M_{\text{res}} = 0.1, M_{\text{cont}} = 0.05$, and $\Gamma = 0.06$ (left) or $\Gamma = 0.09$ (right). The architecture of the NN is the same as before but the multiplier factor is replaced by $\omega^2 \times \omega$ to fit the spectral behavior at the large-ω limit. In Fig. 6, MEM results lose the peak information but our reconstructions can capture it explicitly.

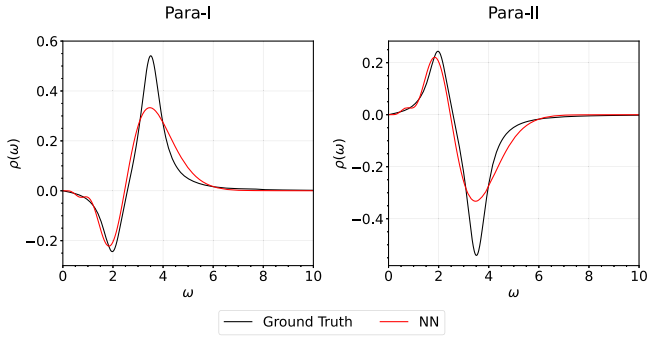

FIG. 5. The predicted spectral functions from NN. The correlators are reconstructed at noise level $\epsilon = 10^{-4}$ with $N_p = 25$ points.

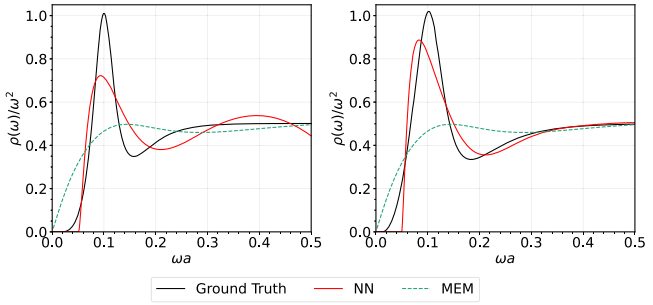

FIG. 6. The predicted spectral functions from NN and MEM at noise level $\epsilon = 10^{-5}$ with $N_\tau = 48$.

VI. SUMMARY

We present an automatic differentiation framework as a generic tool for unfolding spectral functions from observable data. The representations of spectral functions are with two different neural network architectures, in which nonlocal smoothness regularization and modern optimization algorithm are implemented conveniently. We demonstrated the validity of our framework on mock examples from Breit-Wigner spectral functions with single and two peaks. To account for uncertainties from numerical simulation for the propagator observations, we confronted the framework in different levels of noise contamination for the observations. Compared to conventional MEM calculations, our framework shows superior performance especially in two peaks situation with larger noise. Also, the NN-P2P representation gives smooth and well-matched low frequency spectral behavior, which is important in extracting transport properties for the system. Owing to its ill-posedness nature, such an inverse problem cannot be fully solved in our framework. Nevertheless, the remarkable performances of reconstructing spectral functions suggest that the framework and the freedom of introducing nonlocal regularization are inherent advantages of the present approach and may lead to improvements in solving the inverse problem in the future.

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[43] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevD.106.L051502 for machine learning terminology about automatic differentiation and neural networks. Then the details of training set-ups are listed. We also explain how to prepare the mock lattice QCD correlators for doing the tests shown in the section of extensions. Detailed comparisons with the classical MEM method are added in the final part.
[44] It can be conveniently implemented in many deep learning frameworks. In our case, main computations are deployed in Pytorch and released on Github, but also validated in Tensorflow.
[45] It is a stochastic gradient-based algorithm that is based on adaptive estimations of first-order and second-order moments [46].
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