Denoising and Extension of Response Functions in the Time Domain

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Response functions of quantum systems, such as electron Green's functions, magnetic, or charge susceptibilities, describe the response of a system to an external perturbation. They are the central objects of interest in field theories and quantum computing and measured directly in experiment. Response functions are intrinsically causal. In equilibrium and steady-state systems, they correspond to a positive spectral function in the frequency domain. Since response functions define an inner product on a Hilbert space and thereby induce a positive definite function, the properties of this function can be used to reduce noise in measured data and, in equilibrium and steady state, to construct positive definite extensions for data known on finite time intervals, which are then guaranteed to correspond to positive spectra.

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Introduction.—Response functions are critical for the understanding of physics in a wide variety of contexts. They are a natural framework for considering *dynamical* properties that involve excitations [1–4]. Response functions are also measured in experimental setups ranging from low-frequency THz conductivity to magnetic susceptibilities and photoemission spectroscopy. A large body of literature has been devoted to the study of response functions, and a number of field theoretical approaches avoid the calculation of eigenstates entirely, and instead cast the formalism in terms of response functions, called correlation or Green's functions in this context. These include embedding techniques e.g., the dynamical mean field theory [5–7] and cluster extensions [8–11], Monte Carlo approaches for lattice [12] and impurity [13–17] models, self-consistent partial summation methods for real materials and model systems [18–20], and nonequilibrium Green's function methods [21–30].

An important characteristic of correlation functions lies in their analytical properties. The retarded correlation functions have no content at negative times due to causality [1–3]. In the complex frequency domain, they correspond to so-called Nevanlinna functions [31] whose poles are restricted to the lower half of the complex plane. This analytical framework has long been utilized to evaluate integrals that emerge in many-body theory [1–3], such as those occurring in the context of warm dense matter [32] and uniform electron liquids [33]. More recently, it was used to perform analytic continuation from a Wick-rotated frame to a standard frame. Where traditional approaches that rely e.g., on the maximum entropy method [34] have significant uncertainty in the final result, resulting in washed out spectra, explicitly enforcing the highly constraining analytical properties of Nevanlinna functions results in a drastic reduction of the uncertainty, leading to sharp spectral functions [35,36]. It is clear from these examples that encoding this mathematical structure into numerical algorithms can be used to great benefit.

In this Letter, we analyze a fundamental property of correlation functions in the time domain: several correlation functions of interest are *positive definite functions* of their time arguments. This property arises from viewing correlation functions as an inner product in the vector space of operators, combined with the fact that the time translation operator is a unitary representation of the time translation group. This positive definiteness sets a strong constraint on the correlation function, similar to its other analytic properties—in fact, some of these directly follow from the positive definiteness [37]. Moreover, insisting that a correlation function is positive definite enables both the extension of numerical correlation functions to later times, and the extraction of clean spectra from noisy data such as that obtained from Monte Carlo and quantum computing approaches.

We consider a quantum system in a quantum state ρ. In a second quantized formalism, quantum states can be described as states in Fock space [1–3]. The energetics (and dynamics) of the system is described by a Hamiltonian $\mathcal{H}$; in the Heisenberg picture, the time evolution of an operator A is given by $A(t) = e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}$. Expectation values of operators for the state ρ are computed as $\langle A(t)\rangle = \mathrm{Tr}[\rho A(t)]$. In a system with time-translational invariance, $\mathcal{H}$ commutes with ρ, and in the canonical ensemble $\rho = e^{-\beta\mathcal{H}}/\mathcal{Z}$, with β denoting the inverse temperature and $\mathcal{Z} \equiv \mathrm{Tr}e^{-\beta\mathcal{H}}$.

We are primarily interested in time-dependent single-particle correlation functions of the type

$$G_{AB}(t,t') = \langle A^\dagger(t)B(t')\rangle. \tag{1}$$

In a fermion system with creation operators $c_i^\dagger$ creating particles in state i, the so-called "lesser" Green's function [4] $G_{ij}^<(t,t') = i\mathrm{Tr}\left[\rho c_j^\dagger(t')c_i(t)\right]$ and the "greater" Green's function $G_{ij}^>(t,t') = -i\mathrm{Tr}\left[\rho c_i(t)c_j^\dagger(t')\right]$, as well as the charge and spin correlation functions are related to correlation functions of this type. Below, we consider these functions without their usual $\pm i$ prefactors.

Mathematical exposition.—In this section, we will show that $G_{AB}(t,t')$ are *positive definite* functions when $A = B$. First, we observe that the correlation function can be viewed as an inner product of the linear operators that act on Fock space V [we denote this vector space as $\mathcal{L}(V)$]. This fact was also noted in Ref. [38], where it was used to construct strictly positive perturbative approximations. We define an inner product on $\mathcal{L}(V)$ as

$$\langle A, B\rangle := \mathrm{Tr}[\rho A^\dagger B], \tag{2}$$

which is conjugate symmetric, linear in the second component, and positive for $\langle A, A\rangle$ when $A \neq 0$. The properties of conjugate symmetry and linearity are straightforward to verify. The positivity property $\langle A, A\rangle \geq 0$ can be established by noting that (i) if a square matrix M equals the multiplication of a matrix with its Hermitian transpose, i.e., $M = AA^\dagger$, then M is a Hermitian positive semidefinite matrix; and (ii) the trace of the product of two positive semidefinite matrices M and N is always greater than or equal to zero, i.e., $\mathrm{Tr}(MN) \geq 0$. We further restrict our consideration to the cases where A, B are not orthogonal to ρ, which would yield a zero expectation value and is thus not physically relevant for correlation functions. $\mathcal{L}(V)$ together with the inner product of Eq. (2) forms a Hilbert space.

The correlation functions are defined as complex-valued two-time functions ($\mathbb{R}\times\mathbb{R}\to\mathbb{C}$):

$$G_{AA}(t,t') = \mathrm{Tr}[\rho A(t)^\dagger A(t')]. \tag{3}$$

Given the inner product, we can show that the Green's functions arising in the study of equilibrium and nonequilibrium dynamics of many-body physics [1–4] are positive definite functions [39] of two variables. That is, given any (finite) set of arbitrarily spaced time points t, the eigenvalues of the matrix that result from evaluating the Green's function at those points, $[G_{AA}(t_i,t_j)]$, are all positive or zero [40].

We prove this by using an equivalent definition of positive definiteness, which is that, given the aforementioned set of time points t,

$$\sum_{ij} G_{AA}(t_i,t_j)\lambda_i^*\lambda_j \geq 0 \tag{4}$$

for any set of λ_i. This follows from

$$\begin{aligned}\sum_{ij} G_{AA}(t_i,t_j)\lambda_i^*\lambda_j &= \sum_{i,j}\mathrm{Tr}[\rho A(t_i)^\dagger A(t_j)]\lambda_i^*\lambda_j \\ &= \mathrm{Tr}\left[\rho\left(\sum\nolimits_i \lambda_i A(t_i)\right)^\dagger\left(\sum_j \lambda_j A(t_j)\right)\right] \\ &= \left\langle \sum_i \lambda_i A(t_i), \sum_j \lambda_j A(t_j)\right\rangle \geq 0. \end{aligned}\tag{5}$$

The correlation functions (and Green's function as well as self-energies [41,42]) are therefore positive definite functions. This holds for any operator $A\in\mathcal{L}(V)$, and in particular it holds for fermionic creation/annihilation operators $c^\dagger/c$, for densities n, for magnetization operators $n_\uparrow - n_\downarrow$, and trivially for the identity. In multi-orbital systems, the diagonal components of electronic Green's functions $G_{ii}^\lessgtr$ are positive semidefinite. Off-diagonal components can be constructed from linear combinations of $\langle c_i + c_j, c_i + c_j\rangle$, $\langle c_i + ic_j, c_i + ic_j\rangle$, and the diagonal components, all of which are positive definite.

In the presence of time-translation invariance, (i.e., for steady-state and equilibrium systems), the Green's function becomes a function of a single time argument corresponding to the time difference: $G_{AA}(t-t')$, i.e., a positive definite function of a single variable where

$$\sum_{ij} G_{AA}(t_i - t_j)\lambda_i^*\lambda_j \geq 0. \tag{6}$$

In order for time translation to hold, the set of time points t must form a group under addition such as $\mathbb{R}$ or $\mathbb{Z}$. With this additional structure, and as long as ρ commutes with the time evolution operator,

$$\langle A(t), B(t')\rangle = \langle A(t-t'), B\rangle = \langle A, B(t'-t)\rangle \tag{7}$$

follows from the cyclicity of the trace. Additional mathematical details are provided in the Supplemental Material [43].

The positive definiteness of the Green's function sets a strong constraint on the function and has important practical consequences, which we will explore and exploit in the remainder of the Letter. In short, we will show that (i) we can improve the signal-to-noise ratio in noisy data from experiment and theory, and (ii) we can construct causal extensions (with a positive spectrum) from short time data.

Denoising correlation functions.—A first, and natural application of the mathematics presented above, is to take a correlation function from a source that has some inherent noise, and to use the positive definite property to project its values to the nearest positive definite correlation function; in effect, denoising the data. Noisy correlation functions

can arise from Monte Carlo evaluations, from experimental measurements, or from simulations on quantum computers.

We consider a discretized, time-translation invariant correlation function on a regularly spaced time axis t, $G_{AA}(t_i - t_j)$. If we label the elements of the correlation function as $G_{AA}(t_i - t_j) \to f_{i-j}$, then the resulting matrix $\underline{\mathrm{G}}$ with entries $\underline{\mathrm{G}}_{ij} = f_{i-j}$ is a positive semidefinite Hermitian Toeplitz matrix [39],

$$\underline{\mathrm{G}} = \begin{pmatrix} f_0 & f_1 & f_2 & \cdots & f_n \\ f_1^* & f_0 & f_1 & \cdots & f_{n-1} \\ f_2^* & f_1^* & f_0 & \cdots & f_{n-2} \\ \vdots & & & \ddots & \vdots \\ f_n^* & f_{n-1}^* & f_{n-2}^* & \cdots & f_0 \end{pmatrix}. \tag{8}$$

$\underline{\mathrm{G}}$ is commonly known as the Gramian or "Gram" matrix.

In the presence of noise in the correlation function data (f_j), this matrix is not positive semidefinite (PSD). However, an alternating projection to the nearest PSD matrix [44] followed by projections to the nearest Toeplitz matrix [45] and an enforcement of the value at time zero (which is typically known precisely, e.g., from equal-time measurements or sum rules) results in quick convergence to a positive definite function.

The projection to the nearest PSD matrix is achieved by diagonalizing G and setting all negative eigenvalues to zero. The projection to the nearest Toeplitz matrix averages entries diagonally, and the enforcement of the norm consists of fixing the diagonal to a predetermined value. While an alternating projection typically converges in less than 100 iterations, faster converging schemes, see e.g., [46–48], may be substantially more efficient; we have not explored them here.

We illustrate the denoising in Fig. 1 for a positive definite Green's function of a steady-state transport problem simulated by quantum Monte Carlo. Enforcing positive definiteness by the procedure above shows a dramatic improvement of the quality of the data. Details and an error analysis for the analytically solvable Hubbard dimer example are presented in the Supplemental Material [43].

Extending correlation functions to longer times.—A second consequence of positive definiteness is that positive definite extensions of response functions to longer times exist, from which spectral measures can be constructed. We make use of two well-known mathematical facts for positive definite functions. First, functions that are only known on a subset of their domain (e.g., $\mathbb{Z}$ or $\mathbb{R}$) have at least one extension to the full domain [50–52]. This is a consequence of the extension theorems of Kreĭn (in the case of $\mathbb{R}$) and Carathéodory (in the case of $\mathbb{Z}$). Second, according to Bochner's theorem [37], the Fourier transform of a positive definite function (over $\mathbb{Z}$ or $\mathbb{R}$) is guaranteed to have positive real part; moreover, the inverse Fourier transform of a positive spectral function is guaranteed to be positive definite. In the discrete case, these extensions may not be unique; in the continuum case, uniqueness is guaranteed by the analyticity of the Green's function.

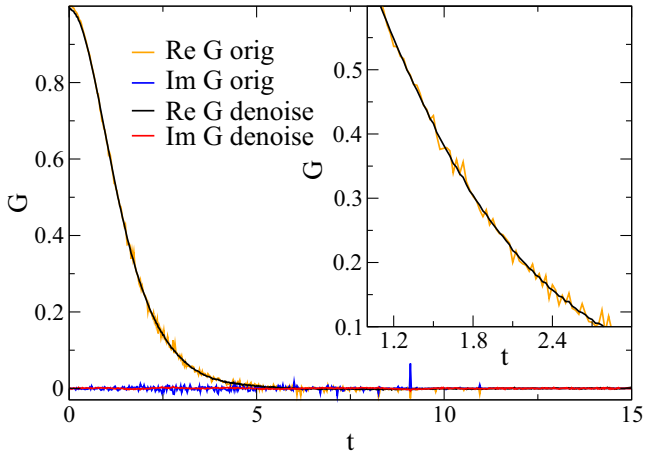

FIG. 1. Denoised quantum Monte Carlo data. Main panel: inchworm [49] quantum Monte Carlo of a steady-state transport problem (for data and parameters see Fig. 1 of [30]), real part (orange) and imaginary part (blue). Denoised data, real part (black) and imaginary part(red). Inset: closeup of the region near $t = 2$ highlighting the effect of denoising.

Conceptually, this realization offers a straightforward methodology to obtain causal spectral functions from finite-time data: in a first step, the function is extended from short to long times by taking advantage of an extension theorem. In a second step, the uniquely defined and positive Fourier transform of the extended data is computed.

Numerically, we can use extension theorems to predict Green's function values at later times from known values at short times [39]. Supplementing a known time series $f_0, \ldots, f_n$ by a single unknown element f_{n+1}, the Gramian of Eq. (8) is a Toeplitz matrix with a single unknown complex number $f_{n+1} = \underline{\mathrm{G}}_{0,n+1} = (\underline{\mathrm{G}}_{n+1,0})^*$. The real and imaginary parts of f_{n+1} can then be obtained in a two-dimensional search in the complex plane for the region where the lowest eigenvalue of G is zero or larger, i.e., G is positive definite; such a value must exist [50] and $|f_{n+1}| \leq f_0$ due to the positive definiteness [53]. Note that this extension may not be unique.

Figure 2 demonstrates the approach for the Green's function of the Hubbard dimer (for details see the Supplemental Material [43]). Once the data is extended to all times, it yields a unique spectral function [37].

More generally, given that the Gram matrix Eq. (8) is a Toeplitz matrix of size n, and assuming a rank of size r, a classical result by Carathéodory and Fejér [54] guarantees the existence of the decomposition $T = APA^\dagger$, where A is a $n \times r$ Vandermonde matrix and P is a $r \times r$ positive diagonal matrix. The columns of A can be interpreted as

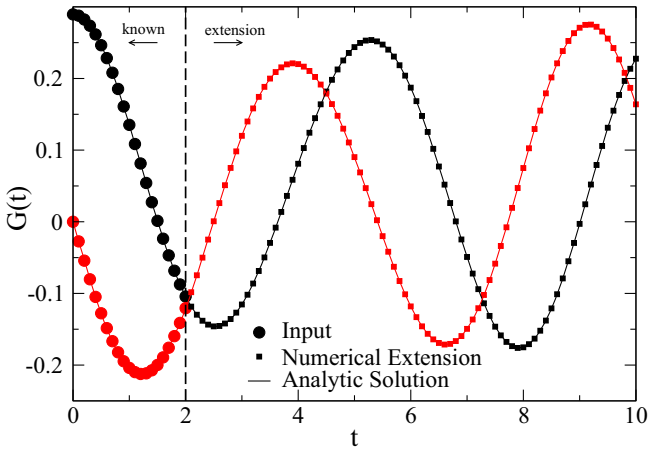

FIG. 2. Extension of the on-site Hubbard dimer Green's function $G^{>}_{11\uparrow}(t)$. Shown are real (black) and imaginary (red) parts of input data up to $t = 2$ (circles), the numerically computed extension from $t = 2$ to $t = 10$ (squares), and the analytically known Green's function up to $t = 10$ (lines).

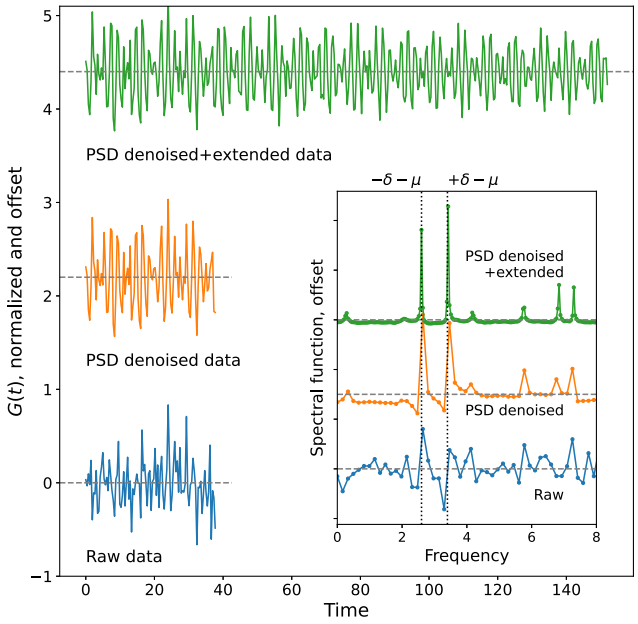

FIG. 3. Main panel: greater Green's function $G^{>}_{k}(t)$ at $k = \pi/2$ of an 8-site Su-Schieffer-Heeger with $\delta = 0.4$ and $\mu = -3$. The figure shows the raw data obtained from the *ibm_auckland* quantum computer (blue), as well as the PSD denoised data (orange), and PSD denoised and extended data (green). Inset: corresponding spectral functions. The Fourier transform used a damping factor $\tau = 100$. The vertical dashed lines indicate the expected analytic frequencies.

uniformly sampled oscillation frequencies, and the entries of P as positive "pole strengths." This approach therefore gives both access to the spectral function in terms of a series of r discrete poles at given frequencies, and a method to construct extensions for all times by enlarging the matrix A with additional frequencies. It also indicates that an extension is unique if a spectrum consists of fewer poles than measurements, which is the typical case in model systems and quantum computing applications.

The decomposition also establishes a connection to signal processing and control theory, where PSD covariance matrices of time-invariant processes are analyzed using this decomposition in super-resolution algorithms such as the multiple signal classification [55], and where thereby approximate extensions from noisy data can be constructed. We will explore this connection, together with connections to reproducing kernel Hilbert spaces [56], in a future paper.

Application to quantum computing.—As a final illustration, we apply the denoising and extension implications of Eq. (6) to a noisy correlation function measured on IBM's quantum computer *ibm_auckland*. We have measured the momentum-space greater Green's function for the empty state $G_k(t) \coloneqq \langle 0|c_k^{\dagger}(t)c_k|0\rangle$ for an 8-site Su-Schrieffer-Heeger model, which is a model for free electrons with a hopping parameter that alternates with an amplitude δ

$$\mathcal{H} = -V_{nn}\sum_i \left[1 + (-\delta)^i\right] c_i^{\dagger}c_{i+1} + \text{H.c} - \mu\sum_i c_i^{\dagger}c_i, \qquad (9)$$

where we set $V_{nn} = 1$. The raw data (originally published in Ref. [57]), is shown in Fig. 3, in the gapped phase with $\delta = 0.4$ at $k = \pi/2$. We report details of the calculation in the Supplemental Material [43]. Because the model is translationally invariant and has two bands, the momentum basis Green's functions should exhibit at most two frequencies. However, due to the hardware noise from the quantum computer, there is significant noise in the time domain signal. This is similarly reflected in the Fourier transform, where peaks can be identified, but only in the power spectrum—the spectral function (shown in Fig. 3) does not show the requisite analytic structure (a consistent sign across all frequencies). We denoise the data by asserting the positive definiteness and performing a point-by-point optimization on the Green's function, where the cost function is the square of the negative eigenvalues, and obtain an improved spectrum. Much of the broad spectrum noise has disappeared and the peaks are clearly visible in the spectral function. We detail the procedure and show the result on additional data from different k points in the Supplemental Material [43]; we find that this iterative procedure is more suitable in the presence of extreme noise than the alternating projection scheme used for Monte Carlo data. The final step is to extend the data as discussed above, which results in a long positive definite signal, with sharp peaks in the spectrum.

Note that applying a PSD projection as done here is conceptually distinct from recent efforts using advanced signals processing approaches to extract a cleaner signal from noisy quantum simulation [58–60], as well as memory

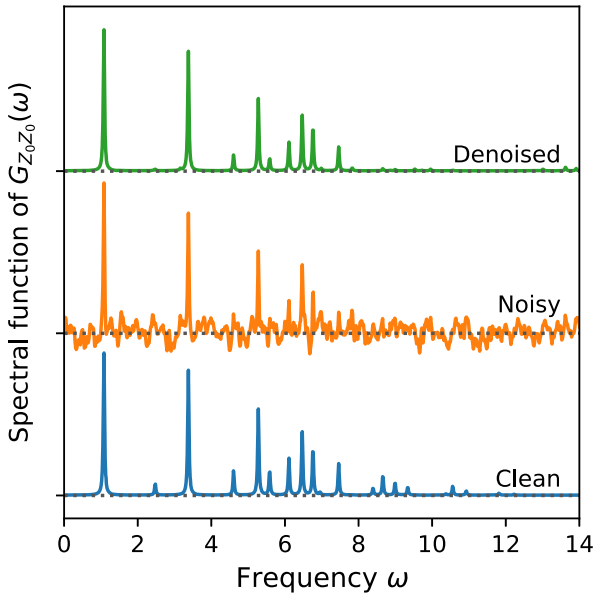

FIG. 4. Spectral function of the $G_{Z_0Z_0}(t)$ correlation function computed for a 16-site Heisenberg chain in the antiferromagnetic regime. The noisy data was polluted by Gaussian noise with $\sigma = 0.5 \cdot G_{Z_0Z_0}(t = 0)$.

kernel approaches [61–66], and in fact can be combined with both.

Discussion.—Positive semidefinite response functions are ubiquitous in many-body physics [1,4,67], as is the desire to reduce systematic or stochastic noise and to obtain corresponding spectral functions. The theory and algorithms presented here are broadly applicable to problems ranging from the analysis of experimental measurements to simulations of quantum systems on classical and quantum hardware.

The Letter and Supplemental Material [43] demonstrate that denoising data yields substantial improvements over analyzing noisy spectra directly, but the approach has its limits. It generates the closest causal solution to the observed data, which may differ from the solution without noise, as seen in Fig. 3 where unphysical peaks appear. For stochastic noise, a careful error assessment through bootstrap or jackknife methods is advised. However, in the presence of systematic noise the method may not correct error directions that are consistent with causality.

Similarly, the extension formalism has limitations, most notably potential ambiguities in defining extensions. Discrete spectra (e.g., Figs. S1 and S2) allow for a unique extension due to the low-rank properties of the Gramian [54]. However, smooth spectra, such as those in Fig. 1, may admit multiple extensions. While one could theoretically generate and examine all causal extensions, an efficient numerical method to do so is not known to us. Empirically, a denser sampling grid tends to offer more accurate extensions, since the corresponding data is closer to the (uniquely determined [51]) continuum case.

Nevertheless, we expect the applications of PSD projection to continue to be applicable as system sizes increase. In addition to the continuum case shown in Fig. 1, in Fig. 4 we demonstrate the denoising of a more complex but still discrete system. We consider the on-site correlation function $G_{Z_0Z_0}(t) = \langle Z(r = 0, t)Z(r = 0, t = 0)\rangle$ for a 16-site Heisenberg chain in the antiferromagnetic regime (time domain data is shown in Fig. S3). As the figure shows, the denoising procedure recovers a proper (positive) spectrum even for this complex system. Although not all peaks are recovered, the denoised signal has peaks in the appropriate places, and much more information is visible than in the noisy signal.

In this Letter, we have demonstrated the efficiency of removing noise with a PSD projection in the examples of synthetic data and real-world quantum computing data, as well as the feasibility of extending data to long time. We believe that a PSD noise filter followed by an extension should be applied much more broadly to any positive definite response function, simulated or measured, before data is analyzed and/or spectra are computed, including data from quantum Monte Carlo, tensor networks, and time-resolved experiments.

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