

Application of Laplace filters to the analysis of lattice time correlators

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The analysis of lattice simulation correlation function data is notoriously hindered by the ill conditioning of the Euclidean time covariance matrix. Additionally, the isolation of a single physical state in such functions is generally affected by systematic contamination from unwanted states. In this paper, we present a new methodology based on regulated Laplace filters and demonstrate that it can be used to address both issues using state-of-the-art simulation data. Regulated Laplace filters are invertible high-pass filters that suppress local correlations in the data, and we show that they can reduce the condition number of covariance matrices by several orders of magnitude. Furthermore, Laplace filters can annihilate functions that decay exponentially with time, which can be used to alter the spectrum of a lattice correlation function. We show that this property can be exploited to significantly reduce excited-state contamination in the determination of matrix elements. The same property can also be used to constrain the spectral content of a correlation function and has the potential to form the basis of new methods to extract physical information from lattice data.

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I. INTRODUCTION

Lattice quantum chromodynamics (QCD), or more generally, lattice field theory, allows one to formulate strongly coupled field theories nonperturbatively. Such a formulation is then often used as the basis for numerical *ab initio* simulations, which provide systematically improvable predictions in particle physics and related fields. Compelling examples of results obtained using lattice QCD can be found in the Flavour Lattice Averaging Group (FLAG) review [1] and the Muon $g - 2$ Theory Initiative White Paper [2]. In lattice QCD, a discretized version of the QCD path integral in Euclidean space-time is numerically estimated using Markov chain Monte Carlo (MCMC) techniques. The quantities typically computed are *correlation functions*, i.e., expectation values of products of local quantum operators. They are generally expressed as functions of the momenta and Euclidean times of the operators involved (time-momentum representation). Assuming all time separations between operators are fixed except one, and assuming a theory with a mass gap $M > 0$, correlation functions are linear

combinations of exponentials of the form e^{-Et} , where t is the variable Euclidean time separation, and $E \geq M$ is the energy of a specific quantum state propagating in the system. The coefficients (or *amplitudes*) of such combinations are related to quantum matrix elements of the operators involved. The energies and matrix elements are physical quantities typically required for predicting a given observable.

A critical step in most lattice analyses is therefore to fit statistical data for correlation functions to a truncated spectral decomposition as described above. This is generally done through a goodness-of-fit optimization of such a model to the data. Although this is in appearance a simple problem, precisely assessing systematic uncertainties on the resulting fit parameters can be challenging, in part due to the two issues below:

- (1) Data points are generally strongly statistically correlated at short time separations, as a consequence of the covariance itself being a correlation function decaying exponentially with time separations. This makes χ^2 goodness-of-fit estimates potentially unreliable due to poor conditioning of the time-covariance matrix.
- (2) Numerous physical observables require the extraction of a single term Ae^{-Et} in the correlation function, typically the one with the smallest energy (ground-state contribution). It is often difficult to distinguish such a term from others in the correlation function, and maximum-likelihood estimators of A

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and E can be systematically biased by the presence of contributions with energies close to E . This issue is generally referred to in the literature as *excited-state contamination*. Additionally, in many lattice correlation functions, the signal-to-noise ratio degrades exponentially fast at large times, which can make this issue extremely challenging to address in a controlled way.

These two issues can combine and result in uncontrollable systematic errors. Indeed, excited-state contamination could, in theory, be addressed by conducting likelihood-ratio tests for the presence of additional states; however, this requires reliable p -values from minimized χ^2 , which is generally hindered by the poor conditioning of the covariance matrix.

The issues above, as well as potential mitigation strategies, have been discussed at length in the lattice QCD literature over the past 30 years. Some original work on the topic can be found in Refs. [3,4], and here we review some of the most recent works on this topic. One approach to addressing the first issue above is to use the better-behaved *Ledoit-Wolf shrinkage* estimators [5] for the covariance matrix. Such an estimator replaces the sample covariance matrix V with a regulated version of the form $V^* = (1 - \lambda)V + \lambda V_{\text{diag}}$, where V_{diag} is the diagonal part of V . It can be proven [5] that the regulator λ can be chosen such that, asymptotically, V^* is a better-conditioned unbiased estimator of the covariance matrix. This approach is commonly used in lattice QCD; see, for example, [6] as one of the earliest works to use it. A key issue with this approach is that although V^* can be shown to be an optimal regularization asymptotically, it may be difficult to estimate the deviation from this behavior at finite statistics. The shrinkage described above was then improved using a nonlinear optimization in Refs. [7,8]. However, without studying the asymptotic properties, Ledoit-Wolf shrinkage becomes essentially an *ad hoc* regularization procedure, and it is difficult to assess its effect on estimating p -values and resulting hypothesis tests.

Another approach proposed in [9] suggests using an alternative statistic to the standard correlated χ^2 , where the covariance matrix is replaced by a better-behaved one, typically the diagonal part of the covariance matrix. This formalism covers other common regularization strategies such as cuts in the singular value decomposition of the correlation matrix (cf., for example Ref. [10]). In this work, the authors derive the appropriate p -value for this modified χ^2 , allowing them to perform hypothesis tests based on a more reliable estimator. While this addresses some shortcomings of more *ad hoc* regularization strategies, the fit parameters obtained by minimizing the modified χ^2 are, strictly speaking, not the maximum-likelihood parameters given the correlated distribution of the data.

Finally, regarding the determination of a single-state contribution (issue 2 above), a number of techniques are commonly employed. First, excited-state contamination can be suppressed at the level of the measurement itself by choosing operators with weaker coupling to the unwanted states. This can be achieved, for example, by smearing operators using Jacobi iterations [11] or more general forms targeting specific physics (see, for example, the recent work [12]). Methods based on operator design may not be confined to purely statistical data analysis and may require remeasuring expensive correlation functions.

Restricting ourselves to methods usable at the data-analysis stage, one can attempt to use the time-translation properties of correlation functions to reconstruct the spectrum. This is historically the aim of Prony's method [13], which was adapted to lattice QCD analysis as a generalized eigenvalue problem (GEVP) in [14,15]. More recently, Wagman proposed a new method [16] using time translations of the correlation function to infer the spectrum of the transfer matrix via the Lanczos algorithm. This was proven later [17] to be equivalent to the Prony GEVP, and this equivalence is further discussed in [18]. Although methods involving solving for a matrix spectrum have been used consistently in lattice QCD [19], they can feature challenging eigenvalue-identification issues due to the noisy nature of the data. There are ways to regularize this problem, including in the previously cited references, or additionally in the recent work [20].

In this paper, we propose a new method to solve the two issues above, with an emphasis on simplicity and minimal deviations from standard statistical frameworks. We stress that this method is complementary to the literature reviewed in this section, in the sense that in cases where it does not by itself overcome the mentioned issues, it can be applied in conjunction with other ways to regularise the resulting covariance matrix. The key concept is to use regulated Laplace filters on correlation functions, which are a discretized version of the second-order differential operator $-\partial_t^2 + \lambda^2$, where λ is an arbitrary real, nonzero regulator that guarantees the invertibility of the filter. Laplace filters are high-pass filters, allowing us to decorrelate data and improve the conditioning of the correlation matrix. Additionally, they annihilate $e^{\pm\lambda t}$ at nonzero times, allowing us to modify and probe the spectrum of a correlation function by varying the regulator. In Sec. II, we give general definitions that will be used in the rest of the paper. In Sec. III, we introduce representative lattice QCD data that will be used for numerical tests of our methods. In Sec. IV, we discuss how Laplace filters can be used to significantly improve the conditioning of covariance matrices. We then demonstrate in Sec. V how statistical constraints on the spectrum of a correlation function can be designed using Laplace filters. Finally, we present in Sec. VI a number of applications to realistic lattice QCD data-analysis examples.

II. GENERAL PROBLEM AND DEFINITIONS

We consider space-time to be a finite discrete hypercubic lattice.¹ We consider an arbitrary quantum expectation value lattice with spacing a and Euclidean metric

$$C[t] = \langle O[t] \rangle \quad (1)$$

depending on a single discrete time separation t , which in units of the time spacing a takes integer values from 0 to $N_t - 1$. The operator O is generally a product of two or more local operators, and may have additional time variables, which are assumed fixed here. Such an object is referred to as a *time correlator*. Unless otherwise specified, all quantities are expressed in units of a . The bracket notation $[t]$ indicates that t is a discrete variable; later, the notation (t) will be used for continuous variables. We also denote by C the column vector whose component at row t is $C[t]$. We always assume that N_t is divisible by 2. Unless otherwise specified, we assume discrete times are periodic in this paper. This means any operation on time indices should be understood as being performed modulo N_t . This assumption is, in principle, arbitrary, and in several cases lattice correlators may be computed with nonperiodic boundary conditions in time. We make this choice primarily for clarity, as several concepts in this paper have known generalizations to nonperiodic boundary conditions. Second, a finite sequence of numbers can always be assumed periodic regardless of its origin, and the boundary condition can be seen as potential additional freedom in several methods presented here.

Generally, C is estimated through a Monte Carlo process, and N samples $C_\alpha[t]$ of $C[t]$ are known, either directly or through a resampling process (e.g., jackknife or bootstrap). It is important to note that we assume α indexes samples of the expectation value C , not the value of the underlying operator O on individual field configurations.² The average

$$\bar{C}[t] = \frac{1}{N} \sum_{\alpha=1}^N C_\alpha[t], \quad (2)$$

is a Monte Carlo estimator of $C[t]$. We define the associated noise function:

$$\eta_\alpha[t] = C_\alpha[t] - \bar{C}[t]. \quad (3)$$

By construction, $\bar{\eta}[t] = 0$. An unbiased estimator of the true time *covariance matrix* $\Sigma[t_1, t_2]$ of $C[t]$ is given by the *sample covariance matrix*

¹This is the most straightforward and common choice in lattice field theory, however every method in this paper can be applied to anisotropic lattices.

²Assuming normally distributed averages, this assumption simply means we do not add a factor of $\frac{1}{N}$ in the sample variance matrix definition in Eq. (4).

$$\begin{aligned} V[t_1, t_2] &= \frac{N}{N-1} (\overline{\eta \otimes \eta}[t_1, t_2]) \\ &= \frac{1}{N-1} \sum_{\alpha=1}^N \eta_\alpha[t_1] \eta_\alpha[t_2]. \end{aligned} \quad (4)$$

and the *sample correlation matrix* is defined as

$$\Gamma[t_1, t_2] = \frac{V[t_1, t_2]}{\sqrt{V[t_1, t_1]V[t_2, t_2]}}. \quad (5)$$

Both V and Γ are symmetric, positive-definite matrices. The correlation matrix can also be defined analogously to Eq. (4) using the *normalized noise function*

$$\gamma_\alpha[t] = \frac{\eta_\alpha[t]}{\sqrt{V[t, t]}}, \quad (6)$$

so that Γ can be written

$$\Gamma[t_1, t_2] = \frac{N}{N-1} (\overline{\gamma \otimes \gamma}[t_1, t_2]). \quad (7)$$

In a typical lattice calculation, one fits $\bar{C}[t]$ to a model $f(t; \theta)$, where θ denotes the parameters of the model. This model is generally determined by a spectral representation of the underlying correlation function. This is often achieved using a χ^2 goodness-of-fit approach as follows. We define the model prediction vector $F(\theta)[t]$ as the column vector with coefficients $f(t; \theta)$, and the model-to-data variation $\Delta(\theta) = F(\theta) - \bar{C}$. The χ^2 function for the fit is then given by

$$\chi^2(\theta) = \Delta(\theta)^T V^{-1} \Delta(\theta). \quad (8)$$

Maximum-likelihood parameters are then found by minimizing $\chi^2(\theta)$ over θ . A key issue in this process is the presence of the inverse covariance matrix in Eq. (8). In a system with strong time correlations, which is often the case with lattice QCD data, V can be badly conditioned, resulting in a numerical inverse that is poorly determined or even impossible to compute with double-precision arithmetic. In such cases, maximum-likelihood parameters or the χ^2 function itself can have unreliable values, compromising the scientific output of the calculation. Additionally, it has become frequent in state-of-the-art lattice calculations to estimate final systematic uncertainties using a model-averaging procedure [21,22]. In such an approach, many candidate predictions for a given observable are combined in a histogram weighted according to some score function, for example the Akaike information criterion (AIC). Score functions will often depend on numerical values of χ^2 , and imprecision in estimating those can have nontrivial effects on the final prediction.

The problem of inverting the covariance matrix can be replaced without loss of generality by the invertibility of the correlation matrix, which is in general better conditioned. We define $D[t] = V[t, t]^{-\frac{1}{2}}$ to be the element-wise inverse square root of the diagonal vector of the covariance matrix. The correlation matrix Γ is then given by

$$\Gamma = \text{diag}(D)V\text{diag}(D), \quad (9)$$

where $\text{diag}(D)$ is the diagonal matrix with coefficients given by the elements of D . Therefore, knowing $(D \otimes D)$ from the data, inverting V can be reduced to inverting Γ , whose coefficients are bounded in the $[-1, 1]$ interval. We now discuss a metric that can be used to quantify the conditioning of Γ .

A. Correlation dynamic range (CDR)

We introduce the notion of *correlation dynamic range* (CDR). We first define the *condition number* of a positive-definite matrix M , given in the usual way by

$$\kappa(M) = \frac{\max_j(\sigma_j)}{\min_j(\sigma_j)}, \quad (10)$$

where the σ_j , $0 \leq j < N_t$, are the eigenvalues of M . The CDR of M is then defined by the value of $\kappa(M)$ in decibels (dB), namely

$$\text{CDR}(M) = 10 \log_{10}[\kappa(M)]. \quad (11)$$

The CDR gives the number of orders of magnitude between the smallest and largest eigenvalues of M , multiplied by 10. A general rule of thumb in interpreting the CDR is as follows: a CDR of x dB implies that the precision of the data will be degraded by $x/10$ significant digits when multiplied by M .

In the case of the correlation matrix Γ , exactly uncorrelated data is equivalent to $\Gamma = 1$, which is equivalent to a CDR of 0 dB. On the other hand, if one data point is an exact linear combination of others, then Γ is singular and has a CDR of $+\infty$ dB. With IEEE 754 double precision arithmetic, a matrix becomes effectively singular for CDRs above approximately $10 \log_{10}(2^{53}) \simeq 156.54$ dB. Let us now define the general problem of optimization of correlations through data transformations.

B. General data transformations

Let ϕ be an arbitrary known function from the data space $\mathbb{R}^{N_t}$ to some *latent space* $\mathbb{R}^{N_\ell}$, with $N_\ell \leq N_t$. We define the latent-space data

$$C_\alpha^{(\phi)} = \phi(C_\alpha) \in \mathbb{R}^{N_\ell}, \quad (12)$$

and we denote with a superscript (ϕ) all quantities derived from C_α (e.g., $\bar{C}$, η_α , V , etc.) as the corresponding

estimators evaluated on the latent-space data $C_\alpha^{(\phi)}$. As defined in data space for Eq. (8), given a model $f(t; \theta)$, we define the latent-space model prediction vector

$$F^{(\phi)}(\theta) = \phi[F(\theta)], \quad (13)$$

where, as previously, $F(\theta)[t] = f(t; \theta)$. One can hence search for best-fit parameters by minimizing the latent-space χ^2 function

$$(\chi^2)^{(\phi)}(\theta) = \Delta^{(\phi)}(\theta)^T (V^{(\phi)})^{-1} \Delta^{(\phi)}(\theta), \quad (14)$$

with $\Delta^{(\phi)}(\theta) = F^{(\phi)}(\theta) - \bar{C}^{(\phi)}$. One can then attempt to find transformations under which, for example, the correlation matrix is better conditioned. We also require that the model predictions and the χ^2 function remain meaningful from a statistical point of view. Therefore, the latent-space data should approximately obey Gaussian statistics for the χ^2 function interpretation to be valid. In general, an important special case is when ϕ is a linear transformation, which will always be the case in this paper. Under this assumption, if the data are Gaussian distributed, then the latent-space data will also be Gaussian with mean and variance given by

$$\bar{C}^{(\phi)} = \Phi \bar{C}, \quad \text{and} \quad V^{(\phi)} = \Phi V \Phi^T, \quad (15)$$

where Φ is the $N_\ell \times N_t$ matrix representation of ϕ . If ϕ is nonlinear, then the Gaussianity of the latent-space data will directly depend on the smoothness of ϕ around $\bar{C}$.

In this paper, we will investigate a unique class of linear transformation, the regulated Laplace filters, presented in the next section. However, the general idea in this section may be of use for future research on different transformations.

C. Regulated Laplace filter definition

We start by considering the discrete Laplacian

$$\Delta C[t] = C[t-1] - 2C[t] + C[t+1]. \quad (16)$$

The data transformation considered here is the operator

$$D_\lambda C[t] = (-\Delta + \lambda^2)C[t], \quad (17)$$

where the regulator λ is a nonzero real number and ensures that D_λ is an invertible matrix. D_λ is translation-invariant and corresponds to the convolution with the impulse response $(-1, 2 + \lambda^2, -1)$. This filter will perform local subtractions in time, which intuitively should reduce correlations in lattice time correlators. In frequency space, this corresponds to the multiplication

$$\mathcal{F}D_\lambda C[\omega] = \left[4 \sin \left(\frac{\pi \omega}{N_t} \right)^2 + \lambda^2 \right] \hat{C}[\omega], \quad (18)$$

where $\mathcal{F}C = \hat{C}$ is the discrete Fourier transform of C

$$\hat{C}[\omega] = \sum_{t=0}^{N_t-1} C[t] e^{-i \frac{2\pi}{N_t} \omega t}, \quad \text{with } \omega \in \{0, \dots, N_t-1\}. \quad (19)$$

In essence, D_λ is a square-law high-pass filter, which suggests it will suppress short-time correlations. Before discussing the practical implication of this statement further, we present the representative lattice QCD data used in this paper.

III. REPRESENTATIVE SAMPLE DATA

In order to exemplify methods in this paper, we apply them to real lattice data on $N_f = 2 + 1$ ensembles generated by the RBC and UKQCD collaborations [23–25]. We consider five datasets corresponding to a selection of typical state-of-the-art lattice applications. In Table I, we list some basic properties of these datasets. In particular, we consider mesonic pseudoscalar two-point functions: one for a pion with physical pion mass (M0M-mes-ll), one for a light-heavy meson between the D and the B masses (F1M-mes-lh), and one for a heavy-heavy meson between the η_c and the η_b masses (F1M-mes-hh). Later, we also consider two-point and three-point functions related to the semileptonic decay of a charm quark to a strange quark with a strange spectator quark (C1M-semi-sc-ss), and to neutral meson mixing between a neutral, unphysically light B_s meson and its antiparticle (F1M-mix-sh). While this is not an exhaustive list, it nonetheless captures several types of datasets to which the ideas presented here can be applied and which are directly relevant to the phenomenological exploitation of lattice QCD simulations.

Regarding the M0M-mes-ll, F1M-mes-lh, and F1M-mes-hh correlation functions, we consider standard operators with the quantum numbers of pseudoscalar mesons of the form

$$\phi_{q_1 q_2}(x) = [\bar{q}_2 \gamma_5 q_1](x), \quad (20)$$

where q_1 and q_2 are quark fields of potentially different flavors. The correlators studied are two-point functions of the form

$$C_2^{q_1 q_2}[t] = \sum_{\mathbf{x}, \mathbf{y}} \langle \phi_{q_1 q_2}(y) \phi_{q_1 q_2}^\dagger(x) \rangle, \quad (21)$$

with $x = (t_{\text{src}}, \mathbf{x})$, $y = (t_{\text{snk}}, \mathbf{y})$, and $t = t_{\text{snk}} - t_{\text{src}}$. Also, we only consider zero-momentum-projected correlation functions, so we do not list any momentum arguments, even though results in this paper equally apply to nonzero momenta.

TABLE I. Representative datasets used in this study. The temporal extents N_t of the M0M, F1M and C1M ensembles are 128, 96 and 64, respectively.

Name	M_π/MeV	a^{-1}/GeV	Flavor	Process
M0M-mes-ll	139	2.3	$\bar{\ell}\ell$	$\pi \rightarrow \pi$
F1M-mes-lh	232	2.7	$\bar{\ell}h$	$D \rightarrow D$
F1M-mes-hh	232	2.7	$\bar{h}h$	$\eta_c \rightarrow \eta_c$
C1M-semi-sc-ss	276	1.7	$\bar{s}c \rightarrow \bar{s}s$	$D_s \rightarrow \eta_s \ell \nu$
F1M-mix-sh	232	2.7	$s\bar{h} \rightarrow \bar{s}h$	$B_s^0 \rightarrow \bar{B}_s^0$

For the semileptonic decay dataset C1M-semi-sc-ss, we additionally consider the temporal component of the local vector current

$$V_{q_1 q_2}(x) = [\bar{q}_1 \gamma_0 q_2](x) \quad (22)$$

and, identifying $t_{\text{snk}} = z_0$, $t_{\text{op}} = y_0$, and $t_{\text{src}} = x_0 = 0$, the correlation functions

$$C_3^{q_1 q_3 \rightarrow q_2 q_3}[t_{\text{op}}, t_{\text{snk}}] = \sum_{\mathbf{x}, \mathbf{y}, \mathbf{z}} \langle \phi_{q_2 q_3}(z) V_{q_1 q_2}(y) \phi_{q_1 q_3}^\dagger(x) \rangle. \quad (23)$$

Finally, for the mixing data set F1M-mix-sh, we consider the Standard Model four-quark bag parameter operator commonly referred to as $O_1 = O_{VV+AA}$ defined as

$$O_1^{q_1 q_2} = (\bar{q}_2 \gamma_\mu q_1)(\bar{q}_2 \gamma_\mu q_1) + (\bar{q}_2 \gamma_\mu \gamma_5 q_1)(\bar{q}_2 \gamma_\mu \gamma_5 q_1), \quad (24)$$

where summation over the index μ is implicit. The corresponding three point functions have the form

$$C_3^{q_1 q_2}[t_{\text{op}}, t_{\text{snk}}] = \sum_{\mathbf{x}, \mathbf{y}, \mathbf{z}} \langle \phi_{q_2 q_1}(z) O_1^{q_1 q_2}(y) \phi_{q_1 q_2}^\dagger(x) \rangle, \quad (25)$$

where we again identify $t_{\text{snk}} = z_0$, $t_{\text{op}} = y_0$ and $t_{\text{src}} = x_0 = 0$. In all cases the spatial sums are performed stochastically using $\mathbb{Z}_2$ -wall sources and local sinks. In the following we give some technical detail about the generation of the data sets, in each case first giving the flavor assignment.

M0M-mes-ll: The flavor assignment is $q_1 = \ell$, $q_2 = \ell$ where ℓ is a physical light quark. For this particular correlation function, the sources were additionally smeared using Jacobi iterations [11]. For further technical details about this data set we refer the reader to Refs. [24,25].

F1M-mes-lh: Here we assign $q_1 = \ell$, $q_2 = h$ where the light quark ℓ takes the unitary value for this ensemble and the heavy quark mass $am_q = 0.68$ lies between the physical charm and bottom quark mass. For the heavy quark we use one of the actions compared in Ref. [26]. More details about the exact parameter

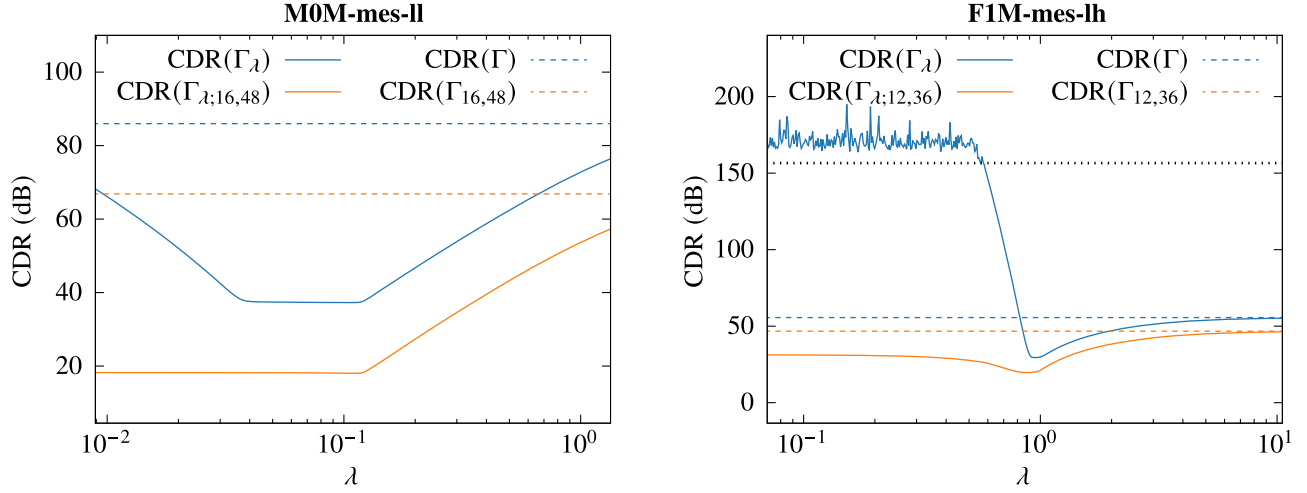


FIG. 1. CDR of the filtered correlators as a function of the regulator λ . The left and right panels show the results for the MOM-mes-ll and F1M-mes-lh correlators, respectively. In each plot, the solid blue and orange curves represent the CDR for the full time range and for the restricted range $\{N_t/8, \dots, 3N_t/8 - 1\}$, respectively. Additionally, the colored dashed lines represent the CDRs of the unfiltered data, and the black dashed line represents the CDR of the restricted range evaluated at the optimal value of the regulator, with values of approximately $\lambda \simeq 0.11$ for MOM-mes-ll and $\lambda \simeq 0.88$ for F1M-mes-lh. In the F1M-mes-lh plot, the dotted line indicates the critical 156.54 dB threshold above which the CDR cannot be resolved using double-precision arithmetic (cf. Sec. II A).

choices are given in Ref. [24] where this dataset was first introduced.

F1M-mes-hh: This is the same as F1M-mes-lh, but with $q_1 = h$ and $am_h = 0.59$ for both quarks. Only the quark-connected part of this correlation function has been considered.

C1M-semi-sc-ss: The assignment of flavors for this dataset is $q_1 = c$, $q_2 = s$, $q_3 = s$. The computational set-up is similar to that of Ref. [27], but using Z_2 -wall sources instead of point sources: At the source propagators for a spectator strange quark (q_3) and a child strange-quark (q_1) are generated, at time t_{snk} the spectator quark is turned into a sequential source from which the parent charm-quark (q_2) is inverted. The charm quark mass is tuned to its physical value and the actions are the same as in the previous dataset. Measurements took place on 180 configurations with 8 sources per configuration.

F1M-mix-sh: We are considering $q_1 = s$, $q_2 = h$ here with $am_h = 0.59$. This dataset has also been introduced in Ref. [24] and the computational set-up is the same as that for F1M-mes-lh.

IV. IMPROVEMENT OF TIME CORRELATIONS

The main question in this section is to find values of λ for which the CDR of the filtered data is significantly reduced. This is in general a nontrivial question since the CDR depends on the spectrum of the correlation matrix.

In practice, one rarely needs to fit the entire time range of a lattice correlator. Instead, fits generally focus on a limited time range. It is therefore useful to define a *restriction operator* R_S , where S is a subset of $\{0, \dots, N_t - 1\}$, that

projects C onto the components indexed by S . If S is an interval $\{t_i, \dots, t_f - 1\}$, we define $R_{t_i, t_f} = R_S$. It is clear that R_S is a linear operator. We additionally define the following shorthand notation

$$C_\lambda = D_\lambda C, \quad C_{t_i, t_f} = R_{t_i, t_f} C, \quad (26)$$

$$\text{and } C_{\lambda; t_i, t_f} = R_{t_i, t_f} D_\lambda C. \quad (27)$$

It is important to note in Eq. (27) that the restriction operation is applied after the Laplace filter. We extend this notation to quantities that depend on C ; for example, Γ_λ is the correlation matrix of C_λ , and so on.

The effect of D_λ can be derived exactly in the limits of large and small λ . For sufficiently large λ the Laplace filter D_λ is, to leading order, proportional to the identity matrix and therefore has no effect on correlations; explicitly

$$\lim_{\lambda \rightarrow +\infty} \text{CDR}(\Gamma_{\lambda; t_i, t_f}) = \text{CDR}(\Gamma_{t_i, t_f}), \quad (28)$$

for any time range from t_i to t_f . On the other hand, when $\lambda \rightarrow 0^+$, D_λ becomes noninvertible, resulting in a singular Γ

$$\lim_{\lambda \rightarrow 0^+} \text{CDR}(\Gamma_\lambda) = +\infty \text{ dB}. \quad (29)$$

However, the above limit is generally expected to remain finite if a nontrivial time restriction is applied. We now discuss how to optimize the value of λ to minimize correlations.

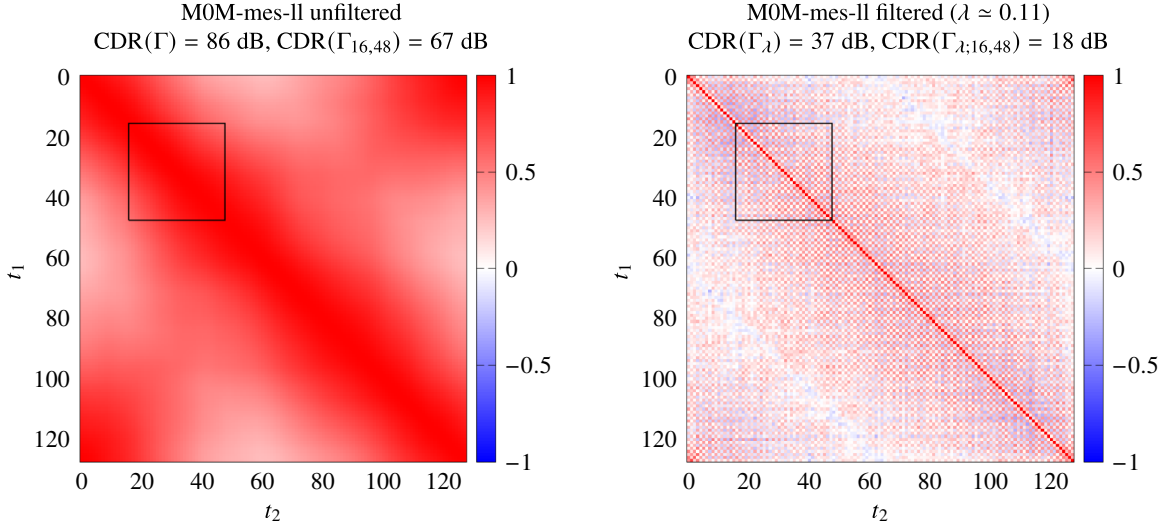


FIG. 2. Correlation matrix of the MOM-mes-II time correlator, in both the unfiltered (left panel) and filtered (right panel) cases. For the filtered case, the optimal value $\lambda \simeq 0.11$ is used (cf., Fig. 1). The titles of the plots provide the CDRs of the full and restricted matrices, using the same time range as in Fig. 1. Finally, the restricted range is represented as a black square in the figure.

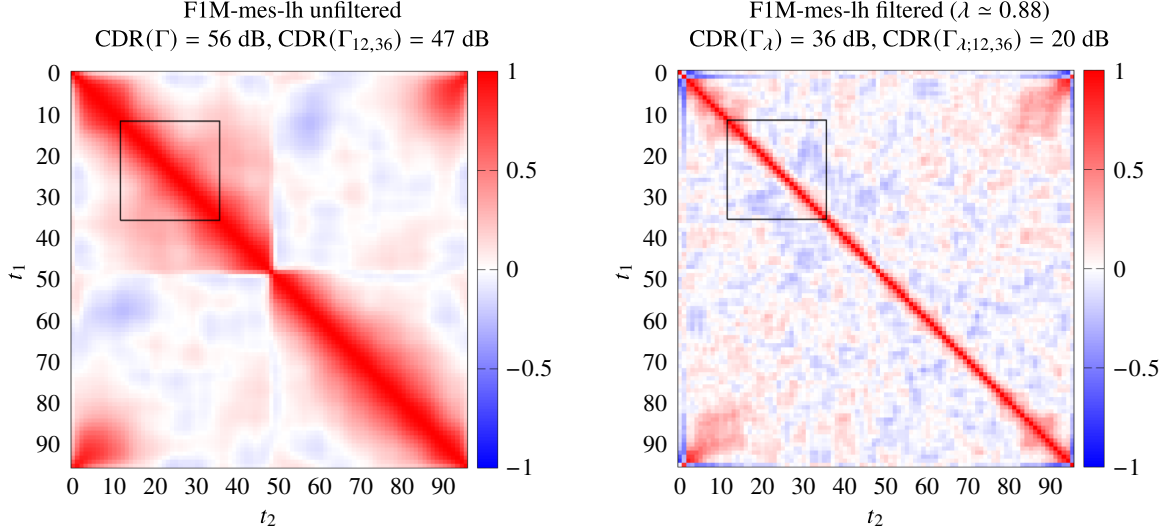


FIG. 3. Representation of the correlation matrix of the F1M-mes-lh time correlator, in both the unfiltered (left panel) and filtered (right panel) cases. In the filtered case, the optimal value $\lambda \simeq 0.88$ is used (cf., Fig. 1). Other details are as in Fig. 2.

A. Filter optimization

In this section, we perform an initial analysis of the effect of the regulated Laplace filter on the statistical correlations in mesonic two-point functions. More specifically, we consider the pseudoscalar correlators labeled MOM-mes-II and F1M-mes-lh in Sec. III. In both cases, we study how the CDR of the filtered correlator varies as a function of λ . We compute the CDR for the full correlation matrices and for the restricted range $\{N_t/8, \dots, 3N_t/8 - 1\}$, which is viewed as a representative fit range.

In all cases, the CDR is computed numerically using a Jacobi singular-value decomposition in double precision. An optimal value of the regulator is then obtained by

numerically minimizing the filtered, restricted CDR as a function of λ . Once a solution λ_0 is obtained, we sample 500 values of the CDR, uniformly spaced on a logarithmic scale between $0.08\lambda_0$ and $12\lambda_0$. The results of this analysis for both MOM-mes-II and F1M-mes-lh are illustrated in Fig. 1. As a first observation, we see that the limits in Eqs. (28) and (29) are satisfied. In the case of the CDR divergence for $\lambda \rightarrow 0^+$, the CDR numerically saturates at the maximum 156.54 dB level for double-precision arithmetic. Second, in both the MOM-mes-II and F1M-mes-lh cases, there are values of λ for which the filtered data exhibit significantly less correlation than the unfiltered data. We also observe that the optimal region is similar for both the full and

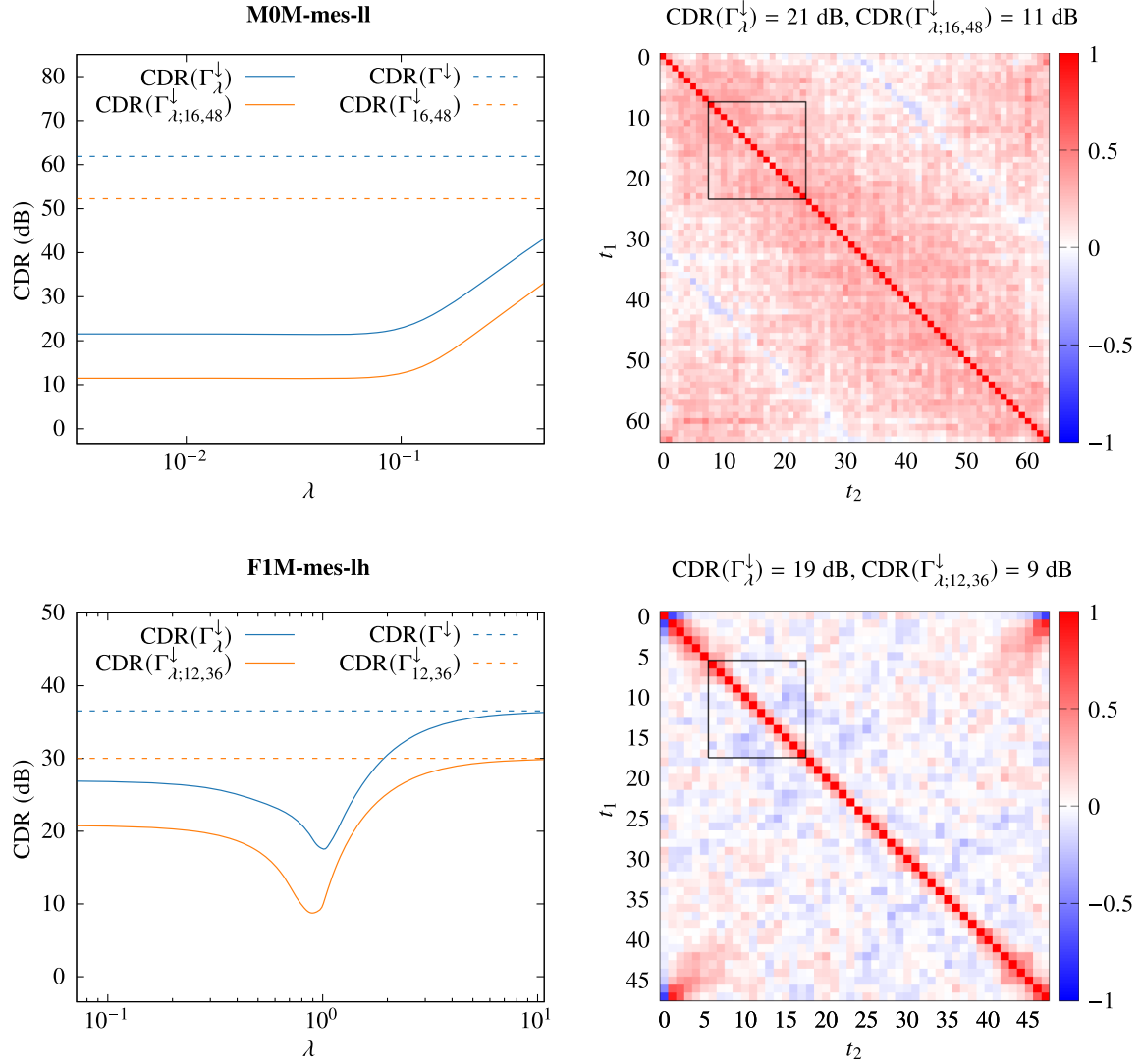


FIG. 4. Laplace filter analysis and optimization when using an additional downsampling step after filtering, as explained in Sec. IV B. The two rows of plots are for the analysis of the M0M-mes-ll and F1M-mes-lh correlators, respectively. Plots on the left represent the dependence of the total and restricted CDR on the filter regulator λ , using identical conventions to Fig. 1. Plots on the right represent the correlation matrix $\Gamma_\lambda^\downarrow$, for the optimal value $\lambda = \lambda_0$, which minimizes the restricted downsampled CDR (i.e., the orange curve on the associated plot on the left). The variables t_1 and t_2 are time indices of the downsampled correlator; that is, they correspond to $2t_1$ and $2t_2$ for the original data, respectively. As in Figs. 2 and 3, the submatrix within the black square is the correlation matrix on the restricted range.

restricted CDRs. In Figs. 2 and 3, we represent the correlation matrices of the M0M-mes-ll and F1M-mes-lh correlators, as well as for the filtered data at the optimal values λ_0 . These figures also provide the numerical values of the full and restricted CDRs for the original and filtered data. In the M0M-mes-ll case, the Laplace filter improves both the full and restricted CDRs by 49 dB. In the F1M-mes-lh case, the full CDR is improved by 20 dB, and the restricted CDR by 27 dB. For all cases, a significant improvement is observed, and for the restricted time range, the condition number of the filtered correlation matrix is at most 100, implying that it is well conditioned.

Following these encouraging initial results, we discuss how additional restriction of the data can further reduce the level of correlation.

B. Additional downsampling step

We define the *downsampled* or *thinned* correlator $C^\downarrow$, of size $N_t/2$, as follows:

$$C^\downarrow[t] = C[2t], \quad (30)$$

i.e., all odd time slices of the original correlator are discarded. Equivalently, $C^\downarrow = R_E C$, where E is the set

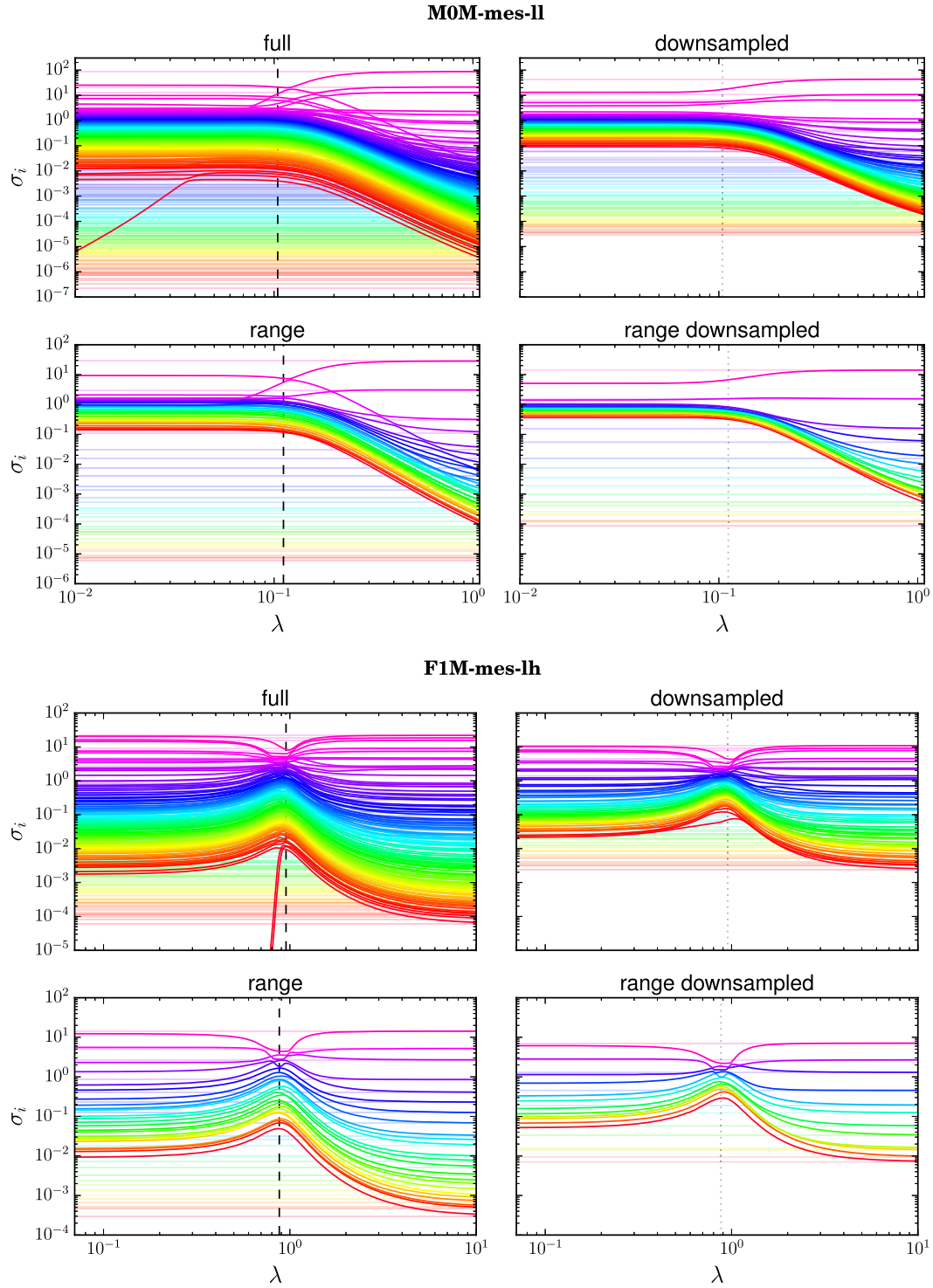


FIG. 5. Behavior of the eigenvalues σ_i of the correlation matrix of the M0M-mes-ll (upper half) and F1M-mes-lh (lower half) correlation functions as a function of Laplace filtering regulator λ . In each half, the top and bottom rows show the spectrum for the full and restricted time ranges, respectively. In the right column, an additional downsampling step is applied. The faint horizontal lines correspond to the spectrum when no filtering is applied.

of even time slices. The choice of discarding specifically odd time slices is arbitrary and made here for the sake of simplicity. In practice, it is also common to skip odd times relatively to a given initial time, or to downsample using a higher factor than 2. When using filtering and range restriction, e.g., $C_{\lambda; t_i, t_f}^\downarrow$, it is always understood that downsampling is applied after restriction or filtering.

Downsampling is commonly used in lattice calculations when fitting correlators. Since correlations are localized in time, discarding neighboring times naturally reduces correlations. Since the Laplace filter also aims to cancel correlations in neighboring time slices, an interesting question is whether its effect is compounded with or redundant to a simple downsampling step.

We repeat the analysis of the previous section, but now for the downsampled correlators $C_\lambda^\downarrow$. The results are summarized in Fig. 4. A first observation is that, without any filtering applied, downsampling already reduces the total CDR by 24 dB and 19 dB for M0M-mes-ll and F1M-mes-lh, respectively. Optimizing the filter, as done in the previous section, leads to an additional decrease in the total CDR by 41 dB and 18 dB for M0M-mes-ll and F1M-mes-lh, respectively. On the restricted range, the CDR is improved by 41 dB and 21 dB for M0M-mes-ll and F1M-mes-lh, respectively. These gains are similar to those obtained without downsampling in the previous section, which suggests that Laplace filtering improves correlations in a way that is not redundant with the additional gains from downsampling. On the restricted range, the optimized CDRs for the downsampled data are 11 dB and 9 dB for M0M-mes-ll and F1M-mes-lh, respectively. In this configuration, the eigenvalues of the correlation matrix vary over roughly one order of magnitude, ensuring that the ill-conditioning in computing the χ^2 function Eq. (8) has been largely eliminated.

We now summarize the various strategies explored for optimizing Laplace filters.

C. Summary of correlation improvements

In Fig. 5 we illustrate how the individual eigenvalues σ_i of the correlation matrix vary as a function of λ for the M0M-mes-ll and F1M-mes-lh correlation functions. The vertical dashed lines correspond to the values that minimise the CDR for the full (top) or range-restricted correlation matrix. The faint horizontal lines correspond to the unfiltered spectrum. We clearly observe the expected asymptotic behavior of recovering the original spectrum for very large values of λ as well as the emergence of a zero mode when considering the full correlation matrix and very small values of λ . In Table II, we summarize the CDRs obtained by filtering and downsampling the M0M-mes-ll and F1M-mes-lh correlators, for both the full time range and a restricted, representative fit range. In all cases, a combination of downsampling and optimized filtering improves

TABLE II. Summary of CDR improvements obtained in Sec. IV for the M0M-mes-ll and F1M-mes-lh correlators. As assumed in all results of Sec. IV, the range-restricted CDRs are evaluated over the representative time interval $\{N_t/8, \dots, 3N_t/8 - 1\}$, and λ_0 denotes the regulator value that minimizes the range-restricted CDR. In principle, optimizing λ_0 for the total range can lead to lower CDR values in the “total” column.

	<i>M0M-mes-ll</i>		<i>F1M-mes-lh</i>	
	Total	Range	Total	Range
CDR(Γ)	86 dB	67 dB	56 dB	47 dB
CDR(Γ_{λ_0})	37 dB	18 dB	36 dB	20 dB
CDR($\Gamma^\downarrow$)	62 dB	52 dB	37 dB	30 dB
CDR($\Gamma_{\lambda_0}^\downarrow$)	21 dB	11 dB	19 dB	9 dB

the condition number of the correlation matrix by at least four orders of magnitude. This is an encouraging result, and we emphasize that this improvement is achieved solely through a linear, invertible transformation of the data and does not introduce any additional systematic error in subsequent fits of the correlators.

The filter optimizations discussed in this section only target improving correlations. We have not discussed the effect of filtering on the statistical accuracy of the data, which is critical for extracting physical information from the correlators. As observed in Figs. 1 and 4, many choices of λ will lead to significant improvements in correlations, which allows for the introduction of additional criteria related to the quality of the filtered data. In the next section, we discuss the physical effect of the regulated Laplace filter on lattice correlators and its impact on fitting spectral decomposition models to these data.

V. SPECTRAL EFFECT OF LAPLACE FILTERS

In this section, we discuss the effect of regulated Laplace filters on the spectrum of a correlation function. We start with a theoretical discussion of this effect, and follow up with applications to data analysis.

A. Theoretical discussion

1. Continuous time

In continuous Euclidean time, the Feynman Green’s function for the propagation of a single spin-0 state with nonzero mass m and momentum $\mathbf{k}$ is given by

$$G_0(t; E) = \int \frac{d\mathbf{k}_0}{2\pi} \frac{e^{-ik_0 t}}{k^2 + m^2} = \frac{e^{-E|t|}}{2E}, \quad (31)$$

where $k = (k_0, \mathbf{k})$ is the Euclidean four-momentum, and $E^2 = \mathbf{k}^2 + m^2$. By construction, $G_0(t; E)$ is a solution to the differential equation

$$(-\partial_t^2 + E^2)G_0(t; E) = \delta(t). \quad (32)$$

A key observation here is that the left-hand side of the equation above is the continuous version of the regulated Laplace filter Eq. (17) with $\lambda = E$. For an arbitrary regulator value,

$$(-\partial_t^2 + \lambda^2)G_0(t; E) = \delta(t) + (\lambda^2 - E^2)G_0(t; E). \quad (33)$$

In a field theory with a nonzero mass gap M , a general scalar two-point function $G(t)$ can be written for $t \neq 0$ using the Källén-Lehmann spectral representation

$$G(t) = \int_M^{+\infty} dE \rho(E) G_0(t; E), \quad (34)$$

where $\rho(E)$ is the associated spectral density. This is the standard result stating that in Euclidean time, a two-point function is related to the Laplace transform of its spectral density. Applying the Laplace filter to $G(t)$, one obtains

$$(-\partial_t^2 + \lambda^2)G(t) = \int_M^{+\infty} dE (\lambda^2 - E^2) \rho(E) G_0(t; E), \quad (35)$$

where the delta function term has been omitted since the spectral representation requires $t \neq 0$.

In conclusion, from a spectral point of view, the Laplace filter with regulator λ is equivalent to transforming the spectral density with $\rho(E) \mapsto (\lambda^2 - E^2)\rho(E)$. Let us now formulate the equivalent statement for discrete and periodic time.

2. Discrete and periodic time

Making the lattice spacing explicit for this subsection, the Laplace filter defined in Eq. (17) in units of a is given by

$$\Delta_\lambda C[t] = a^{-2}[(2 + a^2\lambda^2)C[t] - C[t - a] - C[t + a]], \quad (36)$$

which clearly has the continuum limit

$$\lim_{a \rightarrow 0} \Delta_\lambda = -\partial_t^2 + \lambda^2, \quad (37)$$

when acting on samples of smooth functions. Then, one can show that the discrete version of Eq. (32) is given by

$$\Delta_{\tilde{E}} G_0[t; E] = a^{-1} \delta_{t,0}, \quad (38)$$

where $\delta_{j,k}$ is the Kronecker delta, $G_0[t; E]$ is given by

$$G_0[t; E] = \frac{e^{-E|t|}}{2a^{-1} \sinh(aE)}, \quad (39)$$

and

$$\tilde{E}^2 = 2a^{-2}[\cosh(aE) - 1]. \quad (40)$$

For $a \rightarrow 0$, $\tilde{E}$ converges to E with leading $\mathcal{O}(a^2)$ corrections. Switching back to lattice units (i.e., $a = 1$), the equation above leads to the identity

$$\Delta_\lambda(e^{-E|t|}) = 2 \sinh(E) \delta_{t,0} + (\lambda^2 - \tilde{E}^2) e^{-E|t|}, \quad (41)$$

with $\tilde{E}^2 = 2[\cosh(E) - 1]$ as before. We now consider a quantum field theory with a nonzero mass gap M and a discrete, periodic time dimension of length N_t . At nonzero time separation t , an arbitrary scalar two-point function can be written as

$$C[t] = \sum_n A_n g_0[t; E_n], \quad (42)$$

where A_n and $E_n \geq M$ are finite sets of amplitudes and energies, respectively, and where $g_0[t; E_k]$ is the periodization

$$g_0[t; E] = \sum_{j=-\infty}^{+\infty} e^{-E|t+jN_t|}. \quad (43)$$

Equation (42) is the discrete and periodic equivalent of the Källén-Lehmann spectral representation Eq. (34). For $t \in \{0, \dots, N_t - 1\}$, the expression above can be reduced to the more convenient form

$$g_0[t; E] = \frac{e^{-Et} + e^{-E(N_t-t)}}{1 - e^{-N_t E}}. \quad (44)$$

For $t \neq 0 \pmod{N_t}$, we have

$$\Delta_\lambda g_0[t; E] = (\lambda^2 - \tilde{E}^2) g_0[t; E], \quad (45)$$

and therefore for $t \notin \{-1, 0, 1\} \pmod{N_t}$

$$\Delta_\lambda C[t] = \sum_n (\lambda^2 - \tilde{E}_n^2) A_n g_0[t; E_n], \quad (46)$$

which is the discrete analog of Eq. (35). This last identity is only valid if t is at least two sites away from 0; otherwise, the result will depend on the contact term $C[0]$, which does not necessarily obey the spectral representation Eq. (42).

An important conclusion from Eq. (46) is that the Laplace filter can entirely remove the contribution of a given state from a correlator if the regulator is tuned to the energy $\tilde{E}$ associated with this state. On the one hand, this means that when choosing the regulator, one must be careful to avoid the energies of states of interest. On the other hand, it also implies that the filter can be exploited to remove unwanted states, typically excited-state contamination from hadronic interpolating operators.

3. Summary and generalization

A key ingredient of the discussion above is the identity

$$\Delta_\lambda(e^{\pm Et}) = (\lambda^2 - \tilde{E}^2)e^{\pm Et}. \quad (47)$$

Euclidean time correlators are, however, only linear combinations of such exponentials when all pairs of operators involved have nonzero time separation. This is a particularly important constraint with discrete time, since the filtered correlator $\Delta_\lambda C[t]$ depends on the times $C[t-1]$ and $C[t+1]$. If these neighboring terms are not contact terms, then the Laplace filter is a spectral reweighting according to the equation above. When time is additionally periodic of size N_t , the notion of nonzero time separation must be understood modulo N_t .

These general principles also apply to n -point functions, as well as to correlation functions involving nonzero-spin states. Indeed, an arbitrary n -point time correlator will depend on $n-1$ time separations and can be written as a sum of exponentials if all time separations are nonzero (mod N_t). Additionally, nonzero-spin states also propagate with an exponential time dependence of the form $e^{\pm Et}$. The coefficients of such exponentials will be spin matrices and will generally differ between the backward and forward time directions, however properties of the Laplace filters discussed in this paper can be generalized to these cases.

B. Applications to statistical data analysis

Throughout this section, we assume that the correlator under study is given by Eq. (42), with N_s states of nonzero amplitude and distinct energies indexed by $n \in \{0, \dots, N_s - 1\}$. For $t \notin \{-1, 0, 1\} \pmod{N_t}$, a single application of the Laplace filter yields Eq. (46). For a vector of r regulators $\Lambda = (\lambda_0, \dots, \lambda_{r-1})$, we define

$$C_\Lambda[t] = \Delta_{\lambda_1} \cdots \Delta_{\lambda_r} C[t], \quad (48)$$

i.e., C_Λ is the correlator transformed by r successive Laplace filters. Eq. (46) can be generalized to multiple filters. For $t \notin \{-r, \dots, r\} \pmod{N_t}$, one obtains

$$C_\Lambda[t] = \sum_n \left[\prod_{j=0}^{r-1} (\lambda_j^2 - \tilde{E}_n^2) \right] A_n g_0[t, E_n]. \quad (49)$$

For the remainder of this discussion, we assume that $t \notin \{-r, \dots, r\} \pmod{N_t}$. In order for the formula above to be valid for at least one time slice, we require $r < N_t/2$. Then, Eq. (49) offers an opportunity to determine the energy spectrum $\tilde{E}_n$ by finding a sequence of Laplace filters that annihilate $C[t]$, i.e., that solve the equation

$$C_\Lambda[t] = 0, \quad (50)$$

for all t in a given range satisfying the previous constraints, and containing at least r elements. If the number of filters equals the number of states, i.e., $r = N_s$, then Eq. (50) is satisfied if and only if, for all $j \in \{0, \dots, N_s - 1\}$,

$$\lambda_j = \tilde{E}_j. \quad (51)$$

In this case, the energies E_n are uniquely determined³ by Eq. (50). If $r > N_s$, then necessarily the spectrum is a subset of the solution set of Eq. (50), i.e., $\{\tilde{E}_0, \dots, \tilde{E}_{N_s-1}\} \subset \{\lambda_0, \dots, \lambda_{r-1}\}$. If $r < N_s$, then Eq. (50) has no solution.

In summary, if $N_s < N_t/2$, the spectrum of C can be determined as follows:

- (1) The number of states N_s is given by the minimal r for which Eq. (50) admits a solution;
- (2) The spectrum $\tilde{E}_j$ is given by the unique solution of Eq. (50) for $r = N_s$.

The procedure above can serve as the basis for new methods to determine the energy spectrum of lattice correlators. Although equation Eq. (50) determines the spectrum uniquely, in practice with noisy simulation data it can only be solved up to statistical noise, introducing ambiguities in the above procedure. Therefore, in what follows, we discuss potential hypothesis-testing methods to constrain the spectrum of the correlator.

1. Multistate hypothesis testing

A key observation in the discussion above is that Eq. (50) has no solution if the number of filters is smaller than the number of states, i.e., $r < N_s$. This statement can be reformulated statistically as a hypothesis rejection, which allows us to design tests for the number of statistically significant states in a given time range.

We consider a time range $\{t_i, \dots, t_f - 1\}$ for which the condition $t \notin \{-r, \dots, r\} \pmod{N_t}$ is always satisfied. For sufficiently large statistics, the average restricted correlator $\bar{C}_{t_i, t_f}$ is distributed according to a normal distribution $\mathcal{N}(C_{t_i, t_f}, \Sigma_{t_i, t_f})$ with mean $\bar{C}_{t_i, t_f}$ and covariance Σ_{t_i, t_f} , where Σ is the true covariance matrix estimated in practice by the matrix V defined in Eq. (4). Similarly to Eq. (27), we define

$$C_{\Lambda; t_i, t_f} = R_{t_i, t_f} C_\Lambda, \quad (52)$$

and we denote $\Sigma_{\Lambda; t_i, t_f}$ as its covariance matrix. Since the Laplace filter is linear, we know that $\bar{C}_{\Lambda; t_i, t_f}$ is distributed according to $\mathcal{N}(C_{\Lambda; t_i, t_f}, \Sigma_{\Lambda; t_i, t_f})$. For a given Λ , we can consider the null hypothesis H_Λ defined by

$$C_{\Lambda; t_i, t_f} = 0. \quad (H_\Lambda)$$

³This is a consequence of the fact that functions of the form $t \mapsto e^{-Et}$ are linearly independent for distinct values of E .

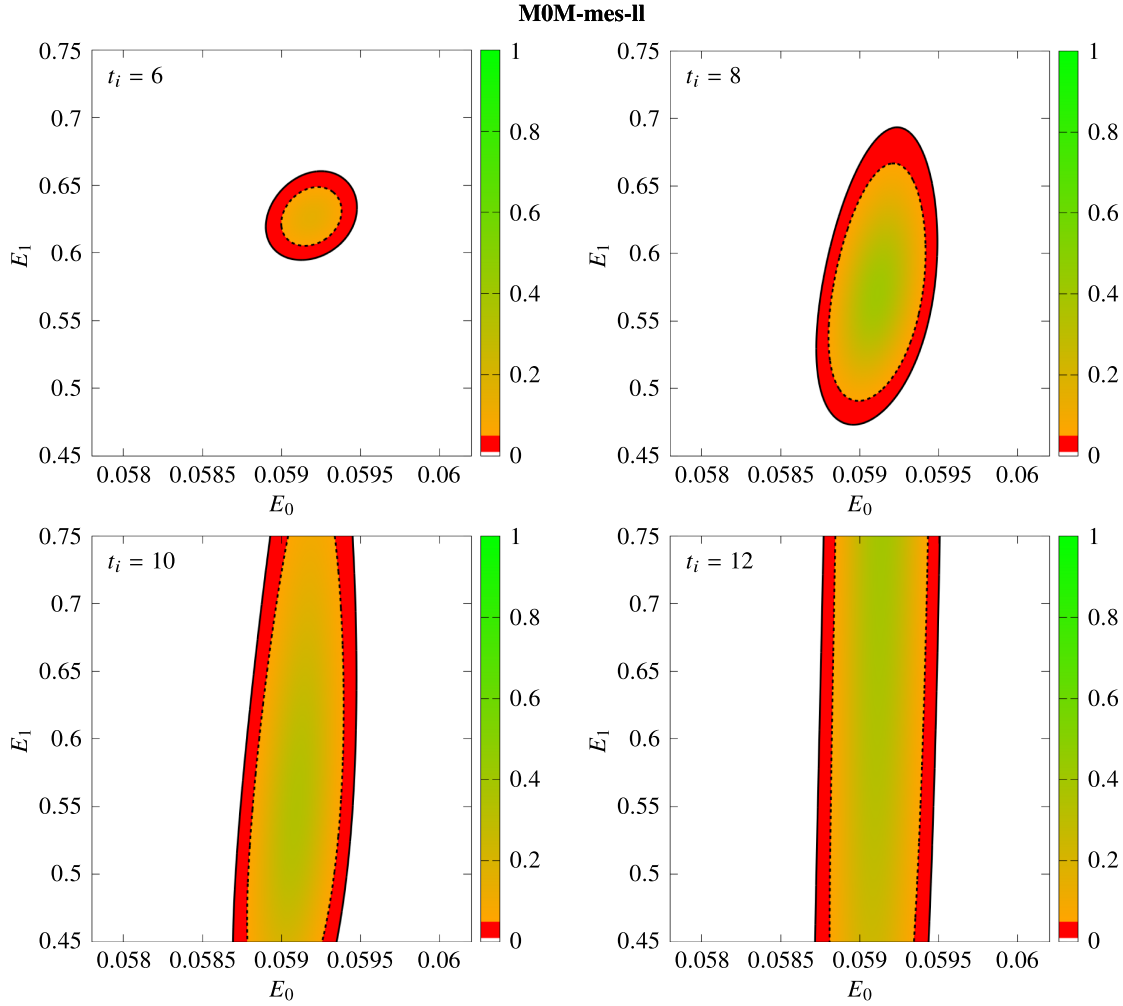


FIG. 6. Representation of the pion correlator M0M-mes-ll 2-state test p_Λ defined in Eq. (54), with $\Lambda = (\tilde{E}_0, \tilde{E}_1)$. The four different plots correspond to various values of the initial time t_i . In all cases, the final time is fixed to $t_f = 48$. Values below 1% are not represented (2-state hypothesis rejected at 99% confidence level), and values above 1% are within the solid black contour. Values between 1% and 5% are represented in red, and values above 5% are within the dashed contour, and represented by a gradient between orange and green.

For a given significance level α , rejecting H_Λ means that there exists at least one element of the spectrum of C which is not part of Λ , with a confidence level of $1 - \alpha$. Since $C_{\Lambda; t_i, t_f}$ is normally distributed, such a test can be performed using the usual T^2 statistic

$$T^2(\Lambda) = \bar{C}_{\Lambda; t_i, t_f}^T V_{\Lambda; t_i, t_f}^{-1} \bar{C}_{\Lambda; t_i, t_f}, \quad (53)$$

which is asymptotically distributed according to a χ^2 distribution with $\Delta t = t_f - t_i$ degrees of freedom. The p -value of the test is then given by the probability

$$p_\Lambda = P[T^2(\Lambda) > T_{\text{obs}}^2(\Lambda)] = 1 - F[T_{\text{obs}}^2(\Lambda), \Delta t], \quad (54)$$

where $T_{\text{obs}}^2(\Lambda)$ is the T^2 statistic observed from the data, and $F(x, \nu)$ is the cumulative distribution function of the χ^2

distribution with ν degrees of freedom. Finally, if $p_\Lambda < \alpha$, then H_Λ is rejected. In the remainder of this section, we will use $\alpha = 0.05$.

As an example, we show in Figs. 6 and 7 representations of p_Λ for two states $\Lambda = (\tilde{E}_0, \tilde{E}_1)$, and for various values of the initial time t_i . At early values of t_i , we observe that H_Λ is systematically rejected except for a well localized $p_\Lambda > \alpha$ region in the (E_0, E_1) plane. In this region, the data can be described up to noise as the sum of two exponentials with well-constrained energies. As the initial time increases, we observe that the $p_\Lambda > \alpha$ region eventually does not constrain the location of E_1 anymore. This suggests, as expected, that for sufficiently large times the correlator can be statistically represented by a single exponential.

The p -value p_Λ allows us to potentially reject Λ as a statistically acceptable spectrum to describe the correlator. However, this is only done at a specific value of Λ , and it is

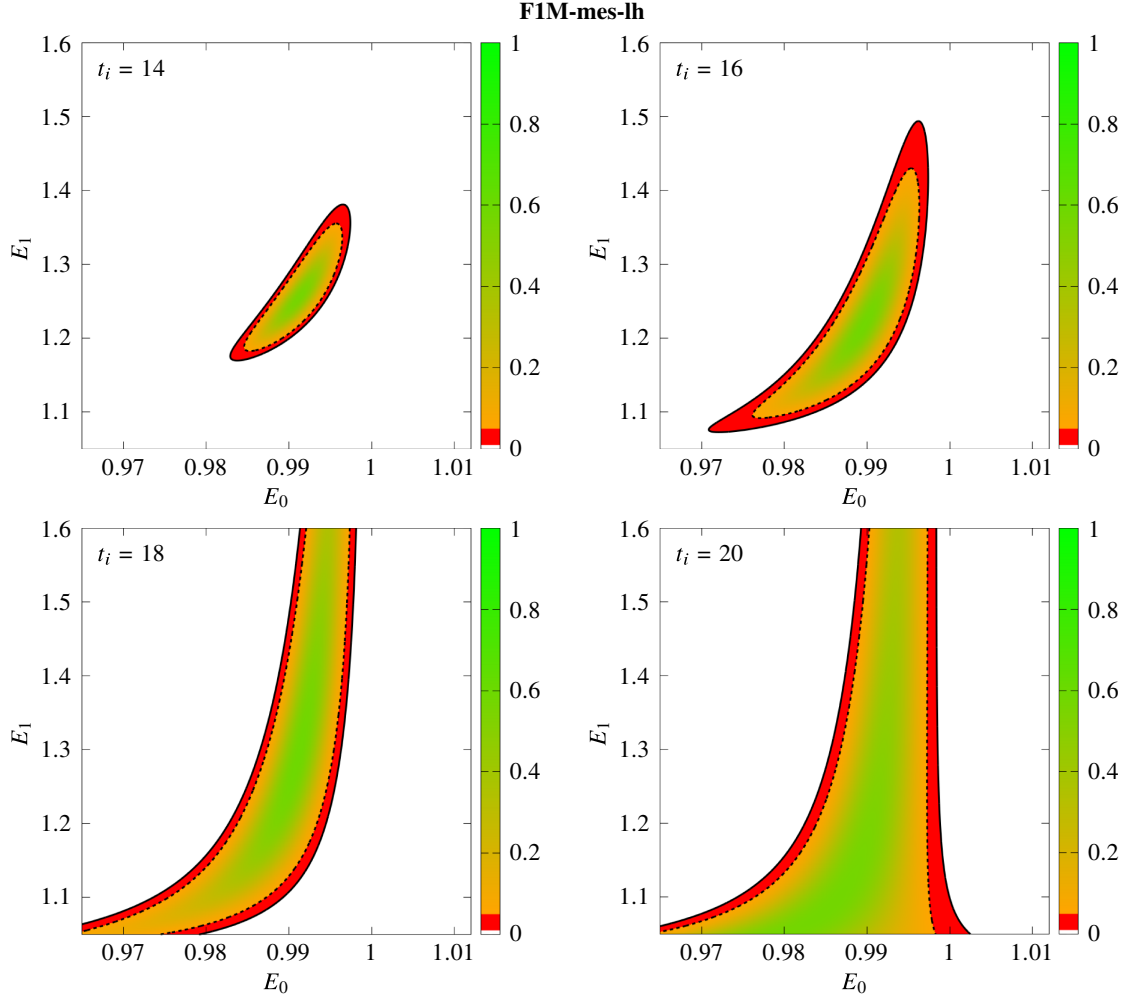


FIG. 7. Representation of the heavy-light correlator F1M-mes-lh 2-state test p -value p_Λ defined in Eq. (54), with $\Lambda = (\tilde{E}_0, \tilde{E}_1)$. The four different plots correspond to various values of the initial time t_i . In all cases, the final time is fixed to $t_f = 36$. Plotting conventions are identical to Fig. 6.

interesting to design a global test for multistate hypotheses. We start by defining the following r -state null hypothesis

$$\text{there exists } \Lambda = (\lambda_0, \dots, \lambda_{r-1}) \text{ s.t. } C_{\Lambda; t_i, t_f} = 0. \quad (H_r)$$

H_r can be tested by minimizing the statistic $T^2(\Lambda)$ over $\Lambda = (\lambda_0, \dots, \lambda_{r-1})$:

$$T_r^2 = \min_{\lambda_0, \dots, \lambda_{r-1}} T^2(\lambda_0, \dots, \lambda_{r-1}). \quad (55)$$

Similarly to curve fitting, such a minimum requires the gradient of $T^2(\lambda_0, \dots, \lambda_{r-1})$ to vanish. This constraint makes T_r^2 a sum of $\Delta t - r$ independent Gaussian random variables squared, and therefore T_r^2 asymptotically obeys the χ^2 distribution with $\Delta t - r$ degrees of freedom. We therefore define the r -state p -value as

$$p_r = P(T_r^2 > T_{r,\text{obs}}^2) = 1 - F(T_{r,\text{obs}}^2, \Delta t - r), \quad (56)$$

where $T_{r,\text{obs}}^2$ is the minimized r -state T^2 obtained from the data. In practice, such a minimum can be computed using standard minimization algorithms with Eq. (53). If one rejects H_r with $p_r < \alpha$, it means that with $1 - \alpha$ confidence level, the data cannot be described as a sum of r exponentials on the chosen time range. However, if H_r is not rejected, it does not necessarily imply that all r exponentials contribute significantly to the correlator—it is possible that a subset of Λ is sufficient. We now discuss an extended procedure to address this.

2. Number of significant states

For a hypothesized number of states r , we want to determine whether a $(r + 1)$ -state description of C over the time range $\{t_i, \dots, t_f - 1\}$ would provide a significant improvement over the hypothesis. This can be done using

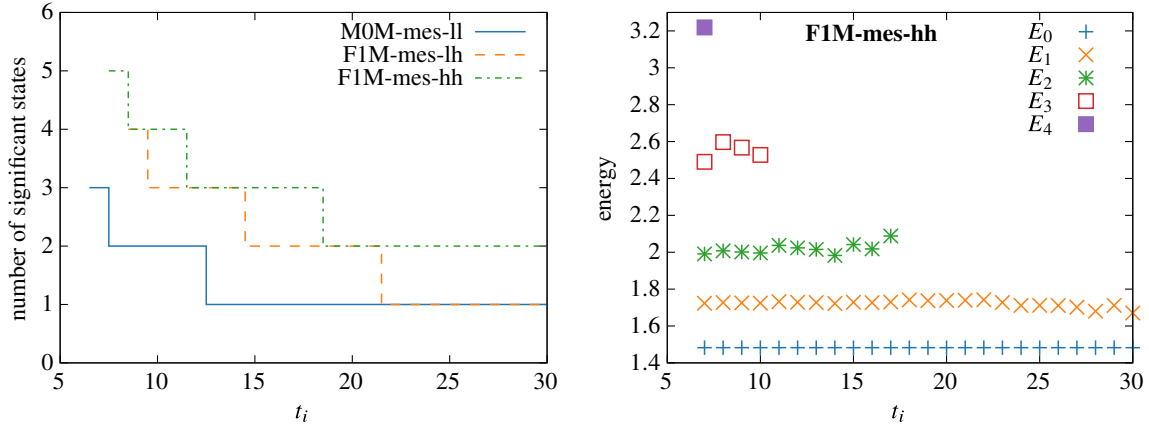


FIG. 8. The left plot represents the number of significant states as a function of the initial time t_i , using the procedure described in Sec. V B 2, at the 95% confidence level, for the pion (M0M-mes-ll), heavy-light (F1M-mes-lh), and heavy-heavy (F1M-mes-hh) pseudoscalar two-point functions. For M0M-mes-ll, the final time is fixed to $t_f = 48$, and $t_f = 36$ in the two other cases. If the procedure is inconclusive (i.e., H_s was rejected at step 3), no points are plotted for the associated values of t_i . The right plot represents the energies of the significant states of the F1M-mes-hh correlator, obtained as a side product of the analysis performed in the left plot.

a standard likelihood-ratio test, considering H_r as the null hypothesis and H_{r+1} as the alternative hypothesis. To achieve this, one first computes the difference in the minimum T^2 statistic between the two models, i.e.,

$$\Delta T_r^2 = T_{r+1}^2 - T_r^2. \quad (57)$$

Wilks' theorem [28] then implies that ΔT_r^2 is asymptotically distributed as a χ^2 distribution with one degree of freedom, and we therefore define the corresponding p -value

$$\bar{p}_r = P(\Delta T_r^2 > \Delta T_{r,\text{obs}}^2) = 1 - F(\Delta T_{r,\text{obs}}^2, 1), \quad (58)$$

where $\Delta T_{r,\text{obs}}^2$ is the observed value of ΔT_r^2 from the data. If $\bar{p}_r < \alpha$, then H_r is rejected in favor of H_{r+1} ; that is, the $(r+1)$ th state is a statistically significant addition to the description of the data. As is usual with ratio tests, it is important to note that only relative significance is tested, which is independent of whether H_r and H_{r+1} can be individually rejected. The values $\bar{p}_r$ allow one to determine the number of significant states in a chosen time range, which we propose to do using the following procedure.

- (1) Choose a maximum number $r_{\text{max}} > 1$ of states to test, and compute the values p_r for $r \in \{1, \dots, r_{\text{max}}\}$ and $\bar{p}_r$ for $r \in \{1, \dots, r_{\text{max}} - 1\}$.
- (2) Using the $\bar{p}_r$ values, find the maximum value s for which H_{s-1} is rejected in favor of H_s . If no such rejection occurs, then $s = 1$.
- (3) If p_s does not result in a rejection of H_s , then the number of significant states is s at the $1 - \alpha$ confidence level.

In step 1, it is important to note that the constraint $t_i > r_{\text{max}}$ must hold to satisfy the requirements of Eq. (49). In step 2, one must be careful that as r_{max} increases, naively

conducting multiple tests of the form $\bar{p}_r < \alpha$ will increase the probability of erroneous rejections, effectively lowering the overall confidence level. This is a well-known issue in statistics generally referred to as *family-wise error rate*. A confidence level of $1 - \alpha$ can be enforced using the Holm-Bonferroni [29] method, which lowers the rejection thresholds to

$$\bar{p}_{r_j} < \frac{\alpha}{r_{\text{max}} + 1 - j}, \quad (59)$$

where $j \in \{1, \dots, r_{\text{max}}\}$ is such that the sequence $\bar{p}_{r_j}$ is ordered from the lowest to the highest p -value. It is important to notice that family-wise error rate control methods generally require deciding in advance the number of hypothesis to be tested, which is part of the justification for step 1. Finally, if H_s is rejected in step 3, we consider the procedure to be inconclusive. This can happen, for example, if r_{max} is too small and not enough states were added to obtain an acceptable description of the data.

In Fig. 8, we show the result of applying the procedure above to M0M-mes-ll, F1M-mes-lh, and F1M-mes-hh. The outcome is as expected: the number of significant states decreases as the initial time increases. Charmoniumlike correlators are well known to generally suffer from considerable excited-state contamination, and we indeed observe from our representative data (F1M-mes-hh) that there are no initial times compatible with a single-state description. We find the procedure to be particularly promising for determining safe minimum times to attempt a single-state fit to the data. Indeed, if the number of significant states is equal to 1, then the procedure above guarantees that the data are compatible with a single-state description at the 95% confidence level. In the data presented in Fig. 8, the earliest safe initial time for

single-state fits is $t_i = 12$ for M0M-mes-ll, and $t_i = 21$ for F1M-mes-lh. It is crucial to note that the proposed procedure is able to establish these results *with no knowledge of the amplitudes* A_n , which makes it more attractive than attempting a nonlinear multiexponential fit test on the data.

3. Possible extensions

As part of the procedure proposed above, one also obtains the energy values for the significant states through the minimization of $T^2(\Lambda)$, opening the way for novel methods to determine energies from lattice data, without requiring multiexponential model fits to the data. For example, we show in the right panel of Fig. 8 the energies of the significant states for the F1M-mes-hh obtained through the analysis described in the previous section. The values obtained are remarkably stable, and an encouraging sign that determining the spectrum through the response of applying Laplace filters is feasible. We will explore this further in future publications. In particular, one needs to understand how to rigorously define the statistical uncertainties of the energies obtained in Fig. 8. Additionally, this new method essentially determines the energies as the coefficients of a finite-difference equation canceling the correlator. This is also the mathematical foundation of the Prony method, and comparison with the outcome of solving a Prony GEVP is an interesting extension. However, due to the iterative nature of our method, we can already state that our method does not suffer from issues or ambiguities related to ordering eigenvalues, which is a known problem with GEVP-based methods.

Finally, in all this section, we based hypothesis testing on asymptotic distributions, assuming a large statistics of independent normally distributed samples. In practice the exact probability distributions of the various estimators used will be affected by the unavoidably finite statistics used in data analysis, as well as the fact that typical MCMC samplers used in lattice QCD produce autocorrelated sequences. We expect that the method presented here can be generalized to using empirical distributions, for example obtained using bootstrap resampling. Such approach is discussed in [30] for standard correlator analysis, and we expect it can be extended to the methodology we discussed in this section.

We now discuss applying the various methods in this paper to realistic data analysis for the extraction of energies and matrix elements from our representative dataset.

VI. APPLICATION EXAMPLES

In this section we discuss how the application of Laplace filtering can be used to improve fits to real lattice data. Lattice correlation functions are generally fit to a model of the form

$$C[t] = \sum_{n=0}^{N-1} A_n e^{-E_n t}, \quad (60)$$

where the amplitudes A_n and energies E_n are model parameters. As discussed in the previous section, the time dependence of an arbitrary n -point function is generally more complicated; however, it is common practice to analyze such functions according to a single time separation, and in an asymptotic time regime where the model above is a suitable description, up to negligible exponential corrections coming from higher-energy states and periodic contributions in time. Energies and amplitudes are then extracted by means of a χ^2 minimization, i.e., by fitting some restricted time range of the data to Eq. (60) for a finite number of states N . As outlined in Sec. II B, this requires the inversion of the estimated correlation matrix between the data points that enter the fit. As discussed in Sec. IV, applying Laplace filtering allows one to find a representation of the data that significantly reduces its CDR, making the numerical inversion of the correlation matrix more reliable. However, to be of practical use, we also require that the statistical uncertainties of extracted observables such as energies and amplitudes remain under control. Anticipating the results from Sec. VI A, we find that for the datasets under consideration here, the value of λ_0 that minimizes the CDR leads to larger statistical uncertainties on the extracted parameters A_n and E_n . However, as can be inferred from Figs. 1 and 4, there is a wide range of values of λ around λ_0 for which the CDR is reduced. In fact, based on the discussion about spectral aspects in the previous section, we will see that in practice there are additional benefits of Laplace filtering that can be exploited.

Most correlation functions in lattice QCD face a signal-to-noise problem as a function of Euclidean lattice time t , where the signal decays faster than the square root of the covariance, rendering earlier time slices statistically more precise than later ones. On the other hand, one is commonly interested in the lowest-lying state of the spectrum with energy E_0 . So any optimal fit is necessarily a trade-off between leveraging early time slices and controlling their contamination by states $n \geq N$ that are not captured in the ansatz. Recalling the effect of Laplace filtering on the correlation function, namely

$$D_\lambda C[t] = \sum_{n=0}^{N-1} A_n (\lambda^2 - \tilde{E}_n^2) e^{-E_n t} = \sum_{n=0}^{N-1} A_{\lambda;n} e^{-E_n t}, \quad (61)$$

where $\tilde{E}_n^2 = 2[\cosh(E_n) - 1]$, we observe that the parameter λ can be chosen to eliminate (or at least significantly reduce) a particular state n by choosing $\lambda = \tilde{E}_n$.

Systems involving a light (u, d, s) and a heavy (b, c) quark are particularly prone to excited-state contamination due to their signal-to-noise properties and the

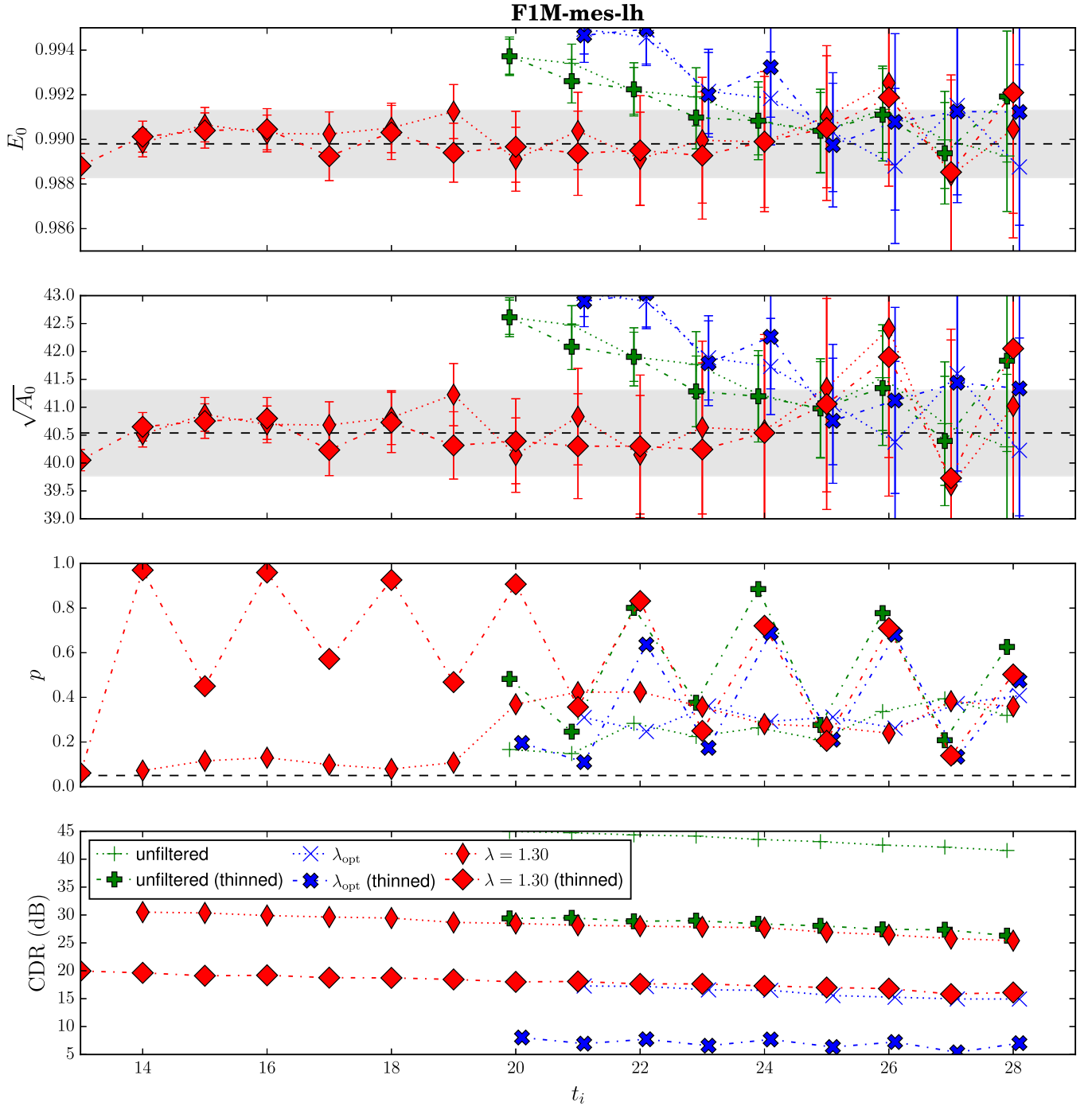


FIG. 9. Fit results for single exponential fits to the F1M-mes-lh dataset as a function of t_i with fixed $t_f = 3/8N_t$. The green pluses, blue crosses and red diamonds represent the fit results to the unfiltered data, the filtered data for which the CDR of the entering time slices is minimized, and the choice $\lambda = 1.3$, respectively. In each case the smaller symbols represent fits to the entire indicated time range, while the larger symbols include an additional down-sampling step. The gray horizontal bands in the top two panels show results obtained from a stability analysis of two-exponential fits to multiple 2 and 3 point functions and serve as validation of the obtained fit results.

relatively small gap between the ground state and the lowest excited states of a system. In the following, we will therefore illustrate the potential of our method on the F1M-mes-lh, C1M-semi-sc-ss, and F1M-mix-sh datasets.

A. Mesonic 2-point functions

In Fig. 9 we show fit results obtained from a simple single-state [i.e., $N = 1$ in Eq. (60)] fit to the F1M-mes-lh dataset. We hold the maximum fit time $t_f = 3N_t/8 = 36$ fixed and vary t_i (shown on the x -axis). Making use of the symmetry present in this particular correlation function, all fits were performed to *folded* data, meaning that the correlation function has been symmetrized for time reversal (i.e., $C[t] \mapsto (C[t] + C[N_t - t])/2$, with the restriction $t \leq N_t/2$) prior to any subsequent operation. This is of practical convenience but not a necessity for the suggested method to work.

Only fits with an acceptable ($\geq 5\%$) p -value are shown. The top panel shows the fit results for the ground state energy, the second panel the value $\sqrt{A_n}$. The third panel reports the p -value associated with this fit and the last the CDR of the correlation matrix that is inverted. Three different types of fits are shown; in each case, the fit is performed once to the full time range (smaller symbols) and once to the down-sampled or thinned version where only every second time slice enters (larger symbols).

The first type (green pluses) are fits to the unmodified data. We observe that the earliest fits with an acceptable p -value occur around $t_i \approx 20$, but the central values still shift until they reach a stable value around $t_i \approx 24$. This is independent of whether the fit is performed to the full or the thinned time range. We note that this is consistent with the determination of the number of significant states presented in Fig. 8 which found that the original correlation function can be described by a single state from $t_i \geq 21$.

The second type of fit (blue crosses) is performed by first determining the value of λ_{opt} that minimizes the CDR of the data entering the fit. Performing the fits to the data filtered by this value, we again observe that the earliest t_i yielding acceptable fits is $t_i \approx 20$ and even larger values of t_i are required in order to reach stable fit results. Furthermore, the statistical uncertainties on these fit results are larger than their unfiltered counterparts. Unfortunately, this implies that the value which minimizes the correlations does not provide a better fit result. However, as can be seen from e.g., Fig. 1, there typically is a region with $\lambda > \lambda_{\text{opt}}$ that still reduces the CDR. Furthermore, it is expected that there is a range where cancellations of the excited-state contributions occur in the correlation function. For the correlation function at hand, we find that a value of $\lambda = 1.3$ (third fit type; red diamonds) achieves both: The CDR is significantly reduced compared to the unfiltered dataset (see bottom panel). At the same time, fit results with

acceptable p -values are already achieved for values $t_i \approx 13$ and stabilize from $t_i \approx 14$. In addition to these benefits, the statistical uncertainty of the fit result is notably reduced compared to the first stable values of the unfiltered or the ‘optimal’ value. This is a promising result: Laplace filtering the data with a suitable choice of filter allows one to reduce the contamination of excited states at comparably early time slices, thereby exploiting statistically more precise data points. These findings are not restricted to the energy of the state (top panel) but apply also to the amplitude, which in many practical applications is the main quantity of interest.

For all three types of fits, when additionally applying thinning (larger symbols), the CDR is further reduced and the p -values of the resulting fits are typically quantitatively better, but the fit results remain largely unchanged. For convenience, results from an extensive stability analysis entirely analogous to the one presented in Ref. [25] are superimposed and shown by the gray bands in the top two panels of Fig. 9. The choice of $\lambda = 1.30$ was initially found by tuning λ with the goal of lowering the t_i for which acceptable fits first occur. However, we can interpret this value by noting that the stability analysis found $E_1 = 1.222(27)$, hence resulting in $\tilde{E}_1 = 1.29946$. Hence filtering with $\lambda = 1.30$ effectively eliminates the first excited state from the correlation function. Furthermore, from Fig. 8 we then expect that after removing the first excited state, the filtered correlation function can be described by a single state from $t_i \approx 15$ in agreement with our findings.

B. Application to semileptonic decays

In the following, we will explore the application of our method to more complicated processes. We start by considering the semileptonic decay of a D_s meson to an η_s meson, where a charm quark decays to a strange quark. For demonstration, we only consider the zero recoil (also known as q_{max}^2) data point, where the initial and the final hadronic states are at rest. In addition to the η_s and D_s 2-point functions [see Eq. (60)], the three point function $C_3^{cs \rightarrow ss}[t_{\text{op}}, t_{\text{snk}}]$ contributes (where we have assumed that $t_{\text{src}} = 0 < t_{\text{op}} < t_{\text{snk}} \leq N_t/2$). The spectral decomposition for this three-point function is

$$C_3^{cs \rightarrow ss}[t_{\text{op}}, t_{\text{snk}}] = \sum_{i,j} B_{ji} e^{-E_j^{\eta_s} t_{\text{op}} - E_i^{D_s} (t_{\text{snk}} - t_{\text{op}})}, \quad (62)$$

where we assumed around-the-world effects to be negligible and defined

$$B_{ji} = \sqrt{A_j^{\eta_s}} M_{ji} \sqrt{A_i^{D_s}}, \quad (63)$$

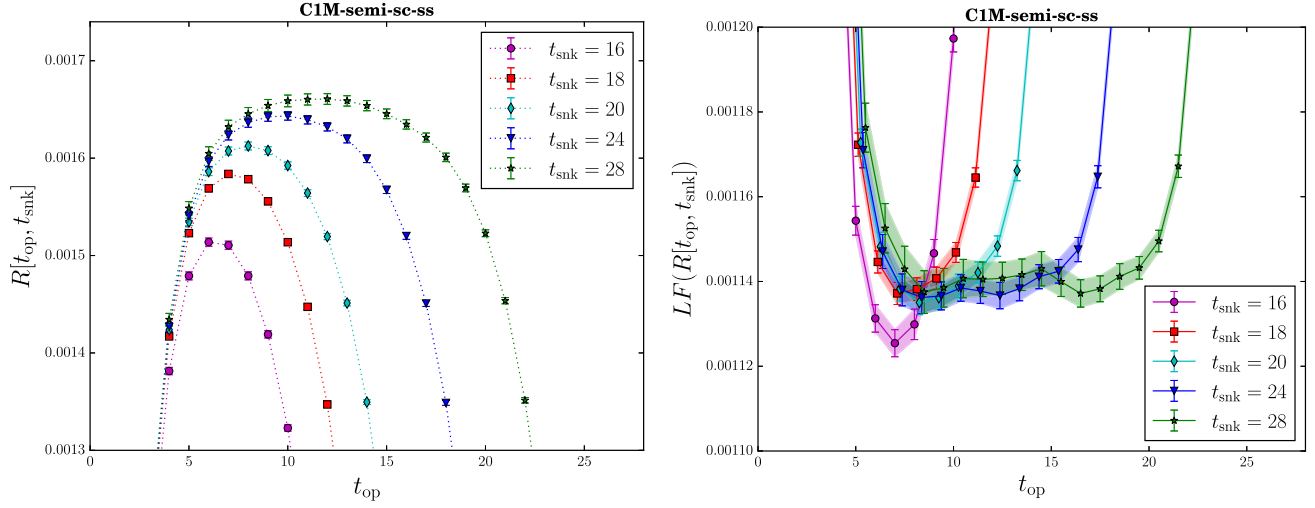


FIG. 10. Illustration on the C1M-semi-sc-ss dataset of ratios that for sufficiently large times t_{op} and t_{snk} should approach an asymptotic value. The left-hand panel shows the unfiltered data, where no region that is independent of t_{snk} can be isolated. The right panel shows the data after Laplace filtering the two point functions that enter this ratio. Here a region for which three different choices of t_{snk} coincide for values $0 \ll t_{\text{op}} \ll t_{\text{snk}}$ can be identified.

where $M_{ji} = \langle \eta_s^j | V_4 | D_s^i \rangle$. In order to compute the non-perturbative form factor that parametrizes this decay, we need to extract the ground state matrix element M_{00} from fits to the two- and three-point functions. A common approach is to construct ratios in which the temporal behavior cancels when the ordering $0 \ll t_{\text{op}} \ll t_{\text{snk}} \ll N_t/2$ is satisfied. One choice of such a ratio is

$$R[t_{\text{op}}, t_{\text{snk}}] = \frac{C_3^{cs \rightarrow ss}[t_{\text{op}}, t_{\text{snk}}]}{C_2^{ss}[t_{\text{op}}] C_2^{cs}[t_{\text{snk}} - t_{\text{op}}]}, \quad (64)$$

which in the above limit approaches the value $M_{00}(A_0^{\eta_s} A_0^{D_s})^{-1/2}$.

In practice, the choice of t_{snk} is restricted by the temporal extent of the lattice, so one has to carefully investigate whether a region for t_{op} and t_{snk} can be found for which R is approximately constant. The left-hand panel of Fig. 10 shows this ratio as a function of t_{op} for 5 choices of t_{snk} . We find that even for the largest values of t_{snk} , we cannot isolate a region where stability in t_{op} and t_{snk} is observed, indicating that for this dataset there is no region where a fit to a single state is sufficient. Following our observations from the previous sections, a natural question is whether applying suitably tuned Laplace filters to the data might allow for a transformation of the data in which the excited states are sufficiently reduced to identify a suitable time range where a single-state description of the data is appropriate.

Since the spectrum of the correlation functions remains unchanged, separate Laplace filters can be applied to any of the three correlation functions entering the construction of Eq. (64). For the sake of simplicity, and because we find

this to be sufficient, we restrict ourselves to filtering the two-point functions that enter. The right-hand panel of Fig. 10 shows the Laplace-filtered version of Eq. (64) where, prior to constructing the ratio, the two-point functions C_2^{cs} and C_2^{ss} have been filtered using $\lambda_{D_s}^2 = 2.9$ and $\lambda_{\eta_s}^2 = 1.2$, respectively. We stress that the asymptotic values these ratios approach are different between the two panels. This is unsurprising since the former should asymptotically plateau to $M_{00}(A_0^{\eta_s} A_0^{D_s})^{-1/2}$, while for the latter we have the replacement $A_0^P \rightarrow A_{\lambda_P;0}^P$ for $P = \eta_s, D_s$ [see Eq. (61)]. However, from the same equation, the relationship between A_0 and $A_{\lambda;0}$ is analytically known once E_0 has been determined, so this does not pose any difficulty in practice. In Fig. 11, we jointly plot the original data (open symbols) together with the appropriately rescaled version of the ratio. For this we use ground state energy estimates from late times of the effective mass. Concretely, we use $E_0^{D_s} = 1.154$ and $E_0^{\eta_s} = 0.4030$. For a full comparison between the filtered and the unfiltered result, the value for the energies should be obtained from fits to the data and their uncertainties should be propagated. However, this is not expected to make a large difference for the particular dataset at hand since the statistical uncertainty on individual late-time effective mass data points is below 2 per-mil in both cases. From the plot we can draw several conclusions:

- (i) The filtered and unfiltered datasets approach the same asymptotic value, lending confidence that the method works.
- (ii) There are (few) data points for which the unfiltered dataset with $t_{\text{snk}} = 28$ is close to being ground-state dominated.

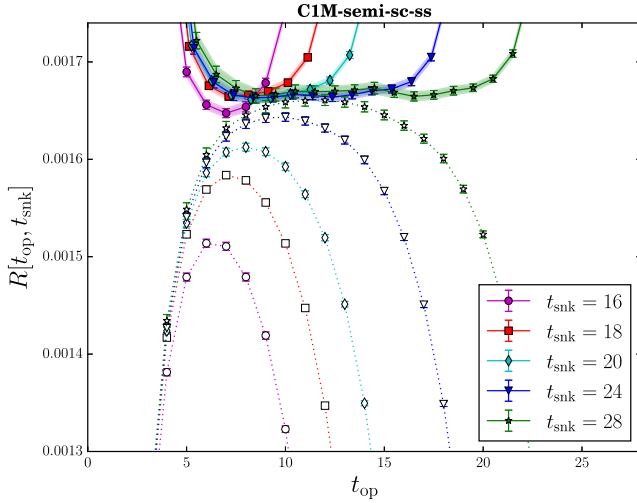


FIG. 11. The same data as in Fig. 10. The unfiltered data is shown with open symbols, while the filtered data has been rescaled by the appropriate factor of $(\lambda_{D_s}^2 - (\tilde{E}_0^{D_s})^2)(\lambda_{\eta_s}^2 - (\tilde{E}_0^{\eta_s})^2)$, assuming $E_0^{D_s} = 1.154$ and $E_0^{\eta_s} = 0.4030$.

- (iii) For the filtered case, there are several values of t_{snk} which admit compatible plateaus for a range of time slices.
- (iv) The statistical uncertainties of the filtered data are of similar size to those of the unfiltered data.

We stress that for sufficiently precise data, the contamination from the first excited state will always be larger than the statistical uncertainties, so the situation displayed in the left panel of the figure *necessarily* arises for large enough statistics. In these situations, the Laplace filter provides a tunable parameter that can be adjusted to eliminate the leading excited state (and the procedure can be iterated as long as the contact term does not propagate into the time slices under consideration). Since the spectral decomposition remains the same, the methodology carries over to other choices of momenta and currents. The procedure can be further refined and extended by also filtering the three-point function.

C. Application to neutral meson mixing

The final dataset we consider describes neutral meson mixing. There are several similarities between this and the case of semileptonic decays, but the required spectral analysis is simplified by the fact that the initial and final state have the same spectrum, so that Eq. (62) becomes

$$C_3^{sh}[t_{\text{op}}, t_{\text{snk}}] = \sum_{i,j} D_{ij} e^{-E_j t_{\text{op}} - E_i(t_{\text{snk}} - t_{\text{op}})}, \quad (65)$$

with $D_{ji} = D_{ij}$. One immediate implication of this is that at fixed t_{snk} the ground state contribution is a constant with respect to t_{op} rather than an exponential decay. Analogous to the case of the semileptonic dataset (see Sec. VIB),

we define suitable ratios at fixed t_{snk} that allow for the comparison of different values of t_{snk} . However, since the temporal dependence with respect to t_{op} cancels when the correlation function is ground-state dominated, the three-point correlation functions are normalized by appropriate two-point functions at single data points, such that the exponential suppression with t_{snk} is removed. For historical reasons, the typical choice is to construct ratios B_{eff} such that the asymptotic value approaches the so-called *bag parameter*, which is achieved by considering the two-point correlation functions C^{PA} with $\gamma_{\text{src}} = \gamma_5$ and $\gamma_{\text{snk}} = \gamma_4 \gamma_5$.⁴ The definition then reads

$$B_{\text{eff}}[t_{\text{op}}, t_{\text{snk}}] = \frac{C_3[t_{\text{op}}, t_{\text{snk}}]}{-C_2^{PA}[0]C_2^{PA}[t_{\text{snk}}]}. \quad (66)$$

Since the generation of this dataset does not require sequential sources and sources were placed on every second time plane (see Refs. [24,25] for details), many choices of t_{snk} are computationally accessible, and our dataset comprises the values $t_{\text{snk}} = 16, 18, \dots, 46$. The left-hand panel of Fig. 12 shows the effective bag parameter as a function of $t_{\text{op}} - t_{\text{snk}}/2$ for different values of t_{snk} . For better readability, we do not display all values for t_{snk} . Clearly, the data point $t_{\text{op}} = t_{\text{snk}}/2$ (plotted as 0 on the x-axis) is furthest away from both source and sink, and hence should have the smallest excited-state contamination. We observe that for this data point, very small values of t_{snk} are statistically incompatible with the larger values of t_{snk} and hence suffer from large excited-state contamination. However, these data points are statistically the most precise, since the uncertainties grow as t_{snk} is increased.

An immediate question is whether Laplace filtering can be used to reduce the contamination by excited states and hence leverage smaller values of t_{snk} . In the previous sections, we saw that the possibility to reduce excited states using our choice of filter relies on the fact that the functional form of exponential decays is unaltered. For that reason, rather than considering C_3^{sh} at fixed t_{snk} , we consider the correlation function along the midpoint between the source at $t = 0$ and t_{snk} . We then recover an exponential decay of the form

$$C_3^{sh}[t_{\text{snk}}/2, t_{\text{snk}}] = \sum_{i,j} D_{ij} e^{-(E_i + E_j)t_{\text{snk}}/2}, \quad (67)$$

so that Laplace filtering is likely to be usable to remove unwanted excited states. A comprehensive stability analysis analogous to that of Ref. [25] has been performed to determine the ground and first excited state parameters of the two- and three-point functions under consideration here, finding $E_0 = 0.94136(27)$, $E_1 = 1.190(21)$, and $B = 0.8341(13)$. Drawing on that knowledge, we apply

⁴More details can be found in Refs. [24,25].

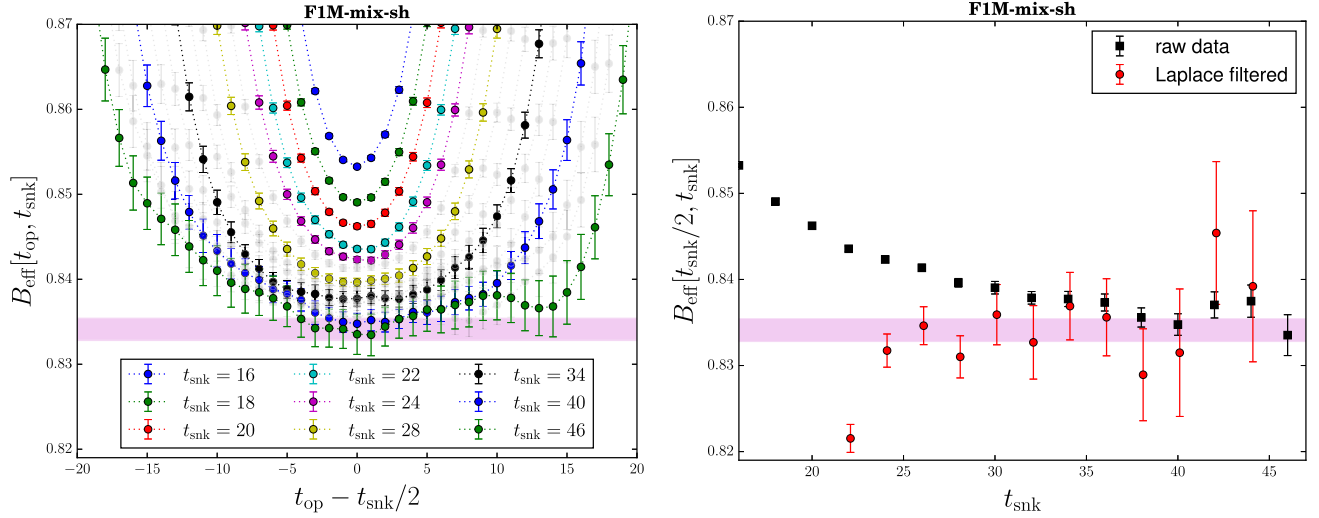


FIG. 12. Analysis of the F1M-mix-sh dataset. The left-hand panel shows the effective bag parameter as a function of t_{op} for a variety of t_{snk} values. The right-hand plot shows the mid-point for the effective bag parameter between the source and the sink for the original data (black) and the Laplace filtered data (red) where the Laplace filter uses the values for the ground and first excited state energies obtained from a stability analysis analogous to that of Ref. [25]. The magenta band corresponds to the bag parameter as extracted from the same stability analysis.

a Laplace filter to cancel the expected leading contamination. For the case of the mesonic two-point function that enters the normalization, we choose $\lambda_{\text{mes}}^2 = \tilde{E}_1^2$. For the three-point function, we note that the leading excited-state contamination in Eq. (67) is $E_{01} = (E_0 + E_1)/2$, and we therefore apply a filter with $\lambda_{\text{mix}}^2 = \tilde{E}_{01}^2$. We then construct the Laplace-filtered version of $B_{\text{eff}}[t_{\text{snk}}/2, t_{\text{snk}}]$. Given that we have knowledge of the spectrum, we can also correct this value by the different normalization incurred from the Laplace filtering and hence present the original and the filtered data on the same scale. This is shown in the right-hand panel of Fig. 12. The black data points show the original data as a function of t_{snk} . There is clear evidence for excited-state contamination for $t_{\text{snk}} \lesssim 36$. For $t_{\text{snk}} \gtrsim 36$ the individual values start to be noisier, which can be understood by referring to the left-hand plot. The red data points show the Laplace-filtered version of the data. As expected, we observe that already for $t_{\text{snk}} \approx 26$ we obtain ground-state dominated data with similar precision to those of the earliest ground-state dominated data points of the unfiltered data. We further find that different choices of t_{snk} fluctuate more for the filtered data, but this is at least partially by virtue of the achieved decorrelation from using a Laplace filter and hence the data points carry more individual information.

While this particular dataset at the current level of statistical uncertainties allows for parameter choices with ground-state dominance, there are many examples where this would not be the case, for example if the statistics were significantly increased, or for operators with larger excited-state contamination and/or ensembles with smaller temporal extent.

VII. DISCUSSION AND CONCLUSION

In this paper, we have addressed two major issues that lattice analysis workflows frequently encounter: the potential ill-conditioning of data-estimated correlation matrices and the extraction of the spectrum from correlation functions in the presence of excited state contamination. Applying a transformation to the data and the model does not involve any *ad hoc* modifications of the spectrum of the correlation matrix and can be used to ameliorate the first problem. As one such transformation, we advocate the use of regulated Laplace filters, as they are linear and invertible, and preserve the exponential form typically encountered in correlation functions.

We find that a suitably chosen Laplace filter significantly improves the condition number of the correlation matrix, and that down-sampling positively interacts with this, i.e., the two effects are additive. This holds in all investigated examples, and a wide parameter range in the regulator λ allows for a reduction of the condition number.

A key observation is that the application of a Laplace filter modifies the amplitudes of all states E_i by a factor $(\lambda^2 - \tilde{E}_i^2)$. This can be exploited in multiple ways:

- (1) Finding the values of λ_i that eliminate the correlation function in a given time range can be used to obtain the spectrum without any need to perform nonlinear multiexponential fits and without needing to fit the corresponding amplitudes, halving the number of parameters that need to be fitted. We find this method to be robust and stable.
- (2) Extending the above, we devised a method to determine the number of statistically significant

states in a given time range. This can be used to choose the appropriate ansatz for a traditional multi-state fit. Combined with the previous point, this method can provide data-driven priors or initial guesses for fit parameters.

- (3) By tuning λ , we can eliminate unwanted excited state contamination. We demonstrated this application for typical state-of-the-art correlation functions. Applying this method allows fits to earlier and hence statistically more precise time slices. We particularly envisage applications to correlation functions with poor signal-to-noise properties and correlation functions that require multiple well-separated timescales. A further advantage is that traditional analysis frameworks can be used to perform the fits, making the method easy to implement and use.

We reiterate that Laplace filtering can be applied in conjunction with the various methods discussed in the Introduction should the resulting correlation matrix not yet be sufficiently well conditioned.

We envisage several further applications of this work in the future. We will apply this method to various ongoing large-scale numerical efforts, such as semileptonic decays and neutral meson mixing. Furthermore, it can be employed to investigate and scrutinize excited state effects, such as those frequently observed in nucleon matrix elements [31,32] and those expected in the heavy-light mesonic sector [33]. This method could also be of great value to finite temperature simulations where the temporal extent has to be small by construction and hence excited state contamination is a big concern. In particular for anisotropic simulations with many points in the temporal direction several Laplace filters could be applied without propagating the contact term into the region of interest.

Finally, we plan to extend the use of the method as a novel way of extracting the spectrum without the need for

multiexponential fits by rigorously attaching statistical uncertainties to the determination of energies and amplitudes obtained from such a maximum likelihood determination.

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DATA AVAILABILITY

Some of the data that support the findings of this article are openly available [35]. Three-point functions are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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