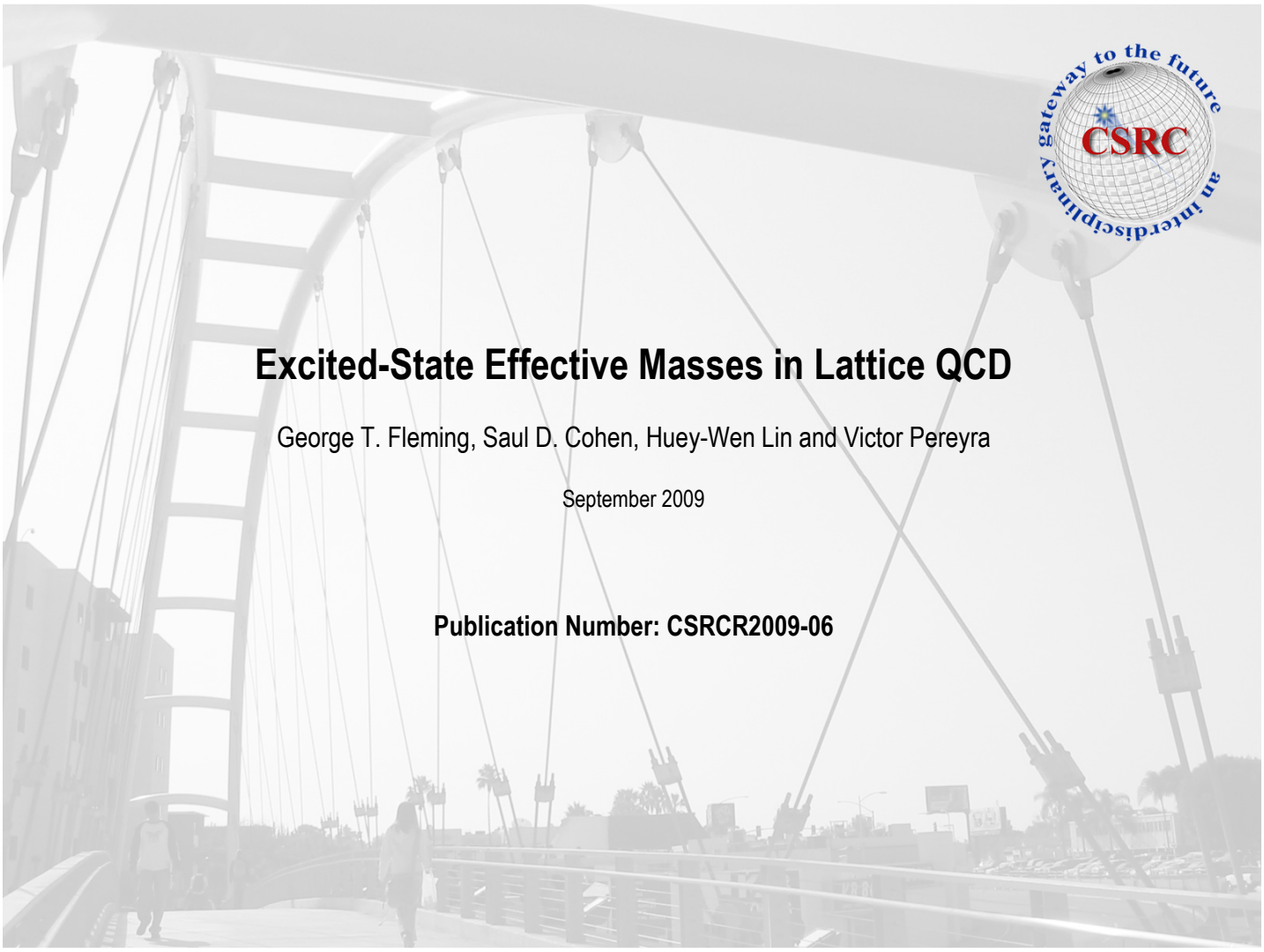

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Excited-State Effective Masses in Lattice QCD

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We apply black-box methods, *i.e.* where the performance of the method does not depend upon initial guesses, to extract excited-state energies from Euclidean-time hadron correlation functions. In particular, we extend the widely used effective-mass method to incorporate multiple correlation functions and produce effective mass estimates for multiple excited states. In general, these excited-state effective masses will be determined by finding the roots of some polynomial. We demonstrate the method using sample lattice data to determine excited-state energies of the nucleon and compare the results to other energy-level finding techniques.

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I. INTRODUCTION

Lattice quantum chromodynamics (LQCD) has been used successfully to compute many experimentally observable quantities from first-principles calculation of Euclidean-time hadron correlation functions, even occasionally predicting experimental results before they are measured. However, the successes of LQCD have mostly been restricted to computation of the physical properties of the lowest-energy states in each quantum number channel by focusing on the large-time behavior of correlation functions where uncertainties due to excited-state contributions are exponentially suppressed. Given that signal-to-noise in correlation functions also falls exponentially at large times, success is often dictated by available computational resources.

Both in meson and baryon spectroscopy there are many experimentally observed excited states whose physical properties are poorly understood that could use theoretical input from LQCD to solidify their identification. Other excited-state quantities that could be computed on the lattice, such as form factors and coupling constants, would be useful to groups such as the Excited Baryon Analysis Center (EBAC) at Jefferson Lab, where dynamical reaction models have been developed to interpret experimentally observed properties of excited nucleons in terms of QCD [1, 2]. In certain cases, input from the lattice may be helpful in determining the composition of controversial states, which may be interpreted as ordinary hadrons, tetra- or pentaquarks, hadronic molecules or unbound resonances.

Among the excited nucleon states, the nature of the Roper resonance, $N(1440)\ P_{11}$, has been the subject of interest since its discovery in the 1960's. It is quite surprising that the rest energy of the first excited state of the nucleon is less than the ground-state energy of nucleon's negative-parity partner, the $N(1535)S_{11}$ [3], a phenomenon never observed in meson systems. There are several interpretations of the Roper state, for example, as the hybrid state that couples predominantly to QCD currents with some gluonic contribution [4] or as a five-quark (meson-baryon) state [5].

Early LQCD calculations using the quenched approximation [6–12], found the computed spectrum inverted relative to experiment, with P_{11} heavier than the S_{11}. A recent study [7] suggested that qualitative agreement between experiment and LQCD in the quenched approximation could be restored provided other simulation effects due to finite volumes and unphysically heavy quarks were properly addressed. The study strongly suggests the nature of the Roper resonance changes dramatically as the quarks are made physically light in LQCD simulations, as in Fig. 1 and Table I. Clearly, future LQCD calculations will require improved analysis techniques for extracting multiple excited-state energies, as well as variational wavefunctions, in the nucleon sector to test the validity of this claim.

Apart from the vast amount of detail about excited states accessible to LQCD computations with advanced analysis methods, the statistical accuracy of ground-state quantities is also enhanced because correlation functions computed at shorter Euclidean times can be used where the signal-to-noise is greater. As current lattice simulations are performed with ever-greater resolution at short Euclidean times as lattice spacings are decreased toward the continuum limit,

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Group	N_f	S_f	a_t^{-1} (GeV)	M_π (GeV)	L (fm)	Method	Extrapolation
Basak et al. [13]	0	Wilson	6.05	0.49	2.35	VM	N/A
Burch et al. [12]	0	CIDO	1.68,1.35	0.35–1.1	2.4	VM	$a + bm_\pi^2$
Sasaki et al. [10]	0	Wilson	2.1	0.61–1.22	1.5,3.0	MEM	$\sqrt{a + bm_\pi^2}$
Guadagnoli et al. [8]	0	Clover [14]	2.55	0.51–1.08	1.85	SBBM	$a + bm_\pi^2 + cm_\pi^4$
Leinweber et al. [9]	0	FLIC	1.6	0.50–0.91	2.0	VM	N/A
Mathur et al. [7]	0	Overlap [15]	1.0	0.18–0.87	2.4,3.2	CCF	$a + bm_\pi + cm_\pi^2$
Sasaki et al. [6]	0	DWF	2.1	0.56–1.43	1.5	VM	$a + bm_\pi^2$

TABLE I: Summary of existing published S_{11} and P_{11} calculations. Due to space limitations, we adopt these abbreviations for fermion actions: Domain-Wall Fermions [16–19] (DWF), Chirally Improved Dirac Operator [20, 21] (CIDO), Fat-Link Irrelevant Clover [22] (FLIC); and for the analysis methods: Variational Method [23, 24] (VM), Constrained Curve Fitting [25] (CCF), Maximum Entropy Method [26, 27] (MEM), Simplified Black Box Method [8, 28] (SBBM). For those works which do not perform extrapolation, we use the lightest pion mass to represent their results.

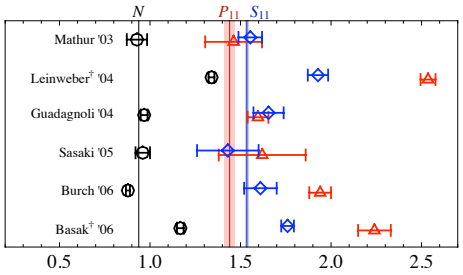

FIG. 1: Summary of previous lattice calculations with extrapolation to the physical pion mass point or the lowest simulated pion point (labeled as "†"). The (black) circles, (red) triangles, (blue) diamonds are the ground-state nucleon, P_{11} and S_{11} states, respectively.

simultaneous extraction of ground and excited-state quantities will be essential to extract full value from such large-scale (and expensive) computations.

A variety of analysis techniques have been applied to extracting the excited-state spectrum from correlation functions. The most widely used method is a nonlinear least-squares (NLLS) fit to a model function, such as a sum over two or more exponentials. Operationally, even such a simple nonlinear fit can be fraught with difficulty, from establishing the range of Euclidean times included in the dataset to stabilizing the convergence of minimization algorithms by careful choices of initial guesses or temporarily freezing selected fit parameters during the minimization process, all of which require intervention by a trained expert.

At such times, the expert typically turns to black-box methods for guidance because they do not require intervention to determine initial guesses and fitting ranges: estimates of correlation functions go into the black box and estimates of hadron energies come out. The main detraction of black-box methods are that the produced estimates are expected to have larger uncertainties, making them *sub-optimal* relative to least squares methods [29]. Marrying the two approaches can effectively combine the best features of both, leading to a highly-automated analysis program producing optimal estimates of energies. Prior to this work, black-box methods were mainly useful for extracting ground-state and, perhaps, first excited-state energies [8, 28]. We believe the method described below will provide the needed black-box method for estimating as many energies from fixed set of correlations functions as are likely to be extracted from a NLLS fit.

The structure of this paper is as follows: Sec. II provides theoretical formulations of the excited-state effective masses for single and multiple correlators; it also explores certain extensions to these techniques: linear prediction and periodic boundary conditions. In Sec. III, we apply the methodology to some characteristic lattice correlators and compare the results with simple fitting and the variational method [23, 24]. Conclusions and future outlook are given in Sec. IV. Numerous details and examples are included in the appendices. Preliminary details of this work were presented in Ref. [30].

II. THEORETICAL BASIS

The hadron spectrum can be calculated in LQCD using two-point hadronic correlation functions

$$C(t_0,t) = \left\langle 0 \left| O(t)\ O^\dagger(t_0) \right| 0 \right\rangle, \tag{1}$$

where the creation and annihilation operators $O^\dagger$ and O transform irreducibly under the symmetries of the lattice space group [31–34]. After taking momentum (and spin for baryons) projection and inserting a complete set of hadronic eigenstates of the Hamiltonian (ignoring the variety of boundary condition choices possible), this becomes

$$C(\vec{p},t_n) = \sum_{m=1}^{M} A_m(\vec{p}) \exp\left[-(t_0+na)E_m(\vec{p})\right] \tag{2}$$

$$n \geq 0, \quad A_m,\ E_m \in \mathbb{R}, \quad 0 \leq E_1 \leq E_2 \leq \cdots \leq E_M.$$

where A_m contains not only the overlap factor between the eigenstate and states created by the operators but also any kinetic factors that do not depend on Euclidean time separation $t_n = na = t - t_0$.

A. Effective Masses

In general, a two-point correlation function computed on $N = 2M$ time-slices t_n will admit an exact algebraic solution having the form of Eq. (2) with M energies E_m and amplitudes A_m. The problem to solve is the nonlinear system of equations $\mathbf{y} = \mathbf{V}(x)\ \mathbf{a}$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ \vdots \\ y_{2M} \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_M \\ x_1^2 & x_2^2 & \cdots & x_M^2 \\ x_1^3 & x_2^3 & \cdots & x_M^3 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{2M-1} & x_2^{2M-1} & \cdots & x_M^{2M-1} \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_M \end{bmatrix} \tag{3}$$

for $x_m = \exp\left[-aE_m\left(\vec{p}\right)\right]$ and $a_m = A_m\left(\vec{p}\right)\exp\left[-t_0E_m\left(\vec{p}\right)\right]$ where $y_n = C\left(\vec{p},t_n\right)$. $\mathbf{V}(x)$ is known as $2M \times M$ rectangular Vandermonde matrix.

By inspection, it appears the problem is of polynomial degree $2M$ and thus by the Abel-Ruffini theorem [35, 36] should not admit a general closed form solution in terms of radicals for $M > 2$. The $M = 1$ solution is simple to compute and is widely known in the lattice QCD literature as the *effective mass* solution. Note already that the simple effective mass problem is linear and has only one solution, suggesting that the polynomial degree is actually of order M.

The $M = 2$ solution was explicitly constructed by one of the authors [28] and was independently constructed some time later by others [8]. It was noted [28] that the problem, when reduced, required only the solution of a quadratic equation and so it was conjectured that the general problem of size M could be reduced to a polynomial equation in one variable of degree M.

An efficient algorithm has been available for some time for solving square Vandermonde systems [37] by making them upper triangular. This approach works equally well for rectangular Vandermonde systems as in Eq. (3). Furthermore, this approach reveals why the solution for the energies E_m can be found without solving for the amplitudes A_m and why the problem is of polynomial degree M.

As a first step toward extracting the energies E from our data, we transform the system so that $V(x)$ is in upper triangular form [37] by pre-multiplying by the lower $2M \times 2M$ bi-diagonal matrices:

$$L_m(x) = \begin{bmatrix} 1 & & & & & & & \\ 0 & \ddots & & & & & & \\ & \ddots & 1 & & & & & \\ & & 0 & 1 & & & & \\ & & & x_m & -1 & & & \\ & & & & \ddots & \ddots & & \\ & & & & & x_m & -1 \end{bmatrix} \tag{4}$$

where the first -1 on the diagonal appears in the $m+1$ row and column. In the appendices, we demonstrate in detail how the general solutions for $M = 2$, 3 and 4 work.

Finding a general approach for $M > 4$ would be a tough challenge. Although Abel's Impossibility Theorem proves there are no general solutions in radicals for polynomials higher than quartic order, there are numerical methods for finding the roots of polynomials of any order. The general form for the polynomial follows from Eqs. (A10), (A22) and (A39) in the appendices:

$$|\boldsymbol{\mathcal{H}}| = \left| \begin{array}{cccc:c} y_1 & y_2 & \cdots & y_M & 1 \\ y_2 & y_3 & \cdots & y_{M+1} & x \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ y_{M+1} & y_{M+2} & \cdots & y_{2M} & x^M \end{array} \right| = 0. \tag{5}$$

The M roots of the polynomial can be labeled x_m and, once known, can be used in Eq. (3) to solve for the a_m.

Prony [38] showed that problems in the form of Eq. (2) implied the following system of equations $\mathbf{y} = \mathbf{H}(y)\ \mathbf{p}$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix} = - \begin{bmatrix} y_2 & \cdots & y_{M+1} \\ y_3 & \cdots & y_{M+2} \\ \vdots & \ddots & \vdots \\ y_{M+1} & \cdots & y_{2M} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_M \end{bmatrix} \tag{6}$$

where the $M \times M$ matrix $\mathbf{H}(y)$ has the special structure of a Hankel matrix and the components p_m of $\mathbf{p}$ are the coefficients of a polynomial

$$P(x) = \prod_{m=1}^{M} (x - x_m) = 1 + \sum_{m=1}^{M} p_m x^m. \tag{7}$$

The Prony-Yule-Walker method (or just Prony's method, for short) [38–40] solves Eq. (6) to find the coefficients and then finds the M roots of the polynomial in Eq. (7). The amplitudes are determined by substituting the roots into Eq. (3) and solving it. Note again that using $2M$ timeslices of correlation function data to determine M effective masses is a problem of polynomial order M.

The general conditions under which the solutions of the Hankel and Vandermonde systems coincide are presented in Ref. [41]. Here we provide a simple demonstration that both solutions are the same under the assumption that there are no complications like degeneracies in the energy spectrum of Eq. (2). Assuming $\mathbf{H}(y)$ is invertible, solving Eq. (6) gives

$$\mathbf{p} = \mathbf{H}^{-1}\mathbf{y}, \qquad P(x) = 1 + \mathbf{p}^\top \mathbf{x} = 1 + \left(\mathbf{H}^{-1}\mathbf{y}\right)^\top \mathbf{x} \tag{8}$$

for the polynomial of Eq. (7) and where $\mathbf{x}^\top = \left(x, x^2, \cdots, x^M\right)$. Recall that the inverse can be written in terms of the adjoint, or matrix of cofactors, $\mathbf{H}^{-1} = \mathbf{C}/\left|\mathbf{H}\right|$, $C_{ij} = (-1)^{i+j}\left|\mathbf{H}(i;j)\right|$, where the notation $\mathbf{H}(i;j)$ means removing row i and column j. For Prony's method, we can rescale $P(x) \to |\mathbf{H}|\, P(x)$ and still find the roots x_m by solving

$$|\mathbf{H}| + (\mathbf{C}\,\mathbf{y})^\top \mathbf{x} = 0 \tag{9}$$

for x.

Returning to the Vandermonde method, the determinant of Eq. (5) can be expanded in terms of its cofactors $\mathcal{C}_{ij} = (-1)^{i+j}\left|\boldsymbol{\mathcal{H}}(i;j)\right|$

$$|\boldsymbol{\mathcal{H}}| = (-1)^M |\mathbf{H}| + \sum_{i=1}^{M} \mathcal{C}_{i+1,M+1} x^i = (-1)^M |\mathbf{H}| + \sum_{i=1}^{M} (-1)^{i+M} \left|\boldsymbol{\mathcal{H}}(i+1;M+1)\right| x^i. \tag{10}$$

As usual, each cofactor can be expanded in terms of further cofactors where additional rows and columns are removed:

$$\left|\boldsymbol{\mathcal{H}}(i+1;M+1)\right| = \sum_{j=1}^{M} (-1)^{j+1} \left|\boldsymbol{\mathcal{H}}(1,i+1;j,M+1)\right| y_j. \tag{11}$$

By eliminating the first row and last column of $\boldsymbol{\mathcal{H}}$ in Eq. (5) we recover $\mathbf{H} = \boldsymbol{\mathcal{H}}(1; M+1)$ and for the cofactors

$$(-1)^{j+1} \left|\boldsymbol{\mathcal{H}}(1, i+1; j, M+1)\right| = (-1)^{j} \left|\mathbf{H}(i; j)\right| \tag{12}$$

so the desired identity is recovered

$$\left|\boldsymbol{\mathcal{H}}\right| = (-1)^{M} \left|\mathbf{H}\right| + (-1)^{M} \sum_{i=1}^{M} \sum_{j=1}^{M} (-1)^{i+j} \left|\mathbf{H}(i; j)\right| y_j x^i. \tag{13}$$

up to a possible overall minus sign for odd M, which is irrelevant for finding roots. There is a unique set of solutions to the Vandermonde and Hankel systems (under the assumption of noise-free correlation functions with non-degenerate energy levels), so other considerations should determine which is the better method to construct the polynomial. It is our experience that computing coefficients from Eq. (5) is preferred to solving Eq. (6) as statistical noise in the correlation functions can lead to nearly singular Hankel matrices which are difficult to invert.

In an earlier work [28], one of the authors showed that Prony's method (also called *linear prediction*) could easily be extended to use more than $2M$ timeslices of a correlation function to extract only M masses by constructing an over-constrained system of equations analogous to Eq. (6). It is not obvious how to construct and solve a similar over-constrained system in the Vandermonde case. Thus, Prony's method has a potential advantage that more time samples of the correlation function can be used to extract the same number of energy levels leading to reduced statistical fluctuations.

B. Solutions with multiple correlation functions

When constructing correlation functions in LQCD, care is taken to ensure that the correlation function transforms irreducibly under the symmetries of the lattice space group [31–34]. For the model function, as in Eq. (2), this implies that the amplitudes depend on the details of the specific correlation function but that the energies depend only on the irreducible representation. Since it is common in lattice QCD simulations to compute at least two distinct correlation functions for each irreducible representation, effective mass solutions which combine data from multiple correlations are also possible.

Assume that there are K correlation functions available as in Eq. (2) that differ only in their amplitudes:

$$C_k(\vec{p}, t_n) = \sum_{m=1}^{M} A_{km}(\vec{p}) \exp\left[-(t_0 + na) E_m(\vec{p})\right] \tag{14}$$

$$n \geq 0, \quad A_{km},\ E_m \in \mathbb{R}, \quad 0 \leq E_1 \leq E_2 \leq \cdots \leq E_M.$$

Data from the same N time slices will be used in the following from each correlation function to construct M effective masses. Under this assumption the condition that there will be equal number of data points as unknowns is $KN = (K+1)M$. In Appendix A are the three solutions that satisfy the condition for $K = 1$, up to quartic order. There are four more solutions (up to quartic order) for $K > 1$: $(K, M, N) = (2, 2, 3)$, $(2, 4, 6)$, $(3, 3, 4)$ and $(4, 4, 5)$ (demonstrated in Appendix B). Relaxing the assumption that the same number of time slices are used from each correlation function will allow for more possibilities up to quartic order. It is straightforward to generalize to these cases if desired.

The general form of the polynomial equation can be inferred by studying the solved examples in Eqs. (B6), (B16), (B23) and (B29). Define K Hankel matrices $H_k^{N \times M_k}$ for each of the correlation functions with the constraints $\sum_{k=1}^{K} M_k = M$ and $N = M + 1$. Then the general form of the polynomial equation is

$$\left| \begin{array}{c:c:c:c:c} & & & & 1 \\ & & & & x \\ H_1^{N \times M_1} & H_2^{N \times M_2} & \cdots & H_M^{N \times M_K} & x^2 \\ & & & & \vdots \\ & & & & x^M \end{array} \right| = 0. \tag{15}$$

As previously discussed, each Hankel matrix is generally of full column rank and, if the correlation functions are linearly independent, then the columns of different Hankel matrices are also linearly independent. So, Eq. (15) will only be satisfied for discrete values of $x_m, m = 1$–M corresponding to the roots of the polynomial.

C. Periodic Boundary Conditions

In practical LQCD calculations, the temporal extent is finite so the choice of temporal boundary conditions affects hadronic correlation functions near the boundary. For simplicity, starting from Eq. (2), set $t_0 = 0$ and identify the points $t_0 = 0$ and $t_N = Na$ which can be done using modular arithmetic, *i.e.* $t_n = (n \bmod N)a$. For anti-periodic boundary conditions, the typical hadronic Euclidean time correlation function is described by the model function

$$C(\vec{p}, t_n) = \sum_{m=1}^{M} A_m(\vec{p}) \exp\left[-(n \bmod N) a E_m(\vec{p})\right] + (-1)^B \sum_{m^\star=1}^{M^\star} A^\star_{m^\star}(\vec{p}) \exp\left[-(N - n \bmod N) a E^\star_{m^\star}(\vec{p})\right] \tag{16}$$

$$n \geq 0, \quad A_m,\ A^\star_{m^\star},\ E_m,\ E^\star_{m^\star} \in \mathbb{R}, \quad 0 \leq E_1 \leq E_2 \leq \cdots \leq E_M, \quad 0 \leq E^\star_1 \leq E^\star_2 \leq \cdots \leq E^\star_{M^\star}.$$

For periodic boundary conditions, set $(-1)^B \to 1$. For mesons, $B = 0$ but more importantly $A_m = A^\star_m$ and $E_m = E^\star_m$, which is not true for baryons ($B = 1$).

Meson correlation functions represent the same M states propagating to the right and left. However, time-reversal symmetry requires $C(\vec{P}, t_n) = C(\vec{P}, t_{N-n})$, up to noise terms, so that only half of the computed timeslices are truly independent. Thus, from a single correlation function computed on N timeslices in a finite box, information about at most $M = N/4$ states in the given quantum number channel can be extracted. As shown in Ref. [28], this can be made explicit by writing the meson correlation function as

$$C(\tau_n) = \sum_{m=1}^{M} A_m \exp(-aNE_m/2) \cosh(anE_m), \quad \tau_n = (n - N/2)a. \tag{17}$$

To write this result in the Vandermonde form of Eq. (3), define the variables

$$a_m = A_m \exp(-aNE_m/2), \quad x_m = \cosh(aE_m), \quad y_n = \frac{1}{2^{n-1}} \sum_{j=0}^{n-1} \begin{pmatrix} n-1 \\ j \end{pmatrix} C(\tau_{n-2j-1}). \tag{18}$$

For baryon ($B = 1$) correlation functions, the states propagating to the left and right are not identical under time-reversal symmetry, *e.g.* $E_m \neq E^\star_m$. Thus, from a single correlation function computed on N timeslices in a finite box, information about at most $M + M^\star = N/2$ states can be extracted in the given channel plus its partner under time-reversal. While the precise numbers of accessible states in each channel may depend on the details of the particular correlation function, in general it is expected that $M \simeq M^\star$ since it is known phenomenologically that the there is not a large gap between partner spectra, *e.g.* $E_m \simeq E^\star_m$. Finally, by choosing a limited range of available timeslices, *i.e.* $n << N$ or $N - n << N$, it is possible to mostly extract the just the properties of either left or right moving states.

When solving Eq. (3), the domain of the solutions x_m will be the real numbers or complex conjugate pairs since real-valued correlation functions are used as input. Complex-valued solutions are clearly unphysical and should be discarded as they are likely due to noise. Real solutions may also be unphysical if they cannot be used to extract a non-negative energy, and this will depend on the details of the model function and hence the boundary conditions. For example, for the basic model of Eq. (2), only the solutions $0 < x_m \leq 1$ will yield non-negative energies. For mesons in periodic boxes, $x_m = \cosh(aE_m)$ so only $x_m \geq 1$ will yield non-negative energies. Finally, for baryons in periodic boxes, the M states propagating to the right have $x_m = \exp(-aE_m)$ and the M states propagating to the left have $x_{M+m} = \exp(aE^*_m)$ so all solutions $x_m > 0$ are physical and $x_m > 1$ means the state is propagating to the left.

For some lattice fermion actions, *e.g.* staggered [42–44] or domain-wall fermions [45, 46], a variation of Eq. (2) is needed as a starting point to account for states which oscillate in time. For example, an appropriate model for staggered mesons on an infinite lattice is

$$C(\vec{p}, t_n) = \sum_{m=1}^{M} \left\{ A_m(\vec{p}) \exp\left[-naE_m(\vec{p})\right] + (-1)^n A^*_m(\vec{p}) \exp\left[-naE^*_m(\vec{p})\right] \right\} \tag{19}$$

$$n \geq 0, \quad A_m,\ A^*_m,\ E_m,\ E^*_m \in \mathbb{R}, \quad 0 \leq E_1 \leq E_2 \leq \cdots \leq E_M, \quad 0 \leq E^*_1 \leq E^*_2 \leq \cdots \leq E^*_M.$$

Note that it is a different symmetry, a shift by one lattice spacing, rather than the time reversal symmetry above, that is responsible for the appearance of a new independently ordered set of states, indicated by E^* instead of $E^\star$ as above,

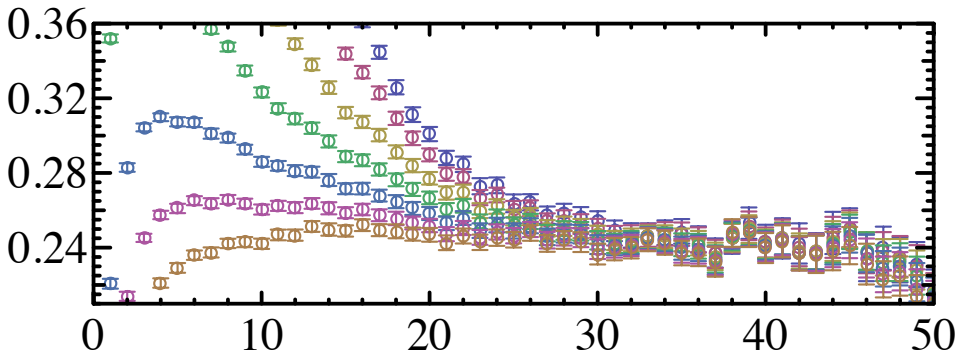

FIG. 2: Effective mass plots from the 7 smeared-point proton correlators used in this work. The horizontal axis shows time and the vertical axis shows the effective masses, both in lattice units.

which oscillate as $(-1)^n$. For symmetry reasons, it is strictly required that the number of states match, *e.g.* $M = M^*$. When solving Eq. (3), such oscillating solutions will have physical solutions if $-1 \leq x_m < 0$. Similarly, for staggered baryons with periodic boundary conditions, physical solutions with $x_m \leq -1$ are certainly expected as oscillating states moving to the left. Thus, in a single correlation function on a periodic lattice, there could be as many as four independently ordered sets of states distinguished by their properties under shift by one lattice spacing or time reversal symmetries, and these can be distinguished by the domain of their solutions: $x < -1, -1 < x < 0, 0 < x < 1, 1 < x$.

Generally speaking, model functions appropriate for the common lattice discretizations and choice of boundary conditions can be formulated and rewritten in the Vandermonde form of Eq. (3). The physical interpretation of the solutions x_m depends on the details of the discretization and boundary conditions. In some cases, all real solutions may have a physical interpretation and thus cannot be immediately discarded without further statistical analysis.

III. NUMERICAL RESULTS

Although the ground-state effective mass has a long tradition of use in the lattice QCD community, not much work has examined excited states and fewer yet their effective masses. In this section, we will demonstrate the application of these effective-mass techniques to some typical lattice correlation functions. At the end, we compare the results with the ones from variational method.

The data on which we demonstrate these methods is from a study done using the quenched approximation to QCD, *i.e.* where the effects of quantum fluctuations of quark-antiquark pairs in the vacuum are ignored, greatly reducing the computational cost but leading to an unknown, but hopefully small, systematic error. We generated an ensemble of $16^3 \times 64$ anisotropic lattices with Wilson gauge action and nonperturbative clover fermion action using Dirichlet boundary condition. The spatial lattice spacing a_s is about 0.125 fm with anisotropy 3 (that is, temporal spacing $a_t^{-1} \approx 6$ GeV). The parameters used in the fermion action give a 720-MeV pion. Specifically, our data are proton correlators using 7 Gaussian smearing parameters, 0.5–6.5 in steps of 1.0, including both smeared-point and smeared-smeared source-sink combinations. Fig. 2 shows the single-state effective-mass plots for these smeared-point proton correlators.

A. Excited-Effective Masses

We now apply the excited-effective masses to our nucleon data. In Fig. 3 we show the results of applying the single-correlator ($K = 1$) excited-effective masses to the nucleon data for all M with analytic solutions in terms of radicals. Notice that as the number of states included increases, the amount of early-time contamination is decreased. As the formulae better account for the exact form of the correlator, more of the time range can be reasonably used to determine the states. However, as the number of roots increases, the occurrence of "bad" roots (those that are negative or imaginary) tends to increase as well. Since these have to be thrown out, this causes gaps in the extracted states where the results are unreliable.

In Fig. 4 we show the results of applying the multiple correlator excited-effective masses to the nucleon data for all combinations of K and M that have solutions in terms of radicals. Notice that as the number of correlators

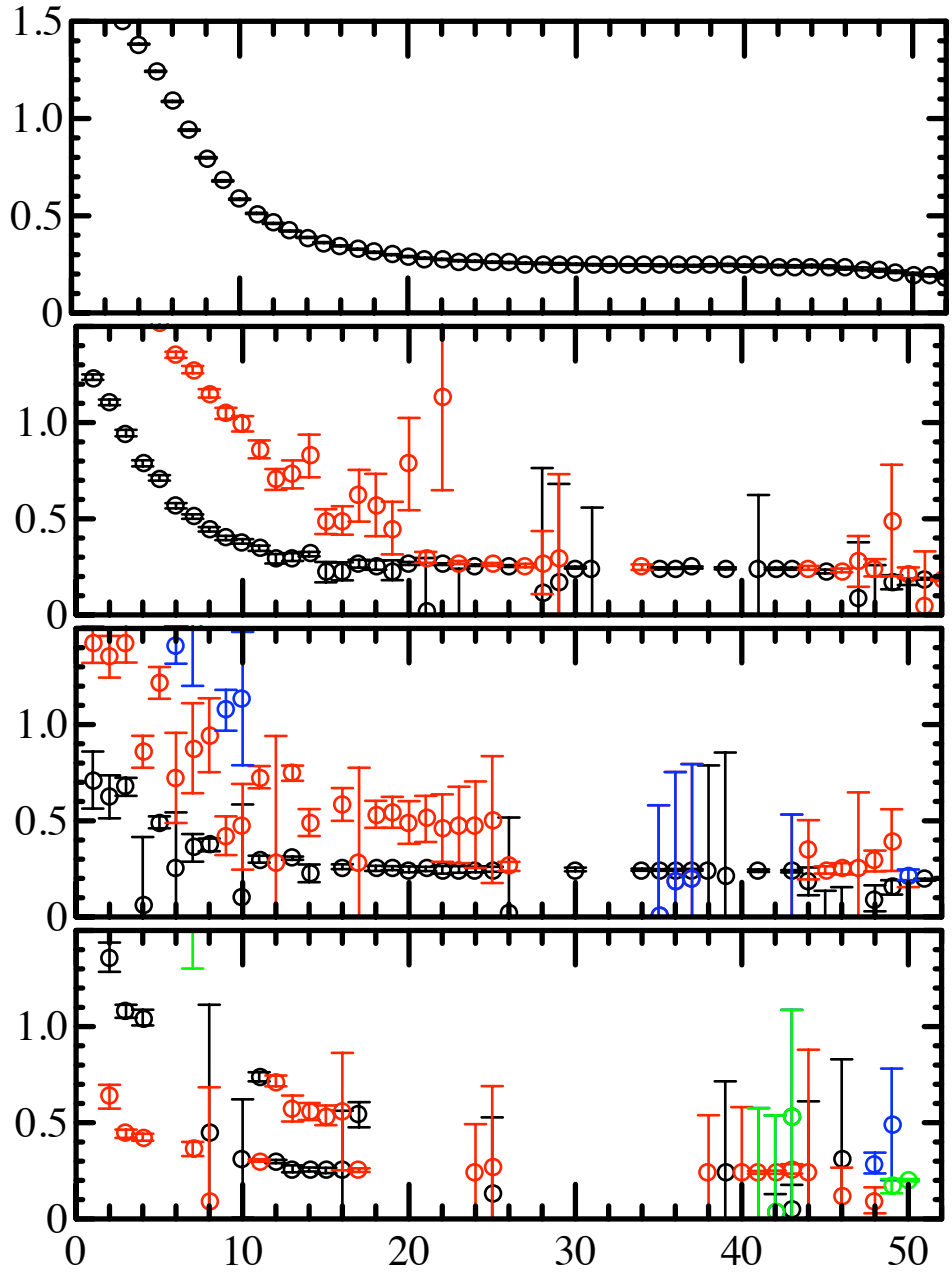

FIG. 3: Higher-effective mass plots with (top-to-bottom) one, two, three and four masses. The colors indicate the (black) ground, (red) first-excited, (blue) second-excited and (green) third-excited states.

increases, the quality of the extracted masses improves. The gaps in the data where bad roots appear become much less noticeable.

We demonstrate this approach using the smallest smearing parameter (0.5) smeared-point correlator. There are a few parameters in the linear prediction method which we can tune: the number of desired states L, the number of time slices used to predict the later time point N, and the order of the polynomial M. In this work, we will show a selection of the better choices in these degrees of freedom. Figure 5 shows the effective mass plot for $L = 2, 3, 4$ from a single Gaussian smeared-point correlator with fixed parameters $N = 20$ and $M = 8$. The excited states are consistent with each other as one increases the value of K. Since we have used a large value of N to form the polynomial, each point uses information extracted from 20 timeslices. Thus, one does not need a large plateau to determine the final mass. One also notes that since we only use a single correlator to extract multiple states, the multiple states

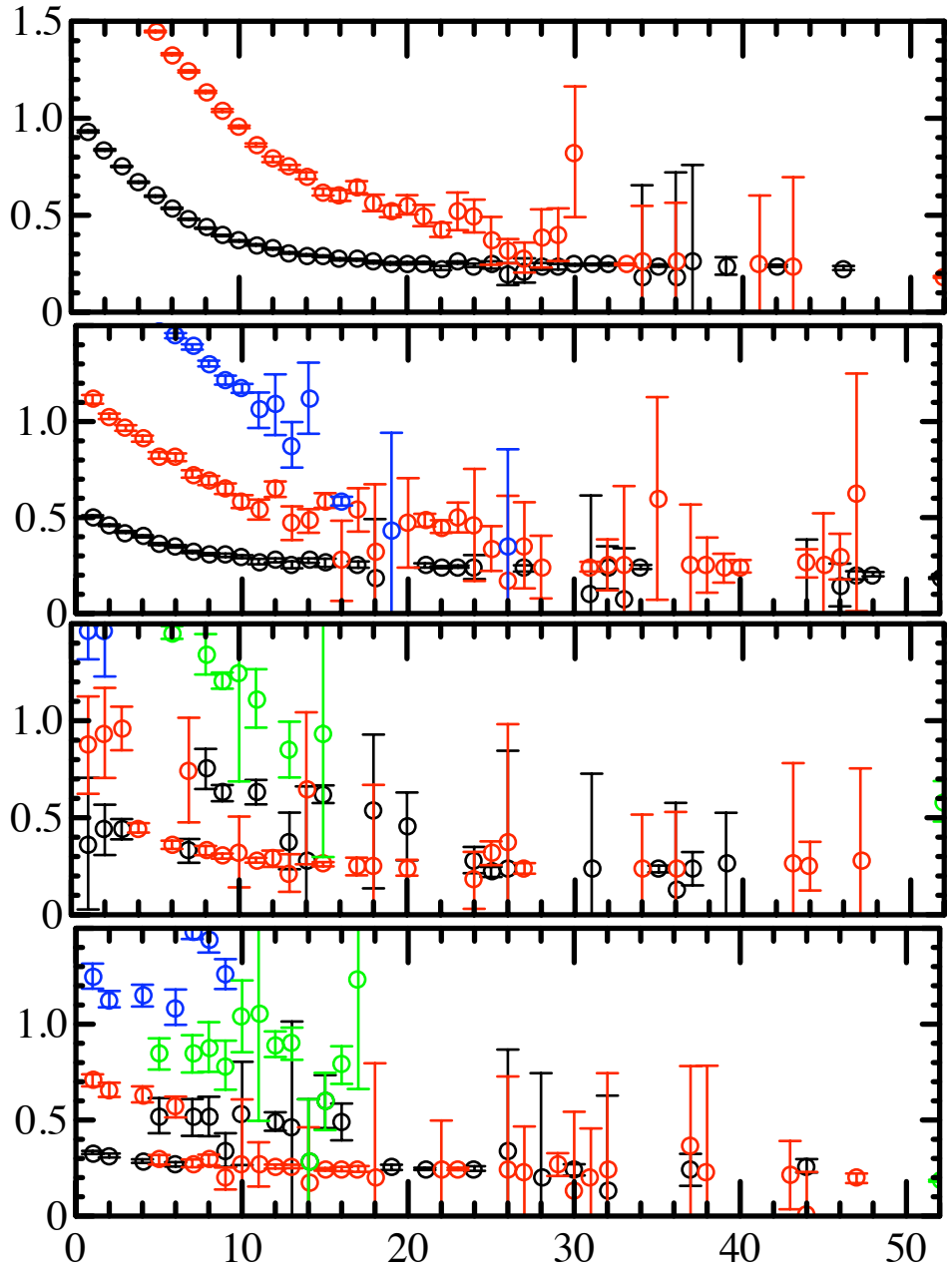

FIG. 4: Multiple-correlator higher-effective mass plots with (top-to-bottom) $\{K, M\}$ equal to $\{2, 2\}$, $\{3, 3\}$, $\{4, 2\}$ and $\{4, 4\}$. The colors indicate the (black) ground, (red) first-excited, (blue) second-excited and (green) third-excited states.

will be correlated; that is, large errors on higher-excited states will make the ground state noisy as well. A future improvement would naturally be to extend this approach to multiple correlators.

B. Variational Method

The variational method [23, 24] is a powerful tool for extracting multi-excited states in lattice QCD. We construct an $r \times r$ spectrum correlation matrix, $C_{ij}(t)$, where each element of the matrix is a correlator composed from different smeared sources or operators $\mathcal{O}_i$ and $\mathcal{O}_j$. Then we consider the generalized eigenvalue problem

$$C(t)\psi = \lambda(t, t_0)C(t_0)\psi, \tag{20}$$

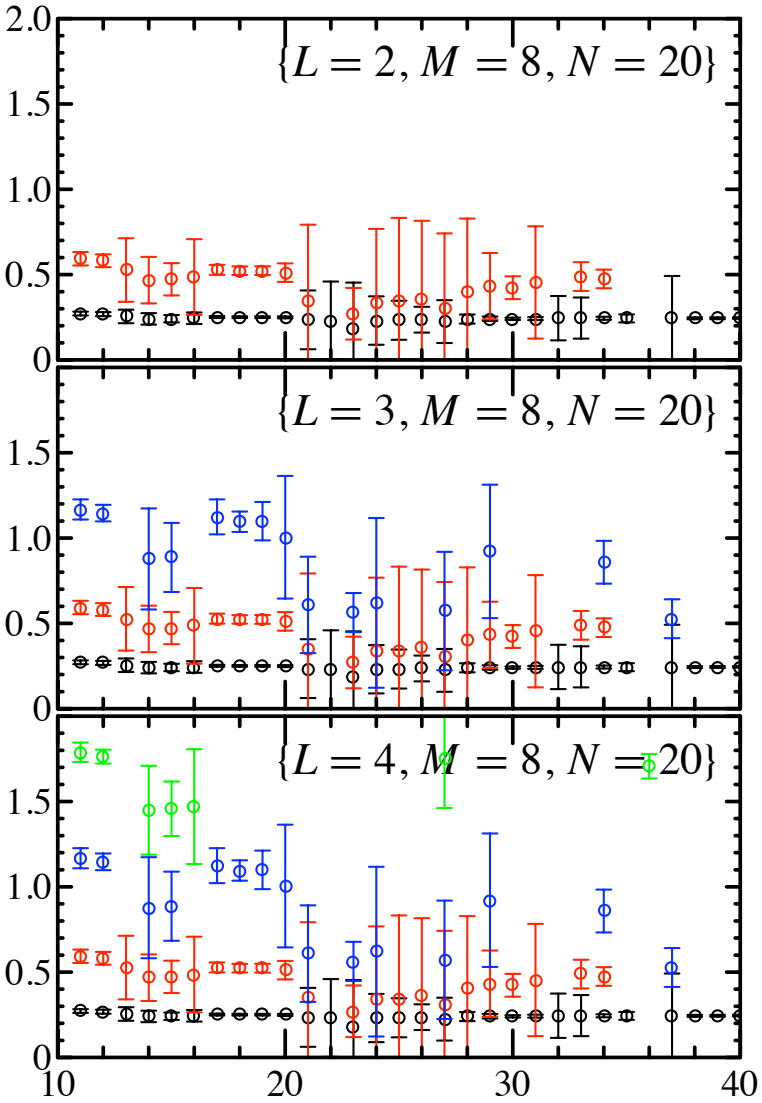

FIG. 5: Effective-mass plots from the linear prediction black-box method at fixed parameters $N = 20$ and $M = 8$. These results were obtained with a single smeared-point correlation function with smearing parameter 0.5.

where t_0 determines the range of validity of our extraction of the lowest r eigenstates. If t_0 is too large, the highest-lying states will have exponentially decreased too far to have good signal-to-noise ratio; if t_0 is too small, many states above the r we can determine will contaminate our extraction. Over some intermediate range in t_0, we should find consistent results.

If the eigenvectors for this system are $\mathbf{v}_n$, $= 1, \ldots, r$, and elements of the eigenvectors are v_{ni} then the correlation matrix can be approximated as

$$C_{ij} = \sum_{n=1}^{r} v_{ni}^* v_{nj} e^{-tE_n} \tag{21}$$

with eigenvalues

$$\lambda_n(t, t_0) = e^{-(t-t_0)E_n} \tag{22}$$

by solving

$$C(t_0)^{-1/2} C(t) C(t_0)^{-1/2} \psi = \lambda(t, t_0)\psi. \tag{23}$$

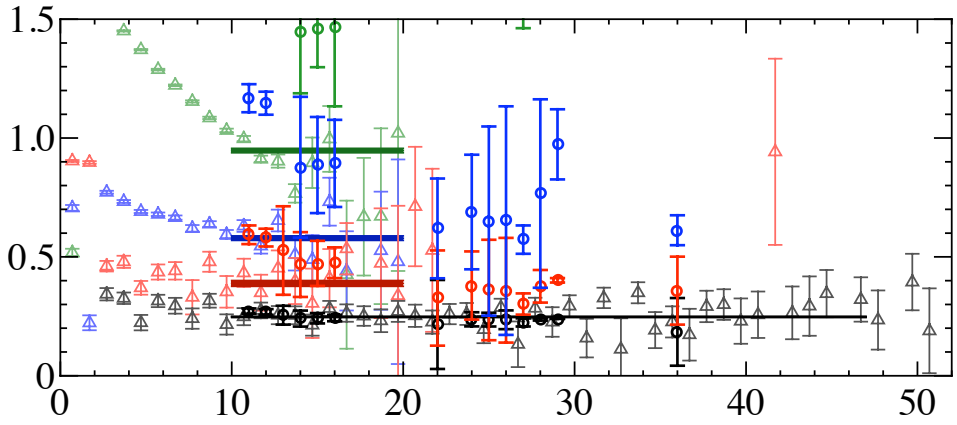

FIG. 6: Comparison between the 4×4 variational method (triangles) and linear prediction with 4 extracted states (circles). The linear prediction results are obtained from a single correlator, while the variational method uses 16 source-sink combinations. The lines indicate the best single-exponential fit to the variational results.

Further analysis on the principal correlators, $\lambda_n(t, t_0)$, reveals information on the energy levels, E_n.

The results from the linear prediction approach in Sec. II A are compared with the variational method (4×4 with smearing parameter ranging 0.5–3.5), as shown in Fig. 6. Here we shift time with respect to the linear prediction plot by 10 to have a better comparison with the plateau region from the variational method. For the ground state, the numbers are consistent with the result from the variational approach, including the size of the error bar. This is remarkable, given that the amount of input information is a factor of 16 less in the linear prediction approach. The first-excited state is consistent but has larger error bar, which is no surprise. As for the second-excited state, it seems to be consistent with the variational ones but definitely needs more statistics. The third-excited state is much larger than expected from the variational approach, which might be caused by contamination from even higher excited states.

IV. CONCLUSIONS

The determination of the physical properties of the excited-state hadrons is currently of great interest due to the construction of the 12 GeV upgrade at Jefferson Lab, where such properties will be measured experimentally. Lattice QCD methods have the potential to predict these properties, provided they can be extracted from the exponential time series, called correlation functions, computed in Monte Carlo simulations. In this work, we demonstrate a powerful, yet easy to use, black-box method for analyzing one or more correlation functions and extracting information about excited states. It can easily be adapted to various choices of boundary conditions and discretizations. While the method can be used by itself to estimate physical properties of excited hadrons, we anticipate that it will also be useful as a method for generating initial guesses for nonlinear least-squares minimizers.

Acknowledgments

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APPENDIX A: GENERAL EFFECTIVE MASS SOLUTION FOR $M = 2$, 3, AND 4

1. General solution for $M = 2$

To reduce the $M = 2$ problem, we pre-multiply by two factors of the bi-diagonal matrices of Eq. (4) to find the reduced equation $L_2 L_1 y = L_2 L_1 V a$. By introducing the auxiliary quantities:

$$\alpha_i = x_1 y_{i-1} - y_i \quad (2 \le i \le 2M) \tag{A1}$$
$$\beta_j = x_2 \alpha_{j-1} - \alpha_j \quad (3 \le j \le 2M) \tag{A2}$$

the reduced system becomes:

$$y_1 = a_1 + a_2 \tag{A3}$$
$$\alpha_2 = a_2 (x_1 - x_2) \tag{A4}$$
$$\beta_3 = 0 \tag{A5}$$
$$\beta_4 = 0 \tag{A6}$$

The first half of the equations, Eqs. (A3) and (A4), involve both the amplitudes A_1, A_2 and the energies E_1, E_2 but the second half involve only the energies. It will be true for any M, in general, that the last M equations can be solved first to find all the energies. Once all the energies are known, the first M equations form a square upper triangular system that can be solved efficiently by backward substitution to find the amplitudes.

To see that Eqs. (A3)–(A6) yield the known solution [28], first substitute Eq. (A2) and eliminate x_2 from Eqs. (A5)–(A6) to find

$$\alpha_2 \alpha_4 - \alpha_3^2 = 0, \quad \text{or} \quad \begin{vmatrix} \alpha_2 & \alpha_3 \\ \alpha_3 & \alpha_4 \end{vmatrix} = 0 \tag{A7}$$

where we note that the l.h.s. is the determinant of a 2×2 Hankel matrix or perhaps the minor of a larger Hankel matrix. After substituting Eq. (A1), this gives the known quadratic equation

$$\left(y_2^2 - y_1 y_3\right) x_1^2 + \left(y_1 y_4 - y_2 y_3\right) x_1 + \left(y_3^2 - y_2 y_4\right) = 0. \tag{A8}$$

Note that this can also be written

$$\begin{vmatrix} y_1 & y_2 \\ y_2 & y_3 \end{vmatrix} x_1^2 - \begin{vmatrix} y_1 & y_2 \\ y_3 & y_4 \end{vmatrix} x_1 + \begin{vmatrix} y_2 & y_3 \\ y_3 & y_4 \end{vmatrix} = 0 \tag{A9}$$

where the coefficients are not determinants of Hankel matrices but minors of a single Hankel matrix. So, it can be written even more compactly as

$$\left|\begin{array}{cc:c} y_1 & y_2 & 1 \\ y_2 & y_3 & x \\ \hdashline y_3 & y_4 & x^2 \end{array}\right| = 0 \tag{A10}$$

where the left block is a Hankel matrix and the right block is a Vandermonde matrix. Note that the choice to eliminate x_2 instead of x_1 in Eq. (A7) was arbitrary and making the opposite choice produces the same polynomial equation. Thus, in Eq. (A10) we use instead the generic variable x and the two solutions should be labeled x_1 and x_2.

2. General solution for $M = 3$

Using the auxiliary quantities defined in Eqs. (A1) and (A2) and a third auxiliary quantity:

$$\gamma_i = x_3 \beta_{i-1} - \beta_i \quad (4 \le i \le 2M) \tag{A11}$$

the reduced system of equations for $M = 3$ is:

$$\begin{aligned} y_1 &= a_1 + a_2 + a_3 && \text{(A12)} \\ \alpha_2 &= a_2\,(x_1 - x_2) + a_3\,(x_1 - x_3) && \text{(A13)} \\ \beta_3 &= a_3\,(x_2 - x_3)\,(x_1 - x_3) && \text{(A14)} \\ \gamma_4 &= 0 && \text{(A15)} \\ \gamma_5 &= 0 && \text{(A16)} \\ \gamma_6 &= 0 && \text{(A17)} \end{aligned}$$

Following the procedure of Sec. A 1, substitute Eq. (A11) into the last three equations to eliminate x_3 and find the (redundant) set of equations

$$\beta_3\beta_5 - \beta_4^2 = 0, \quad \beta_3\beta_6 - \beta_4\beta_5 = 0, \quad \beta_4\beta_5 - \beta_5^2 = 0 \tag{A18}$$

or equivalently

$$\begin{vmatrix} \beta_3 & \beta_4 \\ \beta_4 & \beta_5 \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_3 & \beta_4 \\ \beta_5 & \beta_6 \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_4 & \beta_5 \\ \beta_5 & \beta_6 \end{vmatrix} = 0. \tag{A19}$$

Note the l.h.s. of these three equations are the same as the three coefficients of Eq. (A8) after the substitution $y_i \to \beta_{i+2}$ and thus are minors of a Hankel matrix. Next, substitute Eq. (A2) into these equations to eliminate x_2 and find the equation

$$\alpha_2\alpha_4\alpha_6 + 2\alpha_3\alpha_4\alpha_5 - \alpha_4^3 - \alpha_3^2\alpha_6 - \alpha_2\alpha_5^2 = 0 \quad \text{or} \quad \begin{vmatrix} \alpha_2 & \alpha_3 & \alpha_4 \\ \alpha_3 & \alpha_4 & \alpha_5 \\ \alpha_4 & \alpha_5 & \alpha_6 \end{vmatrix} = 0. \tag{A20}$$

Finally, substituting Eq. (A1) will produce a cubic equation in x_1:

$$\begin{aligned} &Ax_1^3 + Bx_1^2 + Cx_1 + D = 0 && \text{(A21)} \\ &\quad A = y_3^3 - 2y_2y_3y_4 + y_1y_4^2 + y_2^2y_5 - y_1y_3y_5 \\ &\quad B = -y_3^2y_4 + y_2y_4^2 + y_2y_3y_5 - y_1y_4y_5 - y_2^2y_6 + y_1y_3y_6 \\ &\quad C = y_3y_4^2 - y_3^2y_5 - y_2y_4y_5 + y_1y_5^2 + y_2y_3y_6 - y_1y_4y_6 \\ &\quad D = -y_4^3 + 2y_3y_4y_5 - y_2y_5^2 - y_3^2y_6 + y_2y_4y_6. \end{aligned}$$

The coefficients A through D are minors of a Hankel matrix and so Eq. (A21) can also be written compactly as

$$\left|\begin{array}{cccc:c} y_1 & y_2 & y_3 & 1 \\ y_2 & y_3 & y_4 & x \\ y_3 & y_4 & y_5 & x^2 \\ y_4 & y_5 & y_6 & x^3 \end{array}\right| = 0. \tag{A22}$$

The cubic equation can be solved using the method of Scipione del Ferro and Tartaglia [48]. As before, Eq. (A22) gives the polynomial equation in terms of a generic variable x and the three solutions should be labeled $x_m, m = 1$–3.

3. General solution for $M = 4$

Defining a fourth auxiliary quantity:

$$\delta_i = x_4\gamma_{i-1} - \gamma_i \quad (5 \le i \le 2M) \tag{A23}$$

the reduced system of equations for $M = 4$ is:

$$\begin{aligned} y_1 &= a_1 + a_2 + a_3 + a_4 && \text{(A24)} \\ \alpha_2 &= a_2\,(x_1 - x_2) + a_3\,(x_1 - x_3) + a_4\,(x_1 - x_4) && \text{(A25)} \end{aligned}$$

$$\begin{aligned}
\beta_3 &= a_3\,(x_1-x_3)\,(x_2-x_3)+a_4\,(x_1-x_4)\,(x_2-x_4) && \text{(A26)}\\
\gamma_4 &= a_4\,(x_1-x_4)\,(x_2-x_4)\,(x_3-x_4) && \text{(A27)}\\
\delta_5 &= 0 && \text{(A28)}\\
\delta_6 &= 0 && \text{(A29)}\\
\delta_7 &= 0 && \text{(A30)}\\
\delta_8 &= 0 && \text{(A31)}
\end{aligned}$$

Following the now familiar procedure, substitute Eq. (A23) into the last four equations to eliminate x_4 and find the (redundant) set of equations:

$$\begin{aligned}
&\gamma_5^2-\gamma_4\gamma_6=0,\ \ \gamma_4\gamma_7-\gamma_5\gamma_6=0,\ \ \gamma_6^2-\gamma_5\gamma_7=0, \qquad \text{(A32)}\\
&\gamma_6^2-\gamma_4\gamma_8=0,\ \ \gamma_5\gamma_8-\gamma_6\gamma_7=0,\ \ \gamma_7^2-\gamma_6\gamma_8=0
\end{aligned}$$

or as minors of a Hankel matrix:

$$\begin{aligned}
&\begin{vmatrix}\gamma_4 & \gamma_5\\ \gamma_5 & \gamma_6\end{vmatrix}=0,\quad \begin{vmatrix}\gamma_4 & \gamma_5\\ \gamma_6 & \gamma_7\end{vmatrix}=0,\quad \begin{vmatrix}\gamma_5 & \gamma_6\\ \gamma_6 & \gamma_7\end{vmatrix}=0, \qquad \text{(A33)}\\
&\begin{vmatrix}\gamma_4 & \gamma_6\\ \gamma_6 & \gamma_8\end{vmatrix}=0,\quad \begin{vmatrix}\gamma_5 & \gamma_6\\ \gamma_7 & \gamma_8\end{vmatrix}=0,\quad \begin{vmatrix}\gamma_6 & \gamma_7\\ \gamma_7 & \gamma_8\end{vmatrix}=0.
\end{aligned}$$

Substitute Eq. (A11) and eliminate x_3 to find the next set of (redundant) set of equations:

$$\begin{aligned}
\beta_5^3-2\beta_4\beta_5\beta_6+\beta_3\beta_6^2+\beta_4^2\beta_7-\beta_3\beta_5\beta_7 &= 0 && \text{(A34)}\\
-\beta_5^2\beta_6+\beta_4\beta_6^2+\beta_4\beta_5\beta_7-\beta_3\beta_6\beta_7-\beta_4^2\beta_8+\beta_3\beta_5\beta_8 &= 0\\
\beta_5\beta_6^2-\beta_5^2\beta_7-\beta_4\beta_6\beta_7+\beta_3\beta_7^2+\beta_4\beta_5\beta_8-\beta_3\beta_6\beta_8 &= 0\\
-\beta_6^3+2\beta_5\beta_6\beta_7-\beta_4\beta_7^2-\beta_5^2\beta_8+\beta_4\beta_6\beta_8 &= 0
\end{aligned}$$

or as minors of a Hankel matrix:

$$\begin{vmatrix}\beta_3 & \beta_4 & \beta_5\\ \beta_4 & \beta_5 & \beta_6\\ \beta_5 & \beta_6 & \beta_7\end{vmatrix}=0,\quad \begin{vmatrix}\beta_3 & \beta_4 & \beta_5\\ \beta_4 & \beta_5 & \beta_6\\ \beta_6 & \beta_7 & \beta_8\end{vmatrix}=0,\quad \begin{vmatrix}\beta_3 & \beta_4 & \beta_5\\ \beta_5 & \beta_6 & \beta_7\\ \beta_6 & \beta_7 & \beta_8\end{vmatrix}=0,\quad \begin{vmatrix}\beta_4 & \beta_5 & \beta_6\\ \beta_5 & \beta_6 & \beta_7\\ \beta_6 & \beta_7 & \beta_8\end{vmatrix}=0. \qquad \text{(A35)}$$

Again, note that the LHS of these four equations are the same as the four coefficients of Eq. (A21) after the same substitution $y_i \to \beta_{i+2}$. Next, substitute Eq. (A2) and eliminate x_2 to find the equation

$$\begin{aligned}
&\alpha_5^4-3\alpha_4\alpha_6\alpha_5^2-2\alpha_3\alpha_7\alpha_5^2-\alpha_2\alpha_8\alpha_5^2+2\alpha_3\alpha_6^2\alpha_5+2\alpha_4^2\alpha_7\alpha_5 && \text{(A36)}\\
&\quad+2\alpha_2\alpha_6\alpha_7\alpha_5+2\alpha_3\alpha_4\alpha_8\alpha_5-\alpha_2\alpha_6^3+\alpha_4^2\alpha_6^2+\alpha_3^2\alpha_7^2\\
&\quad-\alpha_2\alpha_4\alpha_7^2-2\alpha_3\alpha_4\alpha_6\alpha_7-\alpha_4^3\alpha_8-\alpha_3^2\alpha_6\alpha_8+\alpha_2\alpha_4\alpha_6\alpha_8=0
\end{aligned}$$

As in Eqs. (A7) and (A20) the l.h.s. can be written as a determinant of a Hankel matrix of α_i's:

$$\begin{vmatrix}\alpha_2 & \alpha_3 & \alpha_4 & \alpha_5\\ \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6\\ \alpha_4 & \alpha_5 & \alpha_6 & \alpha_7\\ \alpha_5 & \alpha_6 & \alpha_7 & \alpha_8\end{vmatrix}=0. \qquad \text{(A37)}$$

Finally, substituting Eq. (A1) produces a quartic equation in x_1:

$$\begin{aligned}
&Ax_1^4+Bx_1^3+Cx_1^2+Dx_1+E=0 && \text{(A38)}\\
&A = y_4^4-3y_3y_5y_4^2-2y_2y_6y_4^2-y_1y_7y_4^2+2y_2y_5^2y_4+2y_3^2y_6y_4+2y_1y_5y_6y_4\\
&\quad+2y_2y_3y_7y_4-y_1y_5^3+y_3^2y_5^2+y_2^2y_6^2-y_1y_3y_6^2-2y_2y_3y_5y_6-y_3^3y_7\\
&\quad-y_2^2y_5y_7+y_1y_3y_5y_7\\
&B = y_8y_3^3-2y_5y_6y_3^2-y_4y_7y_3^2+2y_4y_5^2y_3+y_2y_6^2y_3+y_4^2y_6y_3+y_2y_5y_7y_3\\
&\quad+y_1y_6y_7y_3-2y_2y_4y_8y_3-y_1y_5y_8y_3-y_2y_5^3-y_1y_4y_6^2-y_4^3y_5\\
&\quad+y_1y_5^2y_6+y_2y_4^2y_7-y_1y_4y_5y_7-y_2^2y_6y_7+y_1y_4^2y_8+y_2^2y_5y_8
\end{aligned}$$

$$
\begin{aligned}
C =& -y_6y_4^3 + y_5^2y_4^2 + y_3y_7y_4^2 + y_2y_8y_4^2 + y_2y_6^2y_4 - 3y_2y_5y_7y_4 + y_1y_6y_7y_4 \\
&- y_3^2y_8y_4 - y_1y_5y_8y_4 - y_3y_5^3 - y_1y_5y_6^2 + y_2^2y_7^2 - y_1y_3y_7^2 + y_2y_5^2y_6 \\
&+ y_1y_5^2y_7 + y_3^2y_5y_7 - y_2y_3y_6y_7 + y_2y_3y_5y_8 - y_2^2y_6y_8 + y_1y_3y_6y_8 \\
D =& -y_7y_4^3 + 2y_5y_6y_4^2 + y_3y_8y_4^2 - y_5^3y_4 - 2y_3y_6^2y_4 + y_1y_7^2y_4 + y_2y_6y_7y_4 \\
&- y_2y_5y_8y_4 - y_1y_6y_8y_4 + y_1y_6^3 - y_2y_5y_6^2 - y_2y_3y_7^2 + y_3y_5^2y_6 + y_2y_5^2y_7 \\
&+ y_3^2y_6y_7 - 2y_1y_5y_6y_7 + y_1y_5^2y_8 - y_3^2y_5y_8 + y_2y_3y_6y_8 \\
E =& y_5^4 - 3y_4y_6y_5^2 - 2y_3y_7y_5^2 - y_2y_8y_5^2 + 2y_3y_6^2y_5 + 2y_4^2y_7y_5 + 2y_2y_6y_7y_5 \\
&+ 2y_3y_4y_8y_5 - y_2y_6^3 + y_4^2y_6^2 + y_3^2y_7^2 - y_2y_4y_7^2 - 2y_3y_4y_6y_7 - y_4^3y_8 \\
&- y_3^2y_6y_8 + y_2y_4y_6y_8
\end{aligned}
$$

As before, the coefficients A though E are minors of a Hankel matrix of y_n's, so this equation can be written:

$$
\left|\begin{array}{cccc:c}
y_1 & y_2 & y_3 & y_4 & 1 \\
y_2 & y_3 & y_4 & y_5 & x \\
y_3 & y_4 & y_5 & y_6 & x^2 \\
y_4 & y_5 & y_6 & y_7 & x^3 \\
y_5 & y_6 & y_7 & y_8 & x^4
\end{array}\right| = 0. \tag{A39}
$$

The quartic equation can be solved using the method of Ferrari [48]. As before, Eq. (A39) gives the polynomial equation in terms of a generic variable x and the four solutions should be labeled $x_m, m = 1$–4.

APPENDIX B: SOLUTION FOR EXAMPLES OF (K, M, N)

1. Solution for $(K, M, N) = (2, 2, 3)$

The nonlinear equations to solve have a block structure:

$$
\left[\begin{array}{c} y_{11} \\ y_{12} \\ y_{13} \\ \hline y_{21} \\ y_{22} \\ y_{23} \end{array}\right] = \left[\begin{array}{cc|cc} 1 & 1 & & \\ x_1 & x_2 & & \\ x_1^2 & x_2^2 & & \\ \hline & & 1 & 1 \\ & & x_1 & x_2 \\ & & x_1^2 & x_2^2 \end{array}\right] \left[\begin{array}{c} a_{11} \\ a_{12} \\ \hline a_{21} \\ a_{22} \end{array}\right] \tag{B1}
$$

Here, the indices for y_{kn}, x_m and a_{km} are in the ranges $1 \le k \le K$, $1 \le m \le M$ and $1 \le n \le N$. To reduce the system we extend Eq. (4) to block form with K identical blocks $L_m(x)$ on the diagonal. The reduced equations are

$$
\begin{aligned}
y_{k1} &= a_{k1} + a_{k2} && \text{(B2)} \\
\alpha_{k2} &= (x_1 - x_2)\, a_{k2} && \text{(B3)} \\
\beta_{k3} &= 0 && \text{(B4)} \\
& (1 \le k \le 2)
\end{aligned}
$$

where we have added an additional index k to the auxiliary quantities defined in Eqs. (A1) and (A2). Substituting for β_{k3} in Eqs. (B4) and eliminating x_2 gives the equation:

$$
\left|\begin{array}{cc} \alpha_{12} & \alpha_{22} \\ \alpha_{13} & \alpha_{23} \end{array}\right| = 0, \tag{B5}
$$

where we've written the equation as a minor of some matrix, following our experience in Appendix A, yet whose structure is not yet clear. Substituting for α_{kn} gives a quadratic equation in x in determinant form:

$$
\left|\begin{array}{cc:c} y_{11} & y_{21} & 1 \\ y_{12} & y_{22} & x \\ y_{13} & y_{23} & x^2 \end{array}\right| = 0. \tag{B6}
$$

As before, Eq. (B6) gives the polynomial equation in terms of a generic variable x and the two solutions should be labeled $x_m, m = 1$–2.

2. Solution for $(K, M, N) = (2, 4, 6)$

The reduced system of equations for $K = 2$ correlation functions measured on $N = 6$ equally spaced time slices to be solved to extract model parameters for $M = 4$ states is:

$$\begin{aligned} y_{k1} &= a_{k1} + a_{k2} + a_{k3} + a_{k4} && \text{(B7)}\\ \alpha_{k2} &= a_{k2}\,(x_1 - x_2) + a_{k3}\,(x_1 - x_3) + a_{k4}\,(x_1 - x_4) && \text{(B8)}\\ \beta_{k3} &= a_{k3}\,(x_1 - x_3)\,(x_2 - x_3) + a_{k4}\,(x_1 - x_4)\,(x_2 - x_4) && \text{(B9)}\\ \gamma_{k4} &= a_{k4}\,(x_1 - x_4)\,(x_2 - x_4)\,(x_3 - x_4) && \text{(B10)}\\ \delta_{k5} &= 0 && \text{(B11)}\\ \delta_{k6} &= 0 && \text{(B12)}\\ & \qquad (1 \le k \le 2) \end{aligned}$$

Substituting for δ_{kn} and eliminating x_4 gives a set of equations in γ_{kn}:

$$\begin{vmatrix} \gamma_{14} & \gamma_{24} \\ \gamma_{15} & \gamma_{25} \end{vmatrix} = 0, \quad \begin{vmatrix} \gamma_{14} & \gamma_{25} \\ \gamma_{15} & \gamma_{26} \end{vmatrix} = 0, \quad \begin{vmatrix} \gamma_{15} & \gamma_{24} \\ \gamma_{16} & \gamma_{25} \end{vmatrix} = 0, \qquad \text{(B13)}$$
$$\begin{vmatrix} \gamma_{15} & \gamma_{25} \\ \gamma_{16} & \gamma_{26} \end{vmatrix} = 0, \quad \begin{vmatrix} \gamma_{14} & \gamma_{15} \\ \gamma_{15} & \gamma_{16} \end{vmatrix} = 0, \quad \begin{vmatrix} \gamma_{24} & \gamma_{25} \\ \gamma_{25} & \gamma_{26} \end{vmatrix} = 0.$$

Substituting for γ_{kn} and eliminating x_3 gives a set of equations in β_{kn}:

$$\begin{vmatrix} \beta_{13} & \beta_{14} & \beta_{23} \\ \beta_{14} & \beta_{15} & \beta_{24} \\ \beta_{15} & \beta_{16} & \beta_{25} \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_{13} & \beta_{14} & \beta_{24} \\ \beta_{14} & \beta_{15} & \beta_{25} \\ \beta_{15} & \beta_{16} & \beta_{26} \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_{13} & \beta_{23} & \beta_{24} \\ \beta_{14} & \beta_{24} & \beta_{25} \\ \beta_{15} & \beta_{25} & \beta_{26} \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_{14} & \beta_{23} & \beta_{24} \\ \beta_{15} & \beta_{24} & \beta_{25} \\ \beta_{16} & \beta_{25} & \beta_{26} \end{vmatrix} = 0. \qquad \text{(B14)}$$

Substituting for β_{kn} and eliminating x_2 gives an equation in α_{kn}:

$$\begin{vmatrix} \alpha_{12} & \alpha_{13} & \alpha_{22} & \alpha_{23} \\ \alpha_{13} & \alpha_{14} & \alpha_{23} & \alpha_{24} \\ \alpha_{14} & \alpha_{15} & \alpha_{24} & \alpha_{25} \\ \alpha_{15} & \alpha_{16} & \alpha_{25} & \alpha_{26} \end{vmatrix} = 0 \qquad \text{(B15)}$$

Substituting for α_{kn} gives a quartic equation in x:

$$\left|\begin{array}{cccc:c} y_{11} & y_{12} & y_{21} & y_{22} & 1 \\ y_{12} & y_{13} & y_{22} & y_{23} & x \\ y_{13} & y_{14} & y_{23} & y_{24} & x^2 \\ y_{14} & y_{15} & y_{24} & y_{25} & x^3 \\ y_{15} & y_{16} & y_{25} & y_{26} & x^4 \end{array}\right| = 0. \qquad \text{(B16)}$$

As before, Eq. (B16) gives the polynomial equation in terms of a generic variable x and the four solutions should be labeled $x_m, m = 1$–4.

3. Solution for (K,M,N) = (3,3,4)

The reduced system of equations for $K = 3$ correlation functions measured on $N = 4$ equally spaced time slices to be solved to extract model parameters for $M = 3$ states is:

$$y_{k1} = a_{k1} + a_{k2} + a_{k3} \qquad \text{(B17)}$$

$$\alpha_{k2} = a_{k2}(x_1 - x_2) + a_{k3}(x_1 - x_3) \quad \text{(B18)}$$
$$\beta_{k3} = a_{k3}(x_1 - x_3)(x_2 - x_3) \quad \text{(B19)}$$
$$\gamma_{k4} = 0 \quad \text{(B20)}$$
$$(1 \le k \le 3)$$

Substituting for γ_{k4} and eliminating x_3 gives a set of equations in β_{kn}:

$$\begin{vmatrix} \beta_{13} & \beta_{23} \\ \beta_{14} & \beta_{24} \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_{13} & \beta_{33} \\ \beta_{14} & \beta_{34} \end{vmatrix} = 0, \quad \begin{vmatrix} \beta_{23} & \beta_{33} \\ \beta_{24} & \beta_{34} \end{vmatrix} = 0. \quad \text{(B21)}$$

Substituting for β_{kn} and eliminating x_2 gives an equation in α_{kn}:

$$\begin{vmatrix} \alpha_{12} & \alpha_{22} & \alpha_{32} \\ \alpha_{13} & \alpha_{23} & \alpha_{33} \\ \alpha_{14} & \alpha_{24} & \alpha_{34} \end{vmatrix} = 0. \quad \text{(B22)}$$

Substituting for α_{kn} gives a cubic equation in x:

$$\begin{vmatrix} y_{11} & y_{21} & y_{31} & 1 \\ y_{12} & y_{22} & y_{32} & x \\ y_{13} & y_{23} & y_{33} & x^2 \\ y_{14} & y_{24} & y_{34} & x^3 \end{vmatrix} = 0. \quad \text{(B23)}$$

As before, Eq. (B23) gives the polynomial equation in terms of a generic variable x and the three solutions should be labeled $x_m, m = 1$–3.

4. Solution for $(K, M, N) = (4, 4, 5)$

The reduced system of equations for $K = 4$ correlation functions measured on $N = 5$ equally spaced time slices to be solved to extract model parameters for $M = 4$ states is:

$$y_{k1} = a_{k1} + a_{k2} + a_{k3} + a_{k4} \quad \text{(B24)}$$
$$\alpha_{k2} = a_{k2}(x_1 - x_2) + a_{k3}(x_1 - x_3) + a_{k4}(x_1 - x_4) \quad \text{(B25)}$$
$$\beta_{k3} = a_{k3}(x_1 - x_3)(x_2 - x_3) + a_{k4}(x_1 - x_4)(x_2 - x_4) \quad \text{(B26)}$$
$$\gamma_{k4} = a_{k4}(x_1 - x_4)(x_2 - x_4)(x_3 - x_4) \quad \text{(B27)}$$
$$\delta_{k5} = 0 \quad \text{(B28)}$$
$$(1 \le k \le 4)$$

The determinant form of the quartic equation in x is

$$\begin{vmatrix} y_{11} & y_{21} & y_{31} & y_{41} & 1 \\ y_{12} & y_{22} & y_{32} & y_{42} & x \\ y_{13} & y_{23} & y_{33} & y_{43} & x^2 \\ y_{14} & y_{24} & y_{34} & y_{44} & x^3 \\ y_{15} & y_{25} & y_{35} & y_{45} & x^4 \end{vmatrix} = 0. \quad \text{(B29)}$$

As before, Eq. (B29) gives the polynomial equation in terms of a generic variable x and the four solutions should be labeled $x_m, m = 1$–4.

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