

Third moments of nucleon unpolarized, polarized, and transversity parton distribution functions from physical-point lattice QCD

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Using forward matrix elements of local leading-twist operators, we present a determination of the isovector third Mellin moments $\langle x^2 \rangle$ of nucleon unpolarized, polarized, and transversity parton distribution functions. Two lattice QCD ensembles at the physical pion mass are used, which were generated using a tree-level Symanzik-improved gauge action and $2 + 1$ flavor tree-level improved Wilson clover fermions coupling via two-level HEX smearing. Leveraging a wide set of operators, two extraction methods for the matrix elements, and the automatic inclusion of model uncertainties via bootstrapped model averages, we extract values of the third Mellin moments. This is the first direct calculation of these observables performed at the physical pion mass.

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I. INTRODUCTION

Knowledge of parton distribution functions (PDFs) is crucial for making theoretical predictions and interpreting the results of high-energy-physics experiments at hadron colliders. For this reason, several experimental groups have focused on extracting PDFs from global fits of collider data [1–7]. Numerous efforts also come from the lattice QCD community [8–10]. Although a complete determination of PDFs is not possible using the standard tools of Euclidean lattice QCD, a first-principles computation can determine the values of the four first Mellin moments of PDFs. Such a calculation provides useful constraints on the global fits of experimental data. The first [11–37] and second [19,28,35,38–51] isovector Mellin moments have been calculated with high precision in the past, and both

quantities appear in the most recent FLAG review [52]. However, the same level of precision has not yet been achieved for the isovector third Mellin moments.

Direct computations of the isovector third Mellin moments using dynamical fermions have been performed in earlier studies. In recent years, Ref. [53] computed $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+}$ using a subset of the CLS ensembles [54]. The next most recent direct calculation was from 2010 [46], which computed $\langle x^2 \rangle_{u^- - d^-}$ and $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+}$ using $2 + 1$ flavors of staggered sea quarks and domain wall valence quarks. References [55,56] computed $\langle x^2 \rangle_{u^- - d^-}$ using two flavors of clover quarks and two flavors of Wilson quarks, respectively. Reference [57] computed $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+}$ using two flavors of clover quarks and using a nonperturbative renormalization scheme. No previous direct computations of $\langle x^2 \rangle_{\delta u^- - \delta d^-}$ are available, making ours, to the best of our knowledge, the first direct calculation of the isovector third transversity Mellin moment. For a broader overview of prior results, we refer the reader to Table B.10 of Ref. [8].

This work builds upon the techniques employed in [41] for the calculation of the isovector second Mellin moments $\langle x \rangle$. We provide a determination of the isovector third

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Mellin moments $\langle x^2 \rangle$ of unpolarized, polarized, and transversity PDFs. To achieve this, we extract matrix elements at finite momentum for a large number of local twist-two operators. Notably, using nonzero values of momentum is essential in this case, because the operators required to extract the third Mellin moments have vanishing matrix elements at zero momentum. We observed that the amount of excited-state contamination varies significantly among the different operators and momenta employed. Given the large number of operators involved, we developed a procedure to perform a model average automatically in order to accurately extract the matrix elements from all the available data.

Our approach, based on local twist-two operators, is limited to the computation of the first four Mellin moments. For higher moments, power-divergent mixing arises and the same methodology cannot be applied anymore. To overcome this issue, novel methods have been developed. In recent years, these methods have successfully been used to compute Mellin moments. In Refs. [58,59], leveraging the technique of gradient flow [60], the first five Mellin moments for the pion have been computed. Reference [61] computed the fourth Mellin moment for the pion and demonstrated that the heavy-quark operator product expansion method is a viable approach to the study of higher Mellin moments. Using quasi-PDF or pseudo-PDF approaches [62], the first few Mellin moments of the proton have been computed for unpolarized [63–65], polarized [63,65,66], and transversity [63,67–69] PDFs. Except for the gradient flow method, these new methodologies rely on kinematic suppression of higher-twist effects, which is not an issue in the approach we use. More importantly, these new methodologies are not affected by power-divergent mixing. Thus, they are expected to play a central role in future first-principle investigations of PDFs. We then hope that the determination of the isovector third Mellin moments reported in this work can prove to be a useful quantity in the future to assess the compatibility of different lattice QCD calculations.

The rest of the paper is divided into the following sections. In Sec. II, we explain the methodology utilized for the determination of the Mellin moments from lattice data. In Sec. III, we present the available data, and we discuss the extraction of the moment for a subset of all the available operators. In Sec. IV, we summarize the results we obtained and we provide a final estimate for the values of the isovector third Mellin moments. A summary of the current work is provided in Sec. V. Technical details are located in the Appendixes: Appendix A explains in detail how the operators utilized in the analysis were chosen; Appendix B contains the intermediate results for each single operator; Appendix C focuses on the technical details of the model-averaging procedure we used; Appendix D presents the calculation of the renormalization

factors; and Appendix E contains a functional-form study of the continuum estimate.

II. METHODOLOGY

A. Choice of operators

In order to compute third Mellin moments of PDFs, we consider forward matrix elements of local operators of the following kind:

$$\mathcal{O}_{\alpha,\mu,\nu}^X(q) = \bar{q} \Gamma_{\alpha}^X \overleftrightarrow{D}_{\mu} \overleftrightarrow{D}_{\nu} q, \quad X = V, A, T. \quad (1)$$

The moments corresponding to unpolarized, polarized, and transversity PDFs are associated, respectively, with the vector, axial, and tensorial channels, which we distinguish by the use of the symbol $X = V, A, T$. More specifically, this means that the Dirac structure Γ_{α}^X , is given by γ_{α} , $\gamma_{\alpha}\gamma_5$, and $\sigma_{\alpha_1\alpha_2} = i/2[\gamma_{\alpha_1}, \gamma_{\alpha_2}]$, respectively, for the three possible channels (in the tensorial case, α is a compound index). To make sure that our operators have definite transformation properties under charge conjugation, we make use of the forward-backward acting covariant derivative $\overleftrightarrow{D} = \frac{1}{2}(\vec{D} - \overleftarrow{D})$, implemented on the lattice by means of a symmetric finite difference scheme. Furthermore, in order to deal only with connected diagrams, we consider the flavor combination corresponding to the isovector channel. Thus, we look at the difference between operators with up and down quarks, $\mathcal{O}_{\alpha,\mu,\nu}^X(q=u) - \mathcal{O}_{\alpha,\mu,\nu}^X(q=d) \equiv \mathcal{O}_{\alpha,\mu,\nu}^X$.

The particular definition given in Eq. (1) comes from continuum physics. On the lattice, the operators defined in (1) form a closed set under the group of lattice symmetries, the hypercubic group $H(4)$. In order to obtain results that renormalize multiplicatively, we have to select operators that belong to irreducible representations (irreps) of $H(4)$ where mixing with lower- or equal-dimensional operators does not occur. After identifying these irreps, we were able to obtain an explicit expression for the operators, forming them by means of the group-theoretical recipe given in [70] and the matrix representations for the generators of $H(4)$ provided in [71]. The operators we obtained are specific combinations of operators of the form (1). They have been classified according to their trace condition, index symmetry, and charge-conjugation parity, and they match exactly those provided in [72]; more details on this matter can be found in Appendix A. Adopting the common notation, and denoting the a th b -dimensional irrep of $H(4)$ with the symbol $\tau_a^{(b)}$, we can now list the operators we have selected for our analysis together with the irrep they belong to. For the unpolarized (V) and polarized (A) case, there is only one irrep for each case that is not affected by mixing, so the available operators for these two channels are

$$\begin{aligned}
V1. \quad \tau_2^{(4)} \quad O_{\{2,3,4\}}^V, & \quad A1. \quad \tau_3^{(4)} \quad O_{\{2,3,4\}}^A, \\
V2. \quad \tau_2^{(4)} \quad O_{\{1,3,4\}}^V, & \quad A2. \quad \tau_3^{(4)} \quad O_{\{1,3,4\}}^A, \\
V3. \quad \tau_2^{(4)} \quad O_{\{1,2,4\}}^V, & \quad A3. \quad \tau_3^{(4)} \quad O_{\{1,2,4\}}^A, \\
V4. \quad \tau_2^{(4)} \quad O_{\{1,2,3\}}^V, & \quad A4. \quad \tau_3^{(4)} \quad O_{\{1,2,3\}}^A,
\end{aligned} \tag{2}$$

where with the curly brackets $\{\dots\}$ we have denoted the symmetrization of the indices. For the transversity (T) case, three different irreps are free of mixing effects, and the operators we can use are

$$\begin{aligned}
T1. \quad \tau_2^{(3)} \quad 2O_{1,2,\{3,4\}}^T + O_{1,3,\{2,4\}}^T + O_{1,4,\{2,3\}}^T - O_{2,3,\{1,4\}}^T - O_{2,4,\{1,3\}}^T, \\
T2. \quad \tau_3^{(3)} \quad O_{1,2,\{1,2\}}^T - O_{1,3,\{1,3\}}^T + O_{2,3,\{2,3\}}^T, \\
T3. \quad \tau_3^{(3)} \quad 2O_{1,2,\{1,2\}}^T + O_{1,3,\{1,3\}}^T - 3O_{1,4,\{1,4\}}^T - O_{2,3,\{2,3\}}^T + 3O_{2,4,\{2,4\}}^T, \\
T4. \quad \tau_2^{(6)} \quad O_{1,3,\{1,4\}}^T + O_{1,4,\{1,3\}}^T - O_{2,3,\{2,4\}}^T - O_{2,4,\{2,3\}}^T, \\
T5. \quad \tau_2^{(6)} \quad O_{1,2,\{1,4\}}^T + O_{1,4,\{1,2\}}^T + O_{2,3,\{3,4\}}^T - O_{3,4,\{2,3\}}^T, \\
T6. \quad \tau_2^{(6)} \quad O_{1,2,\{2,4\}}^T - O_{1,3,\{3,4\}}^T - O_{2,4,\{1,2\}}^T + O_{3,4,\{1,3\}}^T, \\
T7. \quad \tau_2^{(6)} \quad O_{1,2,\{1,3\}}^T + O_{1,3,\{1,2\}}^T + O_{2,4,\{3,4\}}^T + O_{3,4,\{2,4\}}^T, \\
T8. \quad \tau_2^{(6)} \quad O_{1,2,\{2,3\}}^T - O_{1,4,\{3,4\}}^T - O_{2,3,\{1,2\}}^T - O_{3,4,\{1,4\}}^T, \\
T9. \quad \tau_2^{(6)} \quad O_{1,3,\{2,3\}}^T - O_{1,4,\{2,4\}}^T + O_{2,3,\{1,3\}}^T - O_{2,4,\{1,4\}}^T.
\end{aligned} \tag{3}$$

As we will explain in more detail in a moment, the operators we have selected all have a nonzero kinematic factor and hence also a nonzero matrix element, for at least one of the two momenta available.

Regarding the renormalization, given what we have said before, it is multiplicative and each irrep has its own renormalization factor $Z_a^{(b)}$. Details regarding the computation of the renormalization factors can be found in Appendix D. From now on, we will use the shorthand notation $\mathcal{O}^X$ to denote one of the operators in Eqs. (2) and (3) and Z_{DDX}^ρ to denote the related renormalization factor, with ρ being the relevant irrep of $H(4)$.

B. Matrix elements

Our focus is the forward matrix elements of the selected operators between nucleon states $N(p, \lambda)$, where p is the 4-momentum of the nucleon and λ its spin. As is known [56,73–78], these matrix elements are related to the third Mellin moments $\langle x^2 \rangle$ by the following expression:

$$\langle N(p, \lambda) | \mathcal{S} \mathcal{O}_{\alpha, \mu, \nu}^X | N(p, \lambda') \rangle = \langle x^2 \rangle \bar{u}_{N(p, \lambda)} \mathcal{S} \Gamma_\alpha^X i p_\mu i p_\nu u_{N(p, \lambda')}, \tag{4}$$

where $\mathcal{S}$, formally defined in Appendix D, selects the twist-2 part of the operators by taking the symmetric traceless

combination; symmetrization and trace subtraction leave the operators in Eqs. (2) and (3) unchanged. The established method to extract these matrix elements from lattice data relies on the computation of the ratios of three- and two-point correlation functions [79,80]. In our case, the relevant correlation functions are given by

$$C_{2\text{pt}}(t) = \int d^3\vec{y} e^{-i\vec{p}\cdot\vec{y}} \text{Tr}\{\Gamma_{\text{pol}} \langle \chi(\vec{y}, t) \bar{\chi}(\vec{0}, 0) \rangle\}, \tag{5}$$

$$\begin{aligned}
C_{3\text{pt}}^{\mathcal{O}^X}(t, \tau) = \int d^3\vec{y} d^3\vec{z} [e^{-i\vec{p}'\cdot\vec{y}} e^{i(\vec{p}' - \vec{p})\cdot\vec{z}} \\
\times \text{Tr}\{\Gamma_{\text{pol}} \langle \chi(\vec{y}, t) \mathcal{O}^X(\vec{z}, \tau) \bar{\chi}(\vec{0}, 0) \rangle\}]. \tag{6}
\end{aligned}$$

In the above expressions, $\vec{p}$ and $\vec{p}'$ are, respectively, the momentum at the source and at the sink, $\Gamma_{\text{pol}} = P_+[1 - i\gamma_1\gamma_2]$, with $P_+ = (1 + \gamma_4)/2$, is the polarization matrix we use, and χ is a nucleon interpolating operator, whose explicit expression is

$$\chi_\alpha = \epsilon_{abc} (\bar{u}_a^T C \gamma_5 P_+ \tilde{d}_b) \tilde{u}_{c,\alpha}, \tag{7}$$

where $\tilde{u}$ and $\tilde{d}$ are smeared quark fields. As is clear from Eq. (4), we are interested in forward matrix elements, so in the following we will consider the case $\vec{p} = \vec{p}'$ only.

The ratio of three- and two-point correlation functions is defined as

$$R^{\mathcal{O}^X}(t, \tau) \equiv \frac{C_{3\text{pt}}^{\mathcal{O}^X}(t, \tau)}{C_{2\text{pt}}(t)}. \quad (8)$$

The matrix element is obtained as the following limit of the ratio

$$\mathcal{M}^{\mathcal{O}^X} \equiv \lim_{t \rightarrow \tau, \tau \rightarrow \infty} R^{\mathcal{O}^X}(t, \tau). \quad (9)$$

The associated kinematic factor is derived from the ground-state contribution to the ratio. Its expression is given by

$$K^{\mathcal{O}^X}(p) = -\frac{1}{2E_N(p)} \frac{\text{Tr}\{\Gamma_{\text{pol}}(-i\not{p} + m_N)[C_{a\mu\nu}^{\mathcal{O}^X}\Gamma_a^X p_\mu p_\nu](-i\not{p} + m_N)\}}{\text{Tr}\{\Gamma_{\text{pol}}(-i\not{p} + m_N)\}}. \quad (10)$$

In this expression, $E_N(p)$ is the energy of the nucleon state, m_N is its mass, and $C_{a\mu\nu}^{\mathcal{O}^X}$ are the Clebsch-Gordan coefficients needed to take the appropriate combination of operators of the form (1) such that the final result renormalizes multiplicatively. These coefficients can easily be read from Eqs. (2) and (3), and in the context of this work they have been generated starting from an explicit matrix representation of the generators of $H(4)$; more details on this matter are available in Appendix A. As previously noted, the operators selected for this study are such that the corresponding kinematic factors, calculated using Eq. (10), are nonzero for at least one of the two available momenta.

The matrix element and the kinematic factor are the two ingredients needed to compute the third Mellin moments. The relation between them is given by

$$\mathcal{M} = \langle x^2 \rangle K. \quad (11)$$

The kinematic factor can easily be computed using Eq. (10). The matrix element instead has to be extracted from data. This extraction can be performed in two different ways.

The first way (referred to below as method 2 for consistency with Ref. [41]) relies on the spectral decomposition of the ratio. If we perform the decomposition up to the first excited state, and neglect terms that decay more rapidly than $e^{-t\Delta E}$, we can then rewrite the ratio in the following way:

$$R^{\mathcal{O}^X}(t, \tau) = \mathcal{M}^{\mathcal{O}^X} + R_1 e^{-\frac{t}{2}\Delta E} \cosh\left[\left(\frac{t}{2} - \tau\right)\Delta E\right] + R_2 e^{-t\Delta E}, \quad (12)$$

where $\Delta E = E_1 - E_0$ is the energy difference between the first excited state and the ground state, and the parameters R_1 and R_2 describe the amount of excited-state contamination. These three parameters depend on the specific operator $\mathcal{O}^X$ that has been chosen, and the superscript has been omitted for the sake of readability. By calculating

the ratio of the correlators, and then fitting it to Eq. (12), it is possible to extract the matrix element related to the operator under consideration.

From this fit, one could also extract the energy gap ΔE . However, the right-hand side of Eq. (12) is a truncated sum. The exponentials in its expression effectively approximate contributions from multiple excited states around the first finite-volume energy level. Hence, the fitted energy gap will not equal, in general, the true energy difference between the ground state and first excited state.

A second approach to the matrix-element extraction (referred to below as method 1) revolves around the computation of the summed ratio

$$S^{\mathcal{O}^X}(t, \tau_{\text{skip}}) \equiv a \sum_{\tau=\tau_{\text{skip}}}^{t-\tau_{\text{skip}}} R^{\mathcal{O}^X}(t, \tau) = \mathcal{M}^{\mathcal{O}^X} \times (t + a - 2\tau_{\text{skip}}) + \text{excited states}. \quad (13)$$

The summed ratio has an excited-state contamination that is exponentially suppressed with $t\Delta E$, while instead for the ratio the suppression goes with $t\Delta E/2$ [81,82]. The parameter τ_{skip}/a represents the number of time values we skip around the source and the sink. Neglecting the excited-state contamination, and fixing the value τ_{skip} , we can parametrize the summed ratio as a linear function in the values of the source-sink separation t ,

$$S^{\mathcal{O}^X}(t, \tau_{\text{skip}}) = \mathcal{M}^{\mathcal{O}^X} \times t + \text{const}. \quad (14)$$

The matrix element can then be extracted as the slope from a linear fit.

C. Data analysis

A complete description of the data analysis procedure is given here. Furthermore, the steps of the extraction of the third Mellin moments for the unpolarized, polarized, and transversity channels are explained.

- (1) The first step is the choice of the appropriate operators. As previously discussed, we have chosen

the operators given in Eqs. (2) and (3). It is worth reiterating that these operators all possess a nonzero kinematic factor for at least one of the available momenta, and they all undergo multiplicative renormalization. Furthermore, they are linearly independent of each other.

- (2) The second step consists of the computation of the ratios $R^{\mathcal{O}^x}(t, \tau)$, the summed ratios $S^{\mathcal{O}^x}(t, \tau_{\text{skip}})$, and the kinematic factors $K^{\mathcal{O}^x}$, for each of the selected operators. To compute the kinematic factors, we use the value of the ground-state energy that we have obtained by performing a fit of the two-point correlator $C_{2\text{pt}}(t)$.
- (3) A crucial step is then the extraction of the matrix elements using one of the two methods previously outlined. “Method 1” consists of the determination of the matrix element from the slope of a linear regression of the summed ratio, as expressed in Eq. (14). The linear regression can be repeated with varying initial and final values of t , thereby yielding an additional estimate of the matrix element each time. The results from the various linear regressions have been averaged into one value using the Akaike information criterion [83–85]. “Method 2” consists of the extraction of the matrix element through a direct fit of the ratio based on Eq. (12). Given the significant variability of excited-state contamination among the different operators and momenta, three kinds of fully correlated fits have been performed, and the results have been averaged using again the Akaike information criterion; more details on this matter can be found in Appendix C. At this point, various determinations of the matrix elements are available. We label them by the compound index $j = (\mathcal{O}^x, \vec{p}, \mathbf{m})$, containing the selected operator, the momentum, and the method ($\mathbf{m} = 1, 2$) employed for the matrix-element extraction. For each j associated with a nonzero value of the kinematic factor, we can subsequently compute one value of the bare third Mellin moment

$$\mathfrak{X}_j^2 = \frac{\mathcal{M}_j}{K^{\mathcal{O}^x}(p)}. \quad (15)$$

- (4) Using the renormalization factors, we compute the renormalized moments as $x_j^2 = Z_{DDX}^\rho \mathfrak{X}_j^2$. In order to account for the uncertainty on the renormalization factors, we carry out the renormalization separately for each bootstrap resample. The resamples of the renormalization factors have been generated by sampling from a Gaussian distribution with mean and standard deviation given by the mean and standard deviation of Z_{DDX}^ρ . We computed the renormalization factors in the regularization-independent (symmetric)

momentum subtraction scheme [RI-(S)MOM] and then matched them to the $\overline{\text{MS}}$ scheme at scale 2 GeV; all the details are provided in Appendix D.

- (5) Separately for the three different channels, we combine the results we have obtained into one central value, defined as the following weighted average:

$$\langle x^2 \rangle_X = \sum_j w_j x_j^2, \quad (16)$$

where the sums run over all the available values of j for the given channel. The weights in the average are proportional to the inverse of the variance of the renormalized results, $w_j \propto 1/\sigma_j^2$, and they are normalized in such a way that the weights associated with each of the two methods sum separately to 1/2. The statistical uncertainties σ_j are calculated using a bootstrap resampling over x_j^2 . Bootstrap resampling is further employed to estimate the statistical uncertainty of the final average, with the weights w_j held fixed across all resamples. The choice of weights w_j is the same as the one adopted in our previous work [41]. The rationale behind this choice is to place the two different extraction methods for the matrix element on an equal footing and to avoid excessive dependence on the single method that may yield smaller uncertainties. Different choices for the weights have been explored, and the final results were found not to change significantly.

- (6) As a last point, we estimate the size of the remaining uncertainty due to the excited-state contamination. We provide a proxy of the systematic error by computing the weighted variance of the different results

$$\sigma_{\text{syst}}^2 = \sum_j w_j (x_j^2 - \langle x^2 \rangle_X)^2. \quad (17)$$

This quantity is not computed separately for each bootstrap resample, but is calculated directly on the central values.

D. Simulation parameters

We use a tree-level Symanzik-improved gauge action with 2 + 1 flavor tree-level improved Wilson-clover fermions coupling via two-level HEX smearing. Detailed information about the simulation setup can be found in Refs. [27,86,87]. Key simulation parameters are summarized in Table I.

Two ensembles, coarse and fine, at the physical pion mass are used. These ensembles correspond to lattice spacings of 0.1163(4) and 0.0926(6) fm, respectively. Furthermore, we consider two different momenta,

TABLE I. Details of the used ensembles. For each ensemble, the main simulation parameters are listed. Furthermore, the source-sink separations t and momenta $\vec{p}$ used in the calculation of the ratios are displayed, together with the number of gauge configurations N_{cfg} available for each combination.

Ensemble	Size	β	a (fm)	m_π (MeV)	$m_\pi L$	t/a	$\vec{p}[2\pi/L]$	N_{cfg}
Coarse	48 ⁴	3.31	0.1163(4)	136(2)	3.9	6, 8, 10	(2, 2, 2)	212
						3, 4, 5, 6, 7, 8, 10, 12	(-2, 0, 0)	212
Fine	64 ⁴	3.50	0.0926(6)	133(1)	4.0	8, 10, 12	(2, 2, 2)	221
						10, 13, 16	(-1, 0, 0)	427

$\vec{p}_{\text{low}} = (-2, 0, 0) \frac{2\pi}{L}$, $\vec{p}_{\text{high}} = (2, 2, 2) \frac{2\pi}{L}$ for the coarse ensemble, and $\vec{p}_{\text{low}} = (-1, 0, 0) \frac{2\pi}{L}$, $\vec{p}_{\text{high}} = (2, 2, 2) \frac{2\pi}{L}$ for the fine ensemble. For the low momentum, as described in [27], the smearing is done using Wuppertal smearing [88], $\tilde{q} \propto (1 + \alpha H)^N q$ with H being the nearest-neighbor gauge-covariant hopping matrix, at $\alpha = 3$ and $N = 60, 100$ for the coarse and fine ensemble, respectively. For the high momentum, the smearing is altered by introducing additional phase factors, according to the methodology of Ref. [89] (momentum Wuppertal smearing). In the notation of the reference, we used $\vec{k} = (0.8, 0.8, 0.8) \frac{2\pi}{L}$ and $\vec{k} = (1, 1, 1) \frac{2\pi}{L}$ for the coarse and fine ensemble, respectively. This modification improves statistical precision in the high-momentum data.

For each ensemble, two- and three-point correlation functions are calculated. These calculations involve source-sink separations ranging from approximately 0.3 to 1.4 fm for the coarse ensemble and approximately 0.7 to 1.5 fm for the fine ensemble. Furthermore, we make use of all-mode averaging (AMA) [90,91]. For the low-momentum dataset, the details have already been described in [27]. For the high-momentum dataset, we apply AMA with 96 and 64 sources, respectively, on the coarse and on the fine ensemble. In both cases, there is one high-precision source.

In our previous work [27], the autocorrelation of the gauge configurations was tested and no sizable effect was observed. In addition, we performed a bin-size analysis using delayed binning [92] and found no evidence of significant autocorrelation.

III. EXTRACTION OF MOMENTS

We now present the available data and provide a detailed explanation of the process by which the matrix elements are extracted. This is accomplished by focusing on a single operator for each channel, while the data and results for the complete set of operators are relegated to Appendix B. The selected operators are V2, A2, and T5, the expressions for which can be found in Eqs. (2) and (3). For kinematical reasons, V2 can only be accessed with the high momentum, while A2 and T5 can be accessed with both the high and the low momenta. A summary of which operator can be used with which configuration is given in Appendix B.

In Fig. 1, we show the ratios of these three operators, normalized to the kinematic factor, $\bar{R}(t, \tau) = R(t, \tau)/K$. This normalization is such that from the values of the plateau in these plots one can directly read the values for the bare moments. Note that the largest source-sink separation values (for each lattice and momentum) have been excluded from this plot due to their high noise levels.

As evident from the various panels in Fig. 1, the degree of excited-state contamination exhibits considerable variation across different operators, momenta, and lattices. Consequently, to extract a value for the matrix element reliably from all the ratio data, multiple fully correlated (across all source-sink separations) fits have been done. For each combination of lattice, operator, and momentum, the fits have been done varying both the functional form and the number of included data points. Specifically, three types of functional forms have been employed to perform three distinct types of fits: (i) a fit with 0 excited states, i.e., a fit to a constant, obtained by setting R_1 and R_2 to zero in Eq. (12); (ii) a fit with 1 excited state, where only R_2 has been set to zero; and (iii) a fit with 1 excited state, where R_1 and R_2 are both nonzero. These three types of fits have 1, 3, and 4 free parameters, respectively, for which Bayesian priors were used. The various fits performed have subsequently been averaged using the Akaike information criterion [83–85], as described in greater detail in Appendix C. A visualization of the fit curve obtained from the model average procedure for all operators can be found in Appendix B.

By fitting the ratio data (normalized with respect to the kinematic factor), we derive a single value for the bare moment for each operator and momentum. Specifically, for the operators depicted in Fig. 1, this implies that we obtain one value per lattice for the operator V2, whereas we obtain two values per lattice for both A2 and T5.

The normalized summed ratio data, $\bar{S}(t, \tau_{\text{skip}}) = S(t, \tau_{\text{skip}})/K$, where τ_{skip}/a is fixed at 2, is presented in Fig. 2 for the same set of operators. The normalization is such that to a value of the slope one can directly associate a value of the moment. The summed ratio values are plotted as a function of the source-sink separation. As previously indicated in Table I, a total of eight distinct source-sink separations are available on the coarse lattice for the low momentum, whereas only three are available for all other cases. The summed ratio value at $t/a = 3$ is not displayed

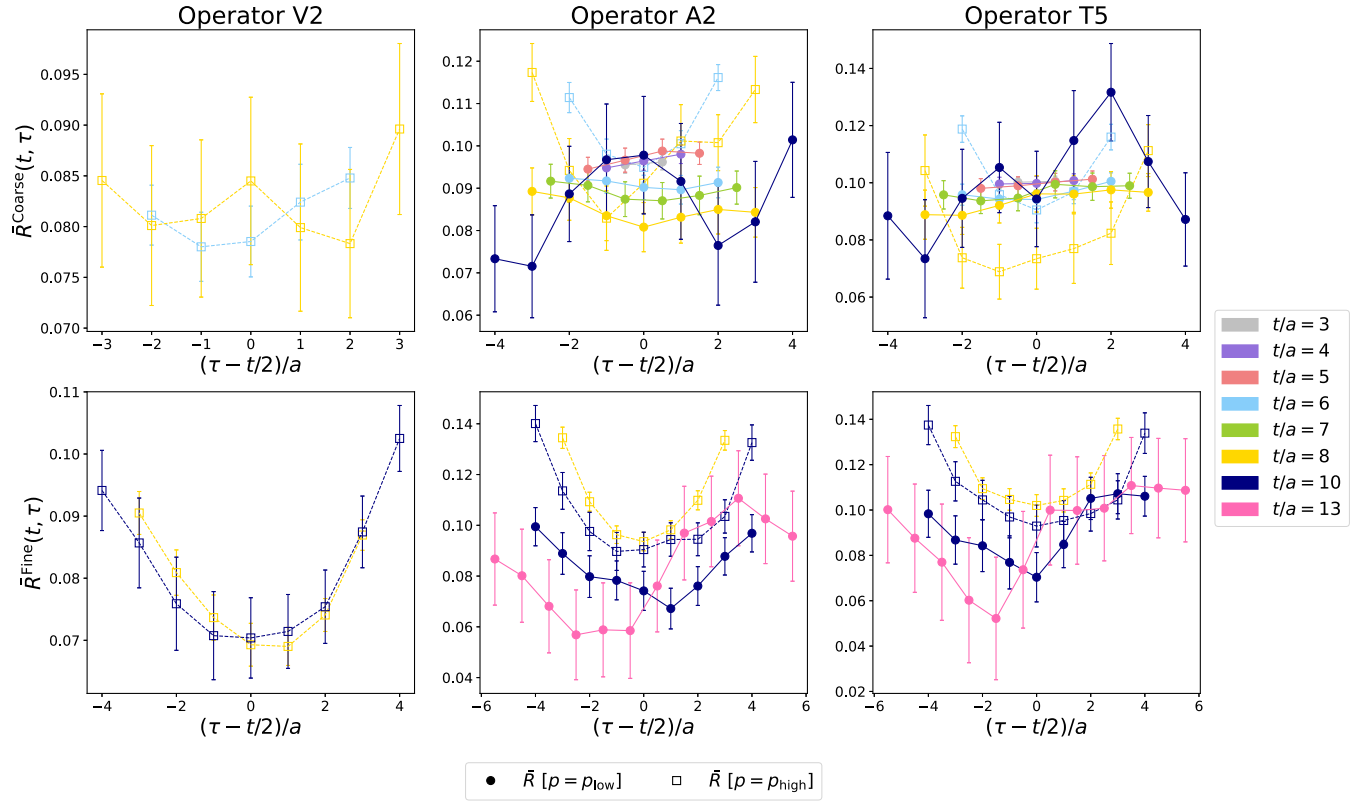


FIG. 1. Ratio data, normalized to the kinematic factor, for the operators V2, A2, and T5 of Eqs. (2) and (3). The data corresponding to high and low momentum are denoted by filled circles and empty squares, respectively. Different values of the source-sink separation t are represented by distinct colors. The three columns are organized by operator, whereas the upper and lower rows display data from the coarse and fine lattice, respectively.

in the plot, as it cannot be computed for $\tau_{\text{skip}}/a \geq 2$. Changing the value of τ_{skip} produced no significant difference in terms of moments. Therefore, all summed ratios were calculated using $\tau_{\text{skip}}/a = 2$.¹

Notably, in every case, the last available value of the source-sink separation is substantially noisier than the others. Consequently, we have chosen to exclude it entirely from our analysis. The smallest source-sink separation, $t/a = 3$, cannot be used with the summed ratio method. Thus, in order to ensure that the two extraction methods rely on the same data, also the source-sink separation $t/a = 3$ has been excluded entirely from our analysis.

Using the remaining data points, we can perform a linear regression and obtain, from the slope, one value of the bare moment. If possible, we repeat the linear regression varying each time the initial and final source-sink separations considered. The results of the various linear regressions are then averaged into one value using the Akaike information criterion. This average yields a result which is consistent with the results of simple linear regressions; more details are available in Appendix B.

¹The same choice was made in our previous work [41], where the value $\tau_{\text{skip}}/a = 1$ was incorrectly specified.

Thus, from this second method, we obtain a single value for the bare moment for each operator and momentum. As for the other method, this implies that we obtain one value per lattice for the operator V2, whereas we obtain two values per lattice for both A2 and T5.

The values of the moments derived from this second methodology are taken as the central value of the wide prior used in the Bayesian fitting procedure we perform on the ratio data, thus enabling us to rely on data for the prior estimation.

IV. RESULTS

By employing the techniques explained in the preceding section, a substantial number of values for the renormalized moments x_j^2 are calculated. Using Eq. (16), these intermediate results are then combined into a final average, for which we compute the statistical uncertainty through bootstrap resampling. Furthermore, the systematic uncertainty on the final average is computed using Eq. (17).

Figures 3–5 display the complete set of all the available renormalized moments, plotted as a function of their respective weights in the final average. This is done separately for the unpolarized, polarized, and transversity channels. The final average is also explicitly reported on the

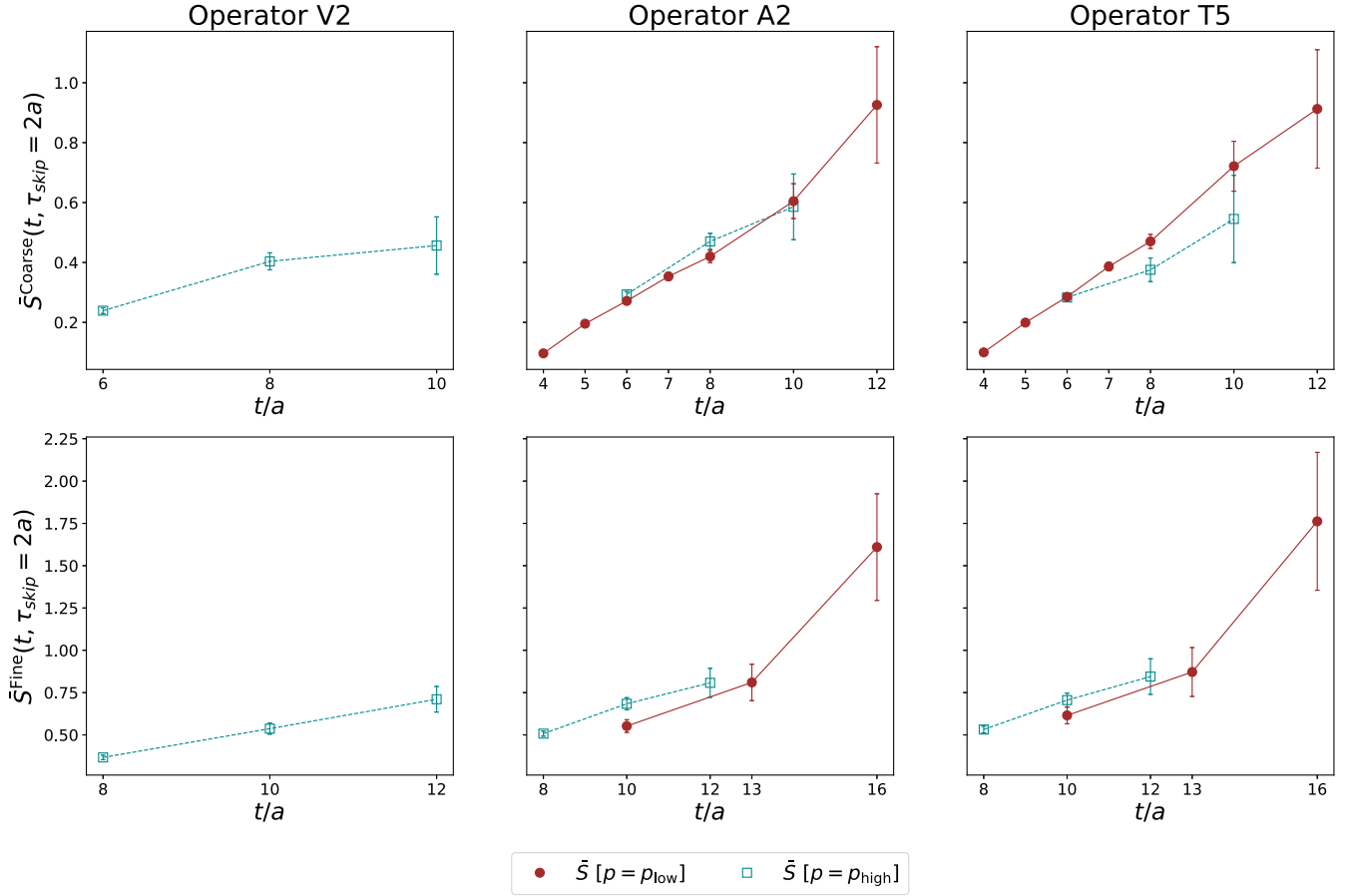


FIG. 2. Summed ratio data with $\tau_{\text{skip}}/a = 2$, normalized to the kinematic factor, for the operators V2, A2, and T5 of Eqs. (2) and (3). The high- and low-momentum data are displayed using filled circles and empty squares, respectively, and are distinguished by different colors. The three columns are organized by operator, while the upper and lower rows represent data from the coarse and fine lattices, respectively.

plots, along with its statistical and systematic uncertainties, enclosed respectively in the first and second parentheses.

For the computation of the final averages, correlations are automatically accounted for by our bootstrap analysis. As an example, Fig. 6 shows the correlation matrices of the renormalized moments related to the polarized channel. Looking at the correlation matrices, it is evident that a strong correlation exists only between results pertaining to the same operator and momentum. This is to be expected, since in these cases the methodology employed to extract different values of the moments varies, but the underlying data remain unchanged. The same behavior is observed for the unpolarized and transversity channels.

The numerical values obtained for the final estimate of the isovector third Mellin moments are summarized in Table II.

The final step of the analysis is the continuum extrapolation. With only two ensembles available, we acknowledge that a continuum extrapolation does not have enough degrees of freedom to judge the quality of the fit. Nevertheless, in order to provide a continuum estimate, we perform a Bayesian fit, where priors on the free parameters are used to stabilize the

fit. The points from the two ensembles are interpreted as partially correlated Gaussian variables. The correlation, we argue, is due to the use of the same operators, and hence to similar excited-state contamination in both cases. Consequently, we conservatively assume that systematic uncertainties are fully correlated and construct a covariance matrix whose off-diagonal entries are the products of single-ensemble systematic uncertainties. The functional form for the extrapolation is the following:

$$\langle x^2 \rangle(a) = \langle x^2 \rangle_{\text{cont}} \cdot (1 + m_1(\alpha_s a \Lambda_{\text{QCD}}) + m_2(a \Lambda_{\text{QCD}})^2). \quad (18)$$

The combination $a \Lambda_{\text{QCD}}$ dictates the size of the discretization effects. The fermion action we use is tree-level $O(a)$ -improved, and the operators we consider are also expected to have no tree-level $O(a)$ errors; thus the above functional form. We expect the dimensionless parameters m_i to be of order 1; thus, we constrain them by the use of two equal Gaussian priors, of the form $\mathcal{N}(0, 2)$. We approximate $\alpha_s \approx 0.3$. A completely flat prior is used for the continuum value $\langle x^2 \rangle_{\text{cont}}$. The continuum value obtained from this procedure is a prior-constrained estimate. To assess the

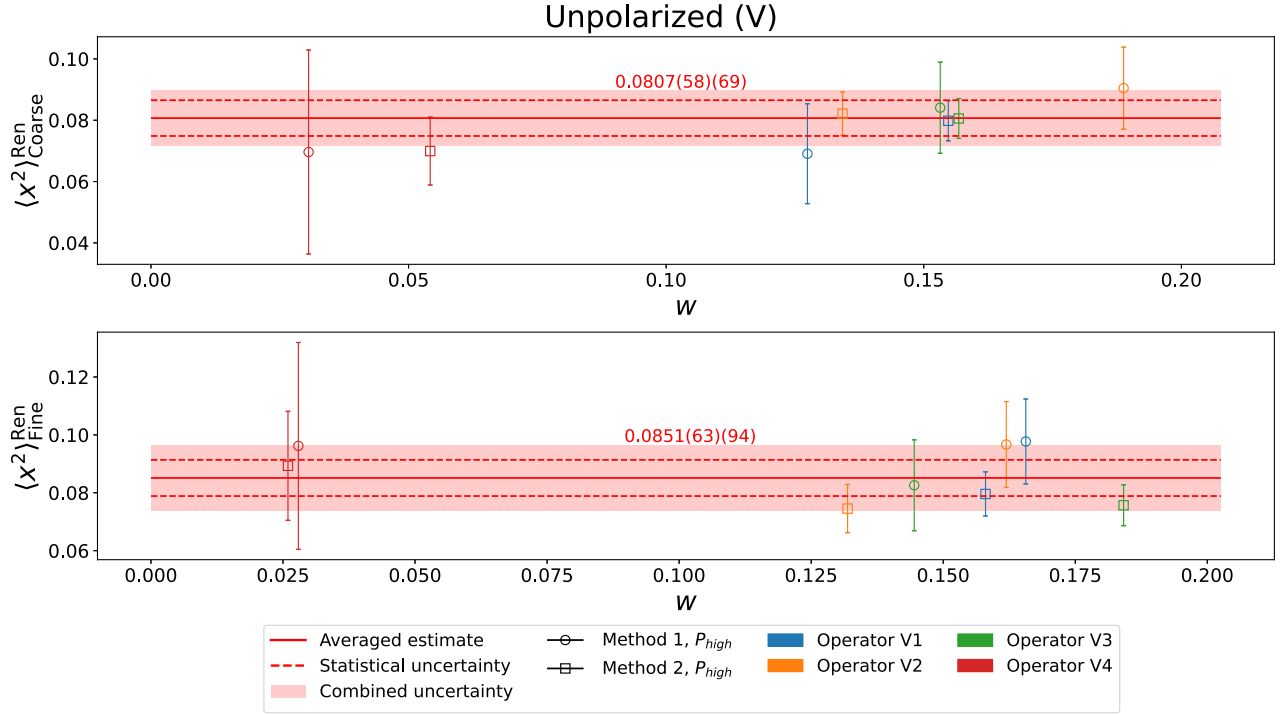


FIG. 3. Estimates of unpolarized x_j^2 versus their weight in the final average. Moments obtained from the coarse and fine lattice are displayed, respectively, on the top and bottom row. They are resolved per operator, momentum, and extraction method, which are represented by different colors and marker styles. The final average is shown in red with a solid line, its statistical uncertainty with a dashed line, and the sum in quadrature of statistical and systematic uncertainty with a red band.

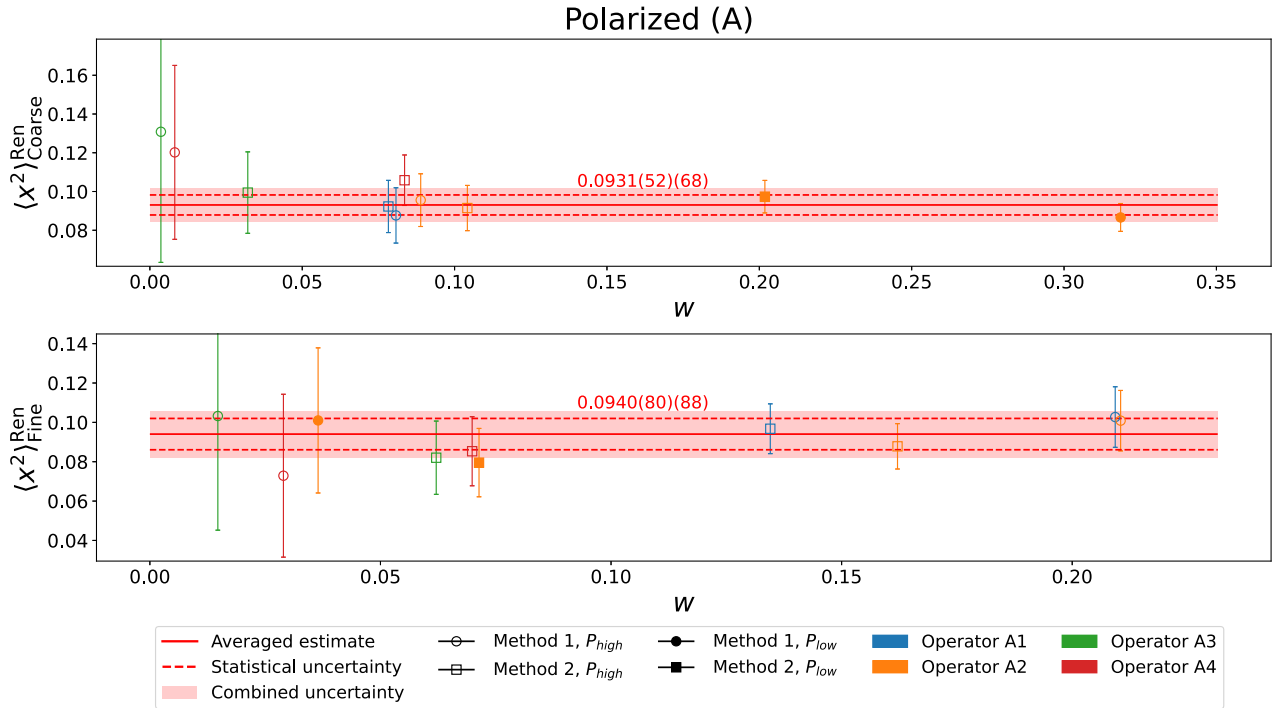


FIG. 4. Estimates of polarized x_j^2 versus their weight in the final average, analogous to Fig. 3.

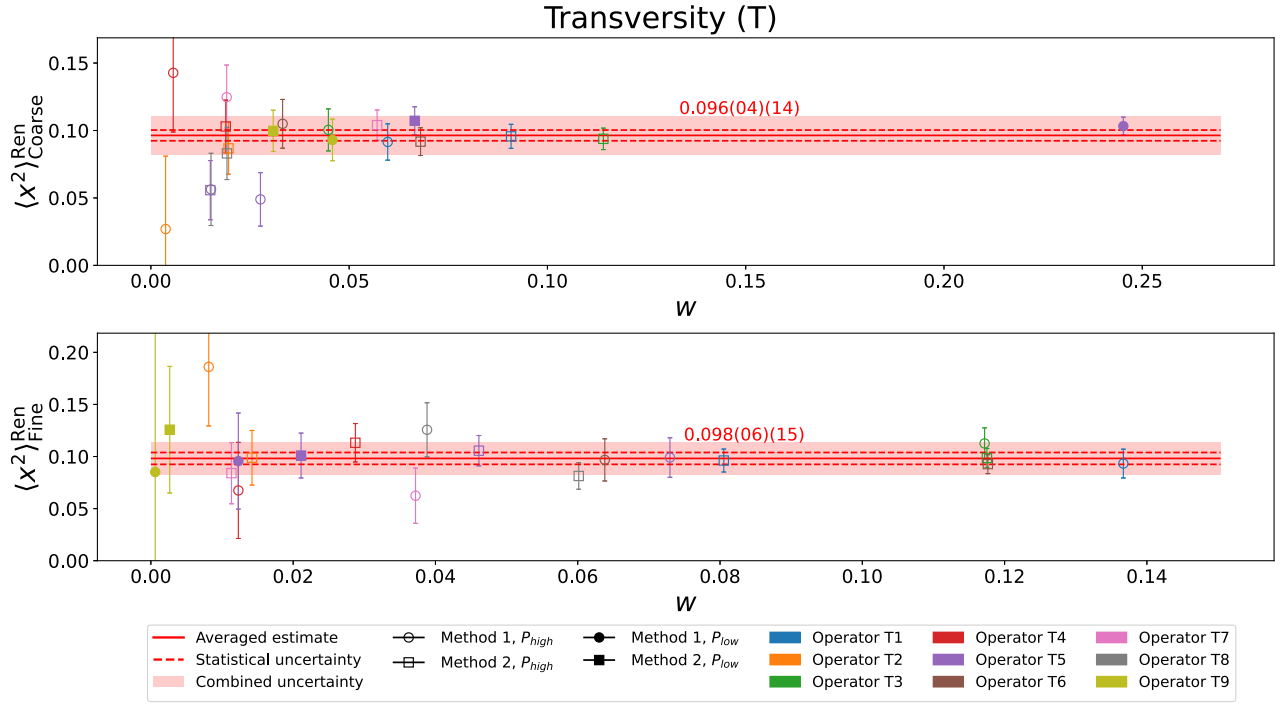


FIG. 5. Estimates of transversity x_j^2 versus their weight in the final average, analogous to Fig. 3.

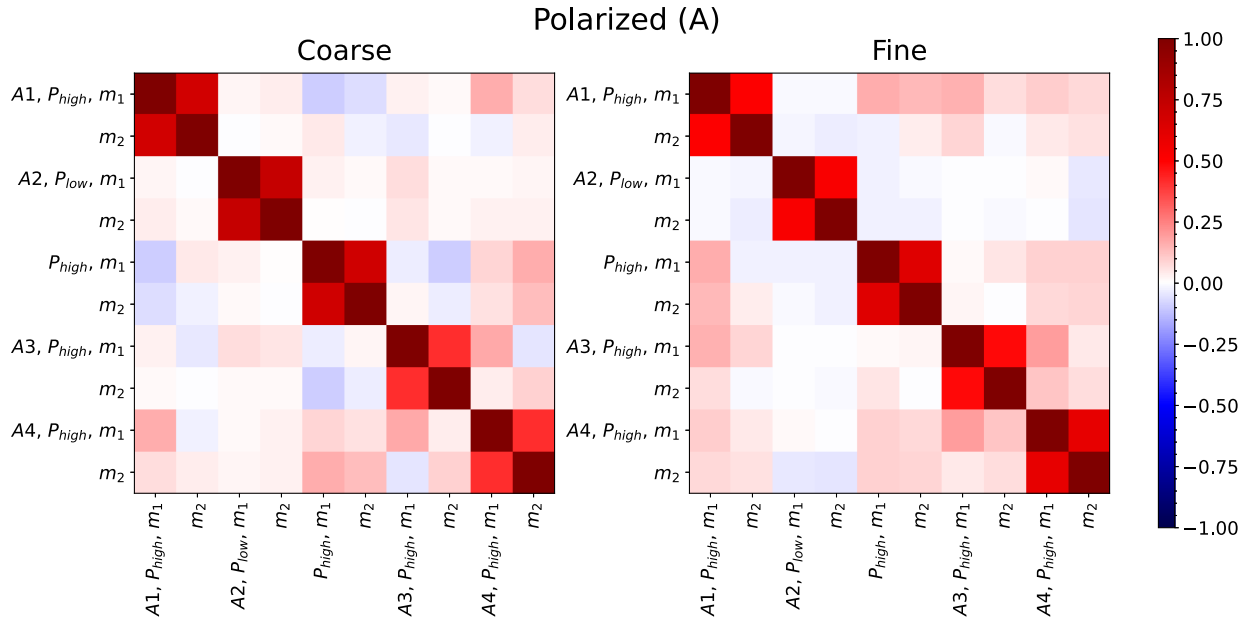


FIG. 6. Correlation matrices of the moments shown in Fig. 4. The moments are labeled by operator, momentum, and extraction method. A strong correlation exists only between results obtained from the same operator and momentum.

robustness of our result, we repeat the extrapolation while varying the width of the prior on m_i within the range $[0.5, 32]$ and observe no sizable effect. We emphasize that the priorred extrapolation results in a more conservative continuum uncertainty. The findings of our prior-width study are reported in Appendix E.

The fit curves are shown in Fig. 7. For each channel, the continuum extrapolation curve is almost completely flat. This is expected because, for each channel, the two available data points are compatible between uncertainties. Indeed, performing a fit to a constant, we find a central value for $\langle x^2 \rangle_{\text{cont}}$ which is completely compatible with the

TABLE II. Final averages for the isovector third Mellin moments for the unpolarized, polarized, and transversity channels. For both the coarse and fine lattices, the central values have been obtained using Eq. (16); the statistical uncertainty, denoted by the value within the first set of parentheses, was calculated through bootstrap resampling; the systematic uncertainty, represented by the value within the second set of parentheses, was obtained using Eq. (17). The continuum values have been extrapolated from the two values at finite lattice spacing using a Bayesian fit. In this case, the values between the three sets of parentheses represent, in order, the statistical uncertainty, the systematic uncertainty related to excited-state contamination, and the systematic uncertainty related to the size of discretization effects. Further details are provided in the main text.

	Ensemble	$\langle x^2 \rangle$
Unpolarized (V)	Coarse	0.081(06)(07)
	Fine	0.085(06)(09)
	Continuum	0.083(04)(09)(10)
Polarized (A)	Coarse	0.093(05)(07)
	Fine	0.094(08)(09)
	Continuum	0.094(04)(08)(12)
Transversity (T)	Coarse	0.096(04)(14)
	Fine	0.098(06)(15)
	Continuum	0.098(03)(15)(11)

one already obtained. However, the uncertainty obtained from a fit to a constant is sizably smaller.

The results of the continuum extrapolation are quoted in Table II. The total uncertainty on the continuum value is obtained using the Bayesian fit procedure described above. To assess which parts of the uncertainty are statistical and which are systematic contributions, we compare the

uncertainties obtained by varying the extrapolation procedure. First, we set the single-ensemble systematic uncertainties to zero and repeat the fit to Eq. (18). We obtain a smaller uncertainty on the continuum value and interpret the difference in quadrature as the excited-state systematic uncertainty. Additionally, keeping the single-ensemble systematic uncertainties to zero, we fit to a constant. The result is again compatible, but the uncertainty is considerably lower. This additional difference in uncertainty is interpreted as the systematic contribution resulting from discretization effects. The uncertainty of the constant fit is taken as the statistical contribution. As an example, we consider the polarized case, where the result of the Bayesian fit is 0.094(15). We rewrite it as 0.094(04)(08)(12). The statistical uncertainty is the value between the first set of parentheses. Inside the second and third parentheses, we have the systematic uncertainties due to excited-state and discretization effects, respectively. The systematic uncertainties appear to be the dominant contribution to the total uncertainty budget. We reiterate that the continuum estimate we provide is not the result of an unconstrained continuum extrapolation. Rather, it is a prior-constrained estimate, obtained with what we believe to be the best option available with the given data.

An overview of the comparison between our results and those of other collaborations is provided in Figs. 8–10. For the unpolarized, polarized, and transversity moment, the lattice calculations are taken from Refs. [56,63,64,93], [53,57,63,66], and [63,67–69], respectively. Some of the quoted results have been derived by us using inputs from the corresponding references. In Refs. [53,57] the polarized moment was given in terms of the matrix element $a_2^{(u-d)}$,

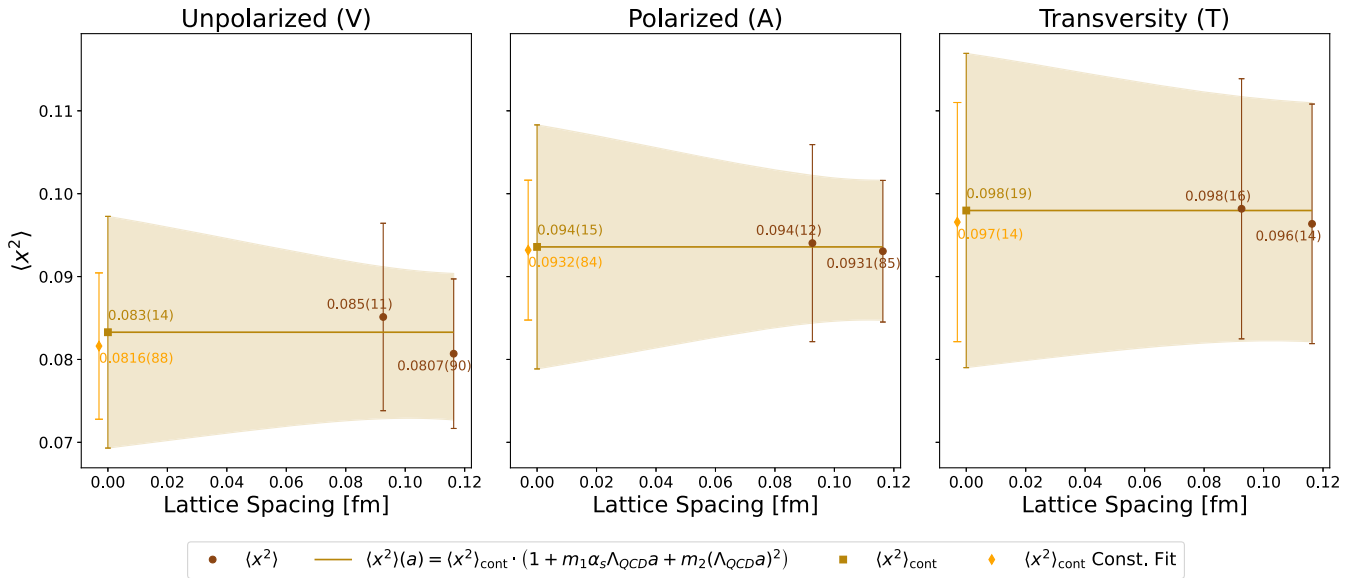


FIG. 7. Continuum extrapolation using a Bayesian fit with the model described in Eq. (18). The limited amount of data makes this extrapolation dependent on the chosen priors for the coefficients m_i . Further details are provided in the main text, and resulting estimates are listed in Table II. For comparison, the continuum value obtained from a constant fit is also shown on the plot, slightly displaced horizontally for visual clarity.

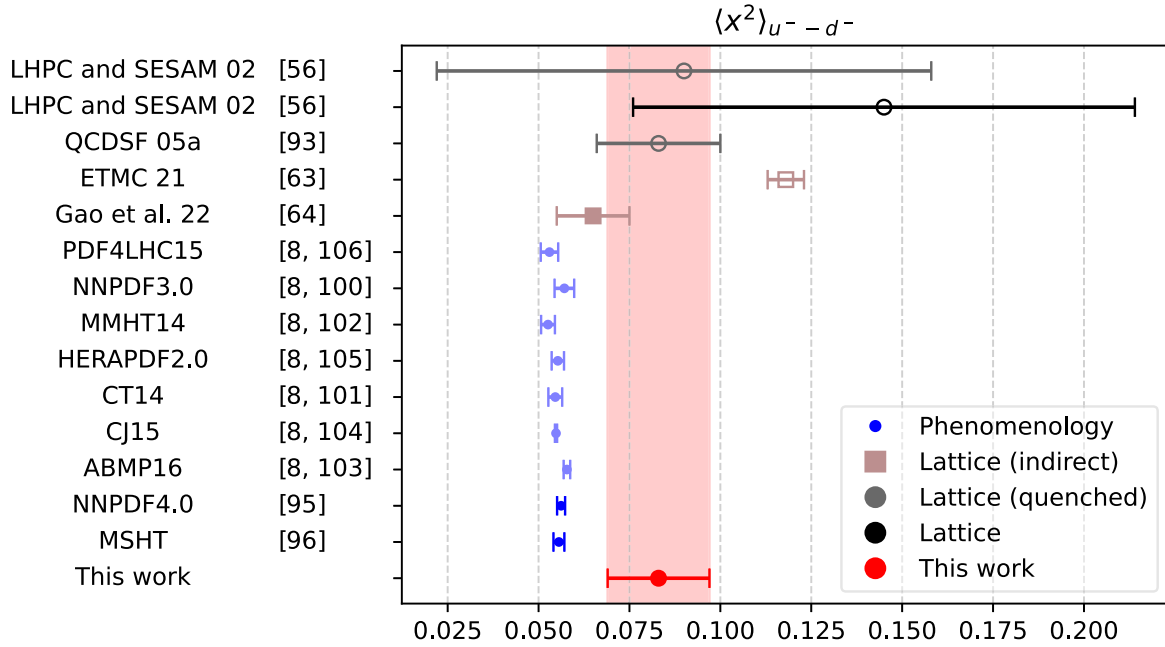


FIG. 8. Comparison of unpolarized isovector third Mellin moments $\langle x^2 \rangle_{u^- - d^-}$ computed by different collaborations. The result obtained in this work is shown as a red circle; the corresponding 1σ region is indicated by a red band. Lattice computations are represented by circles and squares: black circles denote dynamical calculations performed using the same approach adopted here (based on local twist-two operators), gray circles denote quenched calculations using the same approach, and brown squares denote dynamical lattice calculations based on indirect determinations of the moments (e.g., quasi- or pseudo-PDF methods). Empty markers are used for lattice calculations performed on a single lattice with a heavier-than-physical pion mass or with no pion mass below 500 MeV. Phenomenological results are shown as blue dots. A lighter shade of blue is used for values corresponding to older PDF ensembles. Further details and references are provided in the main text.

whose definition differs by a factor of 2 from $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+}$.² The transversity moment was either reported normalized to the tensor charge (Ref. [68]), or at a different renormalization scale (Ref. [63]) or both (Refs. [67,69]); thus, in order to compare with our result, we used the tensor charge from the FLAG review and computed the relevant numerical factors needed for a change of renormalization scale.³ If we exclude calculations performed on single lattice with a heavier-than-physical pion mass and calculations with no pion mass below 500 MeV, we find a good agreement with the results of other collaborations. Reference [53] used our same methodology based on local twist-two operators, and the polarized moment they obtain is in perfect agreement with our result. The authors of Refs. [64,66,68] compute the Mellin moments using the pseudo-PDF approach. For the polarized and transversity cases, their result lies well within 1 standard deviation of our value. In the unpolarized case, the difference is slightly larger.

²For Ref. [57] we considered the combination $3/2(a_2^{(p)} - a_2^{(n)})Z$, where $a_2^{(p)}$ and $a_2^{(n)}$ are the matrix elements, in the $\overline{\text{MS}}$ scheme at scale $\sqrt{5}$ GeV, taken from the reference, and $Z \approx 1.038$ is the factor needed to evolve to our scale of 2 GeV.

³In order to evolve $\langle x^2 \rangle_{\delta u^- - \delta d^-}$ and $\langle x^2 \rangle_{\delta u^- - \delta d^-} / g_T^{u-d}$ from the $\overline{\text{MS}}$ scheme at scale $\sqrt{2}$ GeV to scale 2 GeV, we used the numerical factors $Z \approx 0.865965$ and $Z \approx 0.906225$, respectively.

Results from phenomenology are also available. For the unpolarized and polarized moment, we use the software library LHAPDF [94]. Using the unpolarized PDF sets NNPDF4.0aN3LO [95] and MSHT20aN3LO [96] we obtain the values $\langle x^2 \rangle_{u^- - d^-} = 0.0562(11)$ and $\langle x^2 \rangle_{u^- - d^-} = 0.0556(15)$, respectively. Using the polarized PDF sets NNPDFpol1.1 [97], NNPDFpol2.0NNLO [98], and MAPPDFpol1.0NNLO [99] we obtain the values $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+} = 0.0659(46)$, $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+} = 0.0586(46)$, and $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+} = 0.0666(53)$, respectively. For the unpolarized moment, we also consider the values given in Table C.1 of Ref. [8], where they have been computed using the unpolarized PDF sets provided in Refs. [100–106]. Finally, for the transversity moment, we use the transversity distribution provided by the global analysis JAM3D-22 [107] and obtain the value⁴ $\langle x^2 \rangle_{\delta u^- - \delta d^-} = 0.074(7)$; using the distribution by JAMDiFF [109,110], we obtain the value⁵ $\langle x^2 \rangle_{\delta u^- - \delta d^-} = 0.0704(55)$. In the unpolarized and polarized case, our result exceeds the phenomenological values by approximately 2 standard deviations. For the transversity moment the comparison is more favorable, with our result

⁴The code used to compute this value is based on the Google Colab notebook [108] provided in Ref. [107].

⁵The code used to compute this value is based on the Google Colab notebook [111] provided in Ref. [109].

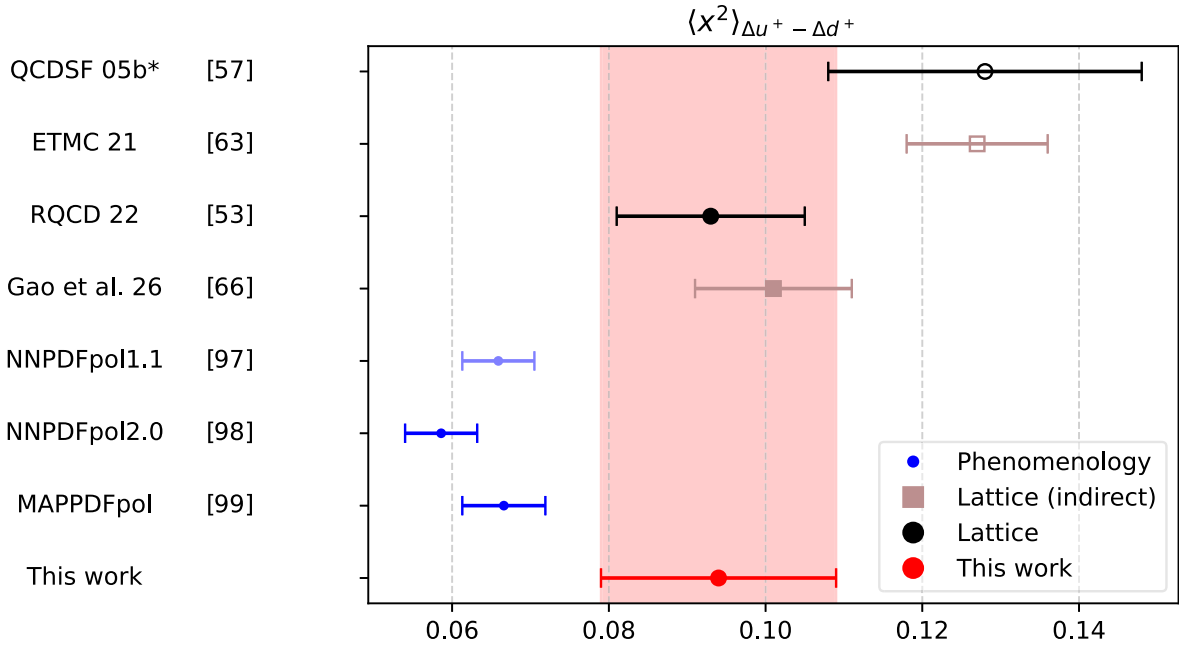


FIG. 9. Comparison of polarized isovector third Mellin moments $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+}$ computed by different collaborations, analogous to Fig. 8. An asterisk next to a collaboration name indicates that the quoted result was derived by us using inputs from the corresponding reference, rather than taken directly from it. Further details and references are provided in the main text.

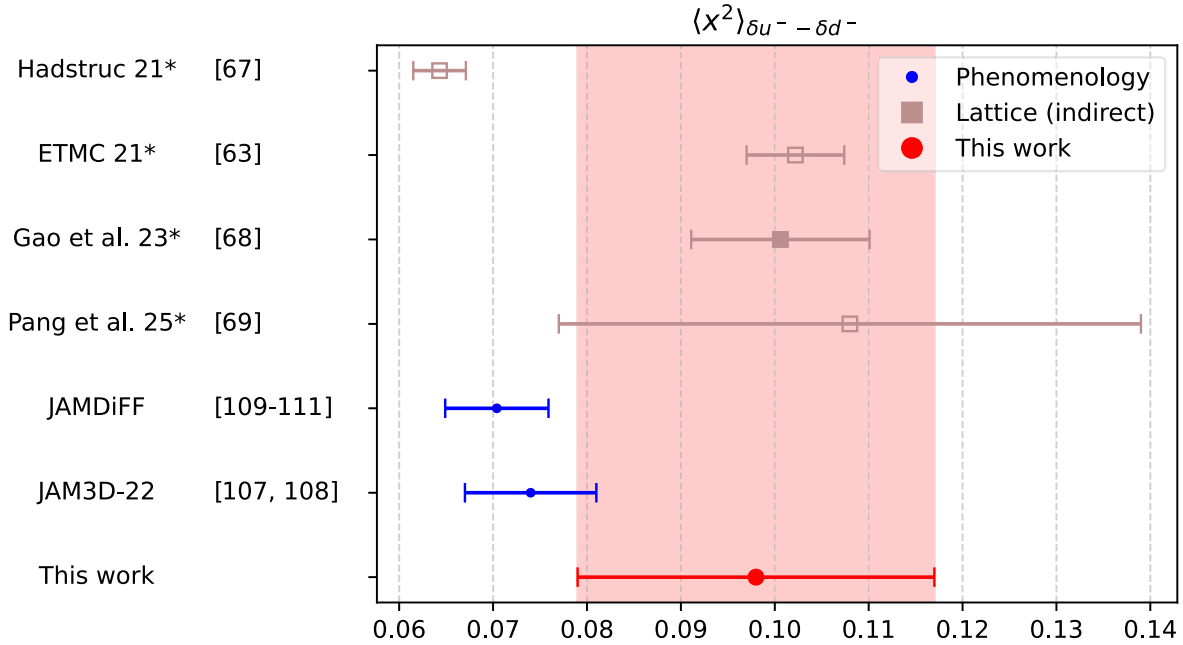


FIG. 10. Comparison of transversity isovector third Mellin moments $\langle x^2 \rangle_{\delta u^- - \delta d^-}$ computed by different collaborations, analogous to Fig. 8. An asterisk next to a collaboration name indicates that the quoted result was derived by us using inputs from the corresponding reference, rather than taken directly from it. Further details and references are provided in the main text.

exceeding the values from phenomenology by less than 2 standard deviations.

V. SUMMARY

In this work, the isovector third Mellin moments $\langle x^2 \rangle$ of unpolarized, polarized, and transversity parton distribution

functions have been computed using two lattice QCD ensembles at the physical pion mass and two different nonzero values of the momentum.

For the computation, we employed a large set of operators. For each kinematically allowed operator-momentum combination, we obtained two estimates of

the Mellin moment. For each ensemble, these intermediate estimates were then combined into a single average. The variety of operators reflected in a variety of excited-state contamination. By applying fit averaging, we were able to consistently extract Mellin moments across all operator choices using the same procedure. The resulting values are mutually compatible, providing a nontrivial cross-check of the robustness of our calculation. Moreover, the large number of operators yields a correspondingly large set of intermediate results. The spread of these results enables a reliable estimate of the systematic uncertainty associated with excited-state contamination.

The continuum limit cannot be reliably performed in an unconstrained way with only two ensembles. To provide a continuum estimate, we performed a Bayesian fit in which the coefficients describing the lattice-spacing dependence were constrained to be natural sized. This procedure provides the following values: $\langle x^2 \rangle_{u^-d^-} = 0.083(14)$, $\langle x^2 \rangle_{\Delta u^+ - \Delta d^+} = 0.094(15)$, $\langle x^2 \rangle_{\delta u^- - \delta d^-} = 0.098(19)$. These results are compatible with the ones at finite lattice spacing.

For both the unpolarized and polarized channels, our result deviates from the corresponding phenomenological estimate by approximately 2 standard deviations. In the transversity channel, the agreement is slightly better, although the phenomenological value still lies more than 1 standard deviation away from our determination. We find good agreement with other lattice results either obtained at or extrapolated to the physical pion mass. However, a comprehensive comparison remains limited, as only a few such lattice calculations exist in the literature. Moreover, this work provides the first direct determination of these observables at the physical pion mass.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: CHOICE OF OPERATORS

Operators of the form given in Eq. (1) can be directly linked to the third Mellin moments by means of Eq. (4). However, these operators are not directly well suited for the computation because, in general, they mix under renormalization with lower- or equal-dimensional operators. Lattice operators can mix if they have the same flavor structure, the same charge-conjugation parity, and the same transformation properties under $H(4)$ (the group of lattice rotations and reflections). For this reason, to avoid mixing, we first classify all irreps of $H(4)$ appearing in the decomposition of operators of the form (1), as well as in the decomposition of operators of equal or lower dimension. We then rearrange the operators of Eq. (1) into irreps of $H(4)$ and focus only on those belonging to an irrep that appears only once (with a given charge-conjugation parity) in the above classification.

In general, all the possible operators of the form (1) span reducible representations of $H(4)$ represented, respectively, for the vector, axial, and tensorial cases, by the tensor products $\tau_1^{(4)} \otimes \tau_1^{(4)} \otimes \tau_1^{(4)}$, $\tau_4^{(4)} \otimes \tau_1^{(4)} \otimes \tau_1^{(4)}$, and $\tau_1^{(6)} \otimes \tau_1^{(4)} \otimes \tau_1^{(4)}$, where $\tau_a^{(b)}$ is the standard symbol used to denote the a th b -dimensional irrep of $H(4)$. These tensor products can be easily decomposed into a sum of irreps by means of the character table of the group $H(4)$ (which one can find, e.g., in Ref. [71]). The decompositions are the following:

$$\begin{aligned} \tau_1^{(4)} \otimes \tau_1^{(4)} \otimes \tau_1^{(4)} &= 4\tau_1^{(4)} \oplus \tau_2^{(4)} \oplus \tau_4^{(4)} \oplus 3\tau_1^{(8)} \oplus 2\tau_2^{(8)}, \\ \tau_4^{(4)} \otimes \tau_1^{(4)} \otimes \tau_1^{(4)} &= \tau_1^{(4)} \oplus \tau_3^{(4)} \oplus 4\tau_4^{(4)} \oplus 2\tau_1^{(8)} \oplus 3\tau_2^{(8)}, \\ \tau_1^{(6)} \otimes \tau_1^{(4)} \otimes \tau_1^{(4)} &= \tau_1^{(1)} \oplus \tau_4^{(1)} \oplus \tau_1^{(2)} \oplus \tau_2^{(2)} \oplus 2\tau_1^{(3)} \oplus \tau_2^{(3)} \\ &\quad \oplus \tau_3^{(3)} \oplus 2\tau_4^{(3)} \oplus 4\tau_1^{(6)} \oplus 2\tau_2^{(6)} \\ &\quad \oplus 3\tau_3^{(6)} \oplus 3\tau_4^{(6)}. \end{aligned} \quad (A1)$$

Comparing such a decomposition to the decomposition of lower- and equal-dimensional operators, we find the irreps that are suitable for a computation that does not involve

mixing. These are: $\tau_2^{(4)}$ for the vector case, $\tau_3^{(4)}$ for the axial case, and $\tau_2^{(3)}$, $\tau_3^{(3)}$, and $\tau_2^{(6)}$ for the tensorial case.

Once these suitable irreps have been identified, we have to find an explicit expression for the operators belonging to them. Such a task can be achieved using the recipe given in Ref. [70], which tells us how to compute the Clebsch-Gordan coefficients of a finite group. In our case, the finite group is $H(4)$, and its Clebsch-Gordan coefficients tell us exactly how to rearrange the operators of the form (1) into a combination which transforms, under $H(4)$, according to one of the selected irreps. To proceed with this computation, one needs to know an explicit matrix representation of each one of the 384 elements of $H(4)$ and for each one of its 20 irreps. These 384×20 matrices can be constructed starting just from an explicit representation, for each irrep, of the three generators of $H(4)$; conveniently enough, these 3×20 matrix representations are given in Table IX of Ref. [71].

Putting everything together we are then able to obtain an explicit expression for our operators of interest, using as input only the explicit matrix representations of the generators of $H(4)$. The results we obtain are shown in Eqs. (2) and (3). We note here that, for the tensorial case, from the three-dimensional $\tau_2^{(3)}$ and $\tau_3^{(3)}$ irreps, we only report 1 and 2 operators, respectively. We omit three operators because their associated kinematic factors vanish for all available momenta.

Finally, we confirm that the bases we obtain for $H(4)$ using this methodology coincide, up to a trivial rearrangement of operators inside the same irrep, with the bases of operators given in Ref. [72], where the same results have been obtained in a different way.

APPENDIX B: RESULTS PER OPERATOR

In this Appendix, we present the complete set of bare moments that enter our final averages. The bare moments are estimated for each lattice, operator, and momentum. Because the extraction of a Mellin moment requires a nonzero kinematic factor, not every operator can be used in combination with every momentum. Operators A2 and T5 can be used with both the high and low momentum. Operators T9 can be used only with the low momentum. All remaining operators can be used solely with the high momentum. For both the vector and axial channels, the employed operators belong to the same irrep. Consequently, a single renormalization factor applies to all operators within each channel. In the tensor channel this simplification does not hold, because the relevant operators transform according to different irreps. Nevertheless, as can be seen from Table III, the tensor renormalization factors are mutually compatible within uncertainties. Hence, agreement among the unrenormalized results in a given channel implies agreement among the corresponding renormalized quantities.

TABLE III. Vector current renormalization factor from Ref. [27] and ratios of renormalization factors computed in this work.

	Coarse	Fine
Z_V	0.9094(36)	0.9438(1)
$Z_{DDV}^{\tau_2^{(4)}}/Z_V^a$	1.2000(100)(181)	1.2134(83)(131)
$Z_{DDA}^{\tau_3^{(4)}}/Z_V^a$	1.2001(102)(221)	1.2168(77)(167)
$Z_{DDT}^{\tau_2^{(6)}}/Z_V^a$	1.1921(108)(138)	1.2017(74)(180)
$Z_{DDT}^{\tau_2^{(3)}}/Z_{DDT}^{\tau_2^{(6)}}$	0.9945(24)(85)	0.9967(31)(57)
$Z_{DDT}^{\tau_3^{(3)}}/Z_{DDT}^{\tau_2^{(6)}}$	1.0044(24)(33)	1.0033(25)(44)

^a $\overline{\text{MS}}$ scheme at scale 2 GeV.

The results of the fits to the ratio data, together with the raw data, are displayed in Figs. 11–14. For each operator, the plotted points have been normalized by the corresponding kinematic factor. The values of the bare moments are indicated by the horizontal bands shown in the figures. The curves that we overlay to the raw data points represent the outcome of the model-averaging procedure. They are not the outcome of a single fit; instead, they have been obtained by averaging the outcomes of the different fits we consider. The average is done, separately for each resample, using the Akaike information criterion (AIC) weights. Then, averaging over the resamples, we obtain the central value and the surrounding 1σ region that we show in the plot. For each channel and lattice, all the values of the bare moments obtained from the fit average procedure agree between uncertainties. The only exception is the bare moment obtained on the coarse lattice from operator T5 with high momentum. As is evident from Fig. 13, this value is not compatible with the other ones obtained on the same ensemble. However, on the fine ensemble, this discrepancy disappears, as shown in Fig. 14. This suggests that the outlier on the coarse ensemble may reflect a statistical fluctuation.

The bare moments extracted with the summed ratio method are shown in Figs. 15 and 16. In the majority of cases only two distinct source-sink separations are available. Consequently, the AIC-averaging procedure we use for the summation method is trivial, and it does coincide with a simple linear regression. For the low momentum on the coarse lattice, however, several source-sink separations are present. In this case, the AIC-averaging procedure is nontrivial and takes into account multiple fits. To illustrate the validity of the procedure, we compare the result we obtain to the results of simple linear regressions performed for different starting values of t . The comparison is made in Fig. 17. Note that a simple linear regression starting at $t/a = 6$ yields results in good agreement with those from the AIC-averaging procedure, without underestimating the associated uncertainties. This suggests that, for the high-momentum data, choosing $t/a = 6$ as the smallest source-sink separation was a sensible choice.

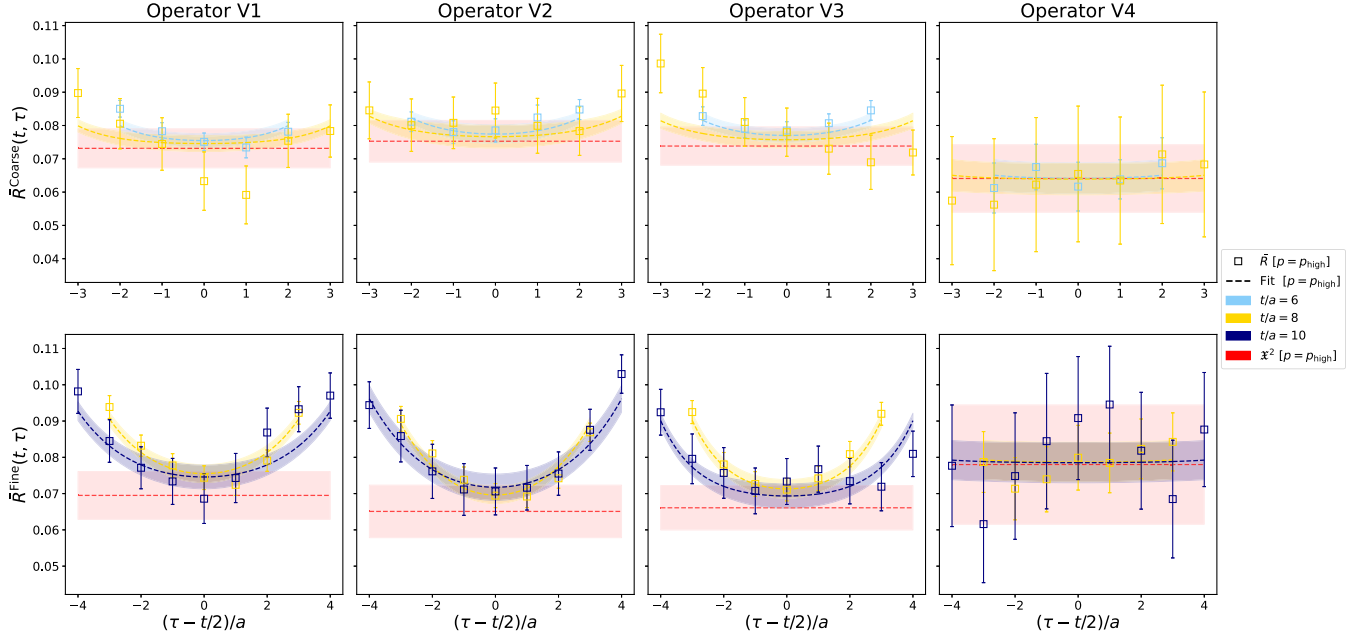


FIG. 11. Normalized ratio for the vector operators versus operator insertion time: different operators (columns) and ensembles (rows). Different source-sink separations are distinguished by distinct colors. The dashed curves illustrate the outcome of the model-averaging procedure. The shaded regions surrounding the curves indicate the 1σ uncertainty interval. The red line denotes the value of the bare moment extracted from the fit average.

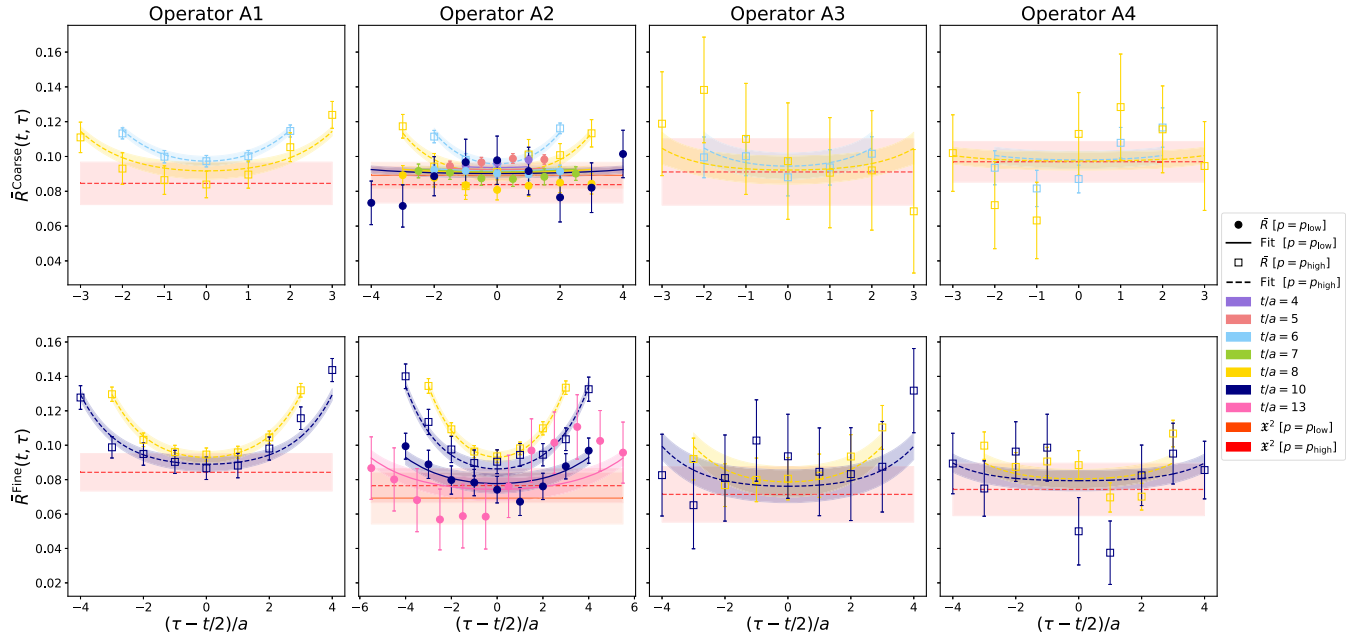


FIG. 12. Normalized ratio for the axial operators versus operator insertion time, analogous to Fig. 11. In the axial case, one operator is also accessible at low momentum. Different momenta are represented by different markers. The outcome of the model-averaging procedure is depicted using solid and dashed lines, respectively, for the high- and low-momentum cases. The fit average over the low-momentum data yields additional values of the bare moment, which are depicted in orange.

APPENDIX C: MODEL AVERAGING

To extract the Mellin moment directly from the ratio data, we perform multiple fits. The different fits are

distinguished by the choice of the functional form and by the data range considered. Each fit yields a different estimate of the Mellin moment. These values are combined

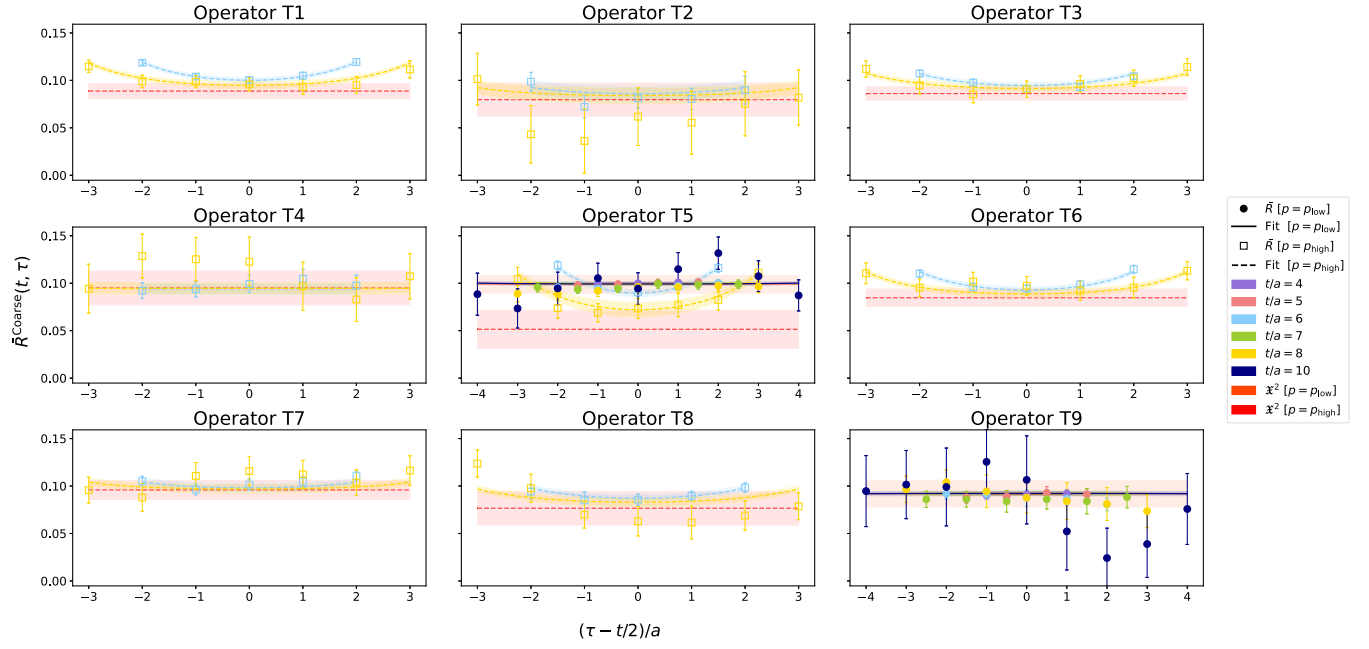


FIG. 13. Normalized ratio, on the coarse lattice, for the tensor operators versus operator insertion time. Analogous to Fig. 12, with two operators being also accessible at low momentum in the tensor case.

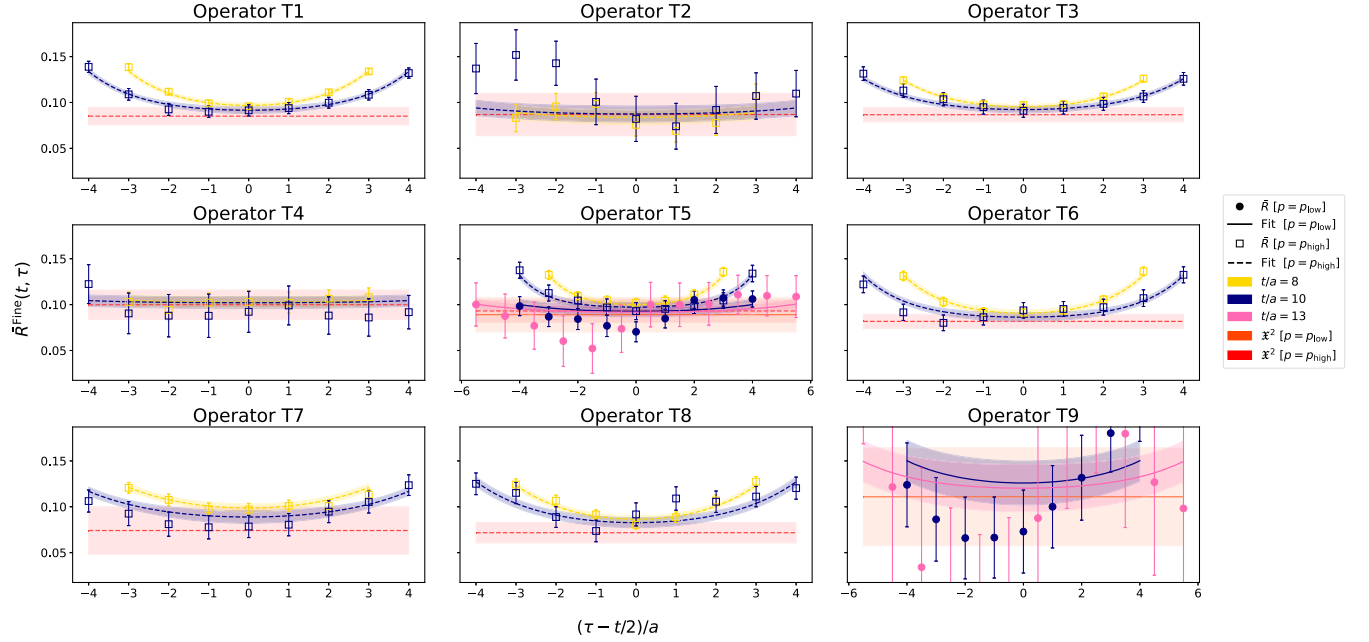


FIG. 14. Normalized ratio, on the fine lattice, for the tensor operators versus operator insertion time. Analogous to Fig. 12, with two operators being also accessible at low momentum in the tensor case.

into one by using the Akaike information criterion [83–85]. The whole procedure is performed under a bootstrap analysis to extract the uncertainties. The fits have been performed on ratios normalized to the kinematic factors. In this way, the fits yield moments instead of matrix elements.

Three different functional forms have been employed to perform the fits

$$\begin{aligned}
 \text{(i)} \quad & \bar{R}(t, \tau) = \mathfrak{X}^2, \\
 \text{(ii)} \quad & \bar{R}(t, \tau) = \mathfrak{X}^2 + \bar{R}_1 e^{-\frac{t}{2}\Delta E} \cosh\left[\left(\frac{t}{2} - \tau\right)\Delta E\right], \\
 \text{(iii)} \quad & \bar{R}(t, \tau) = \mathfrak{X}^2 + \bar{R}_1 e^{-\frac{t}{2}\Delta E} \cosh\left[\left(\frac{t}{2} - \tau\right)\Delta E\right] + \bar{R}_2 e^{-t\Delta E}.
 \end{aligned}
 \tag{C1}$$

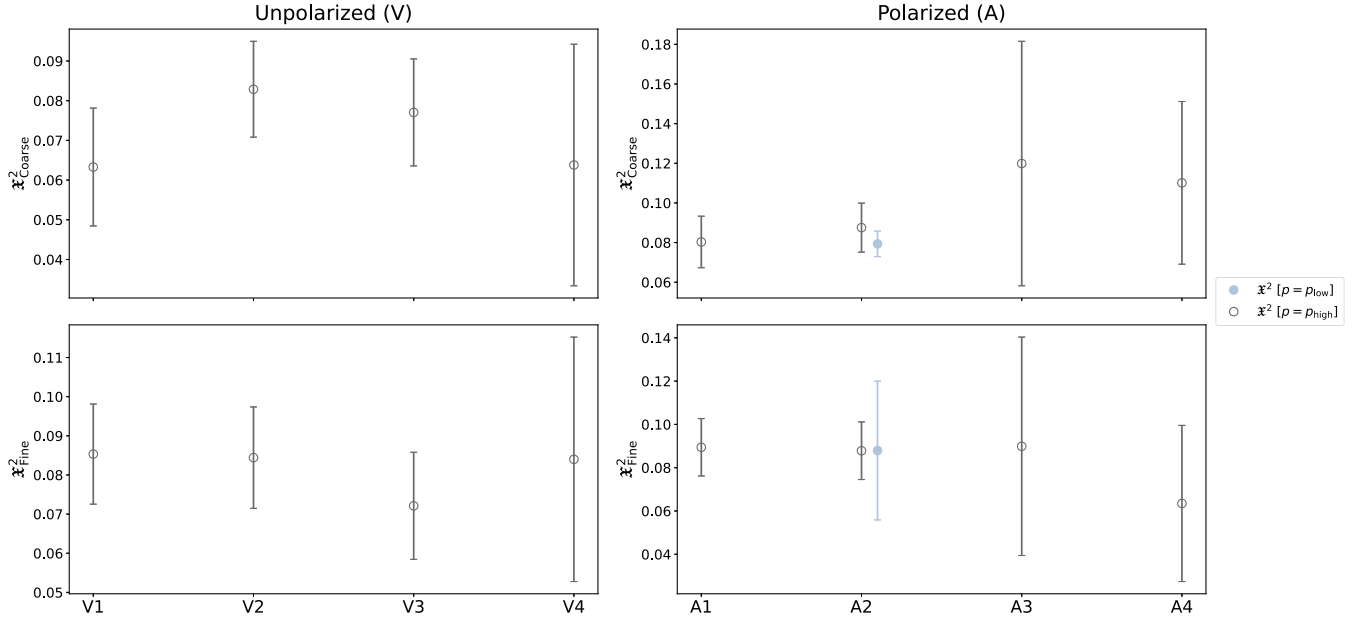


FIG. 15. Overview of the unrenormalized summed ratio results for the vector and axial operators.

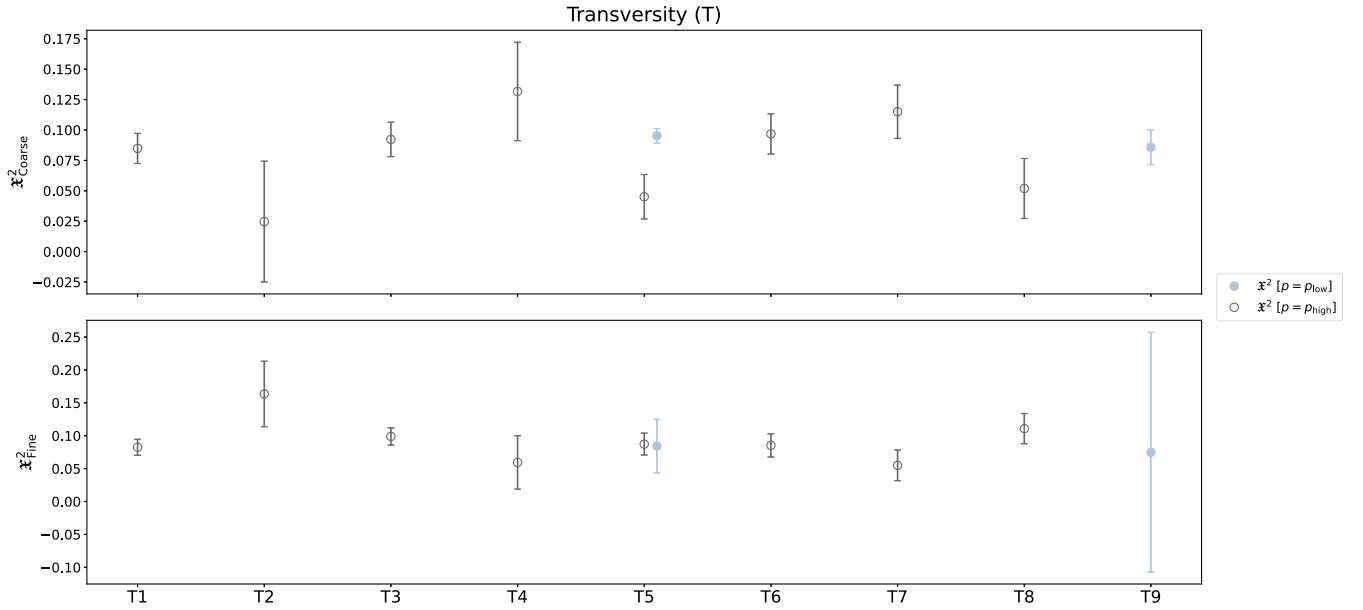


FIG. 16. Overview of the unrenormalized summed ratio results for the tensor operators.

The three functional forms differ in the number of terms retained from the spectral decomposition. For each choice of operator, momentum, and ensemble, we perform one fit for each of three functional forms, repeated for several different data ranges. Given that the ratio depends on two variables, the selection of the data ranges is not unique. We choose to prioritize points (t, τ) with larger values of t and with τ close to $t/2$. This choice is motivated by the expectation that the ratio converges to the matrix element in the limit $t - \tau, \tau \rightarrow \infty$, as stated in Eq. (9). Furthermore,

given the symmetry of the functional forms in Eq. (C1) about the midpoint $\tau = t/2$, we restrict to ranges which are symmetrical about this point. Accordingly, the initial range is chosen as a subset of the points corresponding to the two largest source-sink separations. For each value of t , the initial points are $(\tau - t/2)/a = 0, \pm 1$ if t/a is even and $\pm 1/2, \pm 3/2$ if t/a is odd. The range is then expanded iteratively, cycling continuously from the largest to the smallest values of t until all available points have been considered. For a given t , we add the pair of points (or the

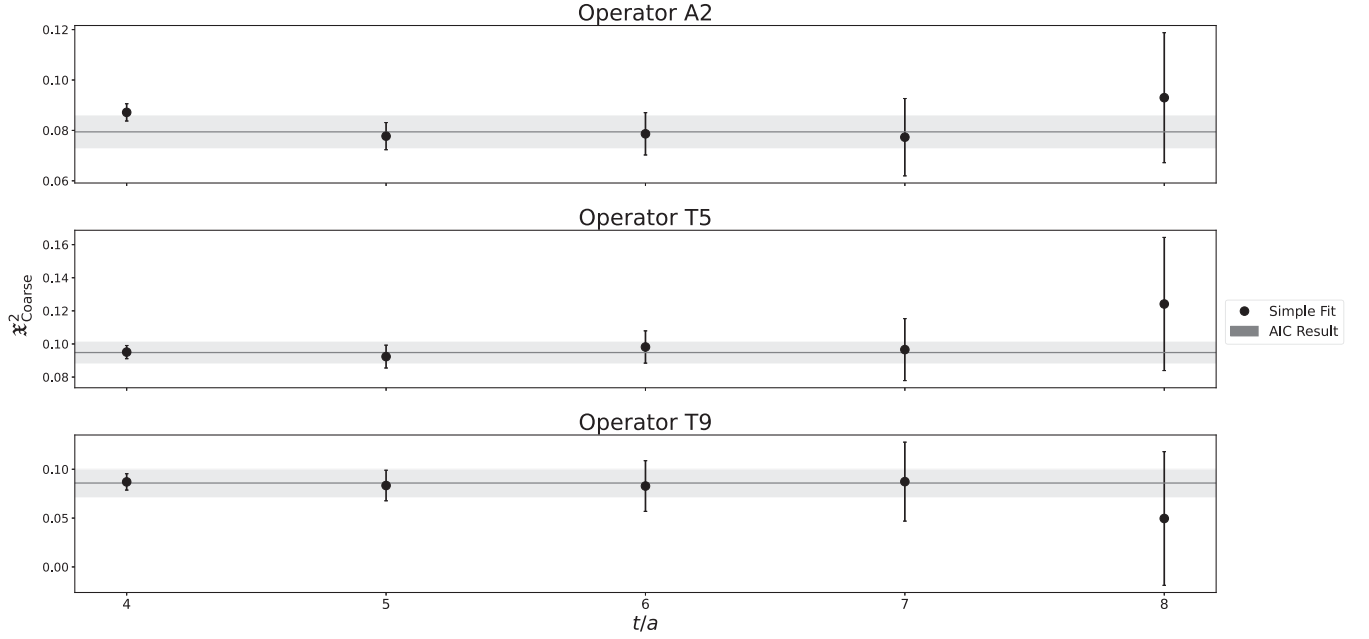


FIG. 17. Comparison of the unrenormalized summed ratio results obtained with the AIC-averaging procedure and results obtained from a simple fit. The gray band indicates the result of the AIC-averaging procedure. The black dots are the result of a single linear regression; they are displayed as a function of the lowest source-sink separation considered.

point) with the smallest value of $|\tau - t/2|$ not yet included. Each time new points are added, a fit is performed. The last fit always includes all the available points. Using this procedure, we perform, for each functional form, a number of fits that goes from a minimum of 4 to a maximum of 16, depending on the number of data points available for each lattice and momentum combination.

The free parameters in the fits are χ^2 , ΔE , $\bar{R}_1$, and $\bar{R}_2$. All parameters exhibit an implicit dependence on the choice of the operator. For $\bar{R}_1$ and $\bar{R}_2$ we used the prior $\mathcal{N}(0, 1)$, i.e., the normal distribution with mean 0 and standard deviation 1. For ΔE , in order to exclude negative energies from the fitting procedure, we used a log-normal prior and enforced a minimum energy gap $\Delta E_{\min} = 100$ MeV. To do so, we have rewritten the energy gap as $\Delta E = \Delta E_{\min} + \Delta E'$ and used $\log \Delta E'$ as the free parameter of the fit. The prior on $\log \Delta E'$ is modeled on the energy gap obtained from the fit of the two-point function. Denoting the latter with ΔE_{2p} , the chosen prior is such that $\log \Delta E' \sim \mathcal{N}(\log \Delta E'_{2p}, 1/2)$, with $\Delta E'_{2p} = \Delta E_{2p} - \Delta E_{\min}$. Depending on the choice of lattice and momentum, ΔE_{2p} ranges approximately from 1 to 1.6 GeV. Regarding χ^2 , the prior is modeled on the value obtained from the summed ratio method. Denoting the central value and standard deviation on the latter with χ^2_S and σ_S , respectively, the chosen prior is a Gaussian distribution with central value χ^2_S and with width $\max(\chi^2_S, \sigma_S)$.

For a given operator, depending on the amount of excited-state contamination, certain kinds of fits, with a given functional form and a given data range, will work

better than the others. To assess which fit is the most relevant, we use the Akaike information criterion [83]

$$\text{AIC} = \chi^2 + 2N_{\text{params}} - 2N_{\text{data}}. \quad (\text{C2})$$

This allows us to combine the estimates we have for the free parameters of the fit, $p \in (\chi^2, \Delta E, \bar{R}_1, \bar{R}_2)$, into one single average

$$\langle p \rangle = \frac{\sum_i e^{-\frac{1}{2}\text{AIC}_i} p_i}{\sum_i e^{-\frac{1}{2}\text{AIC}_i}}, \quad (\text{C3})$$

where the index i runs over all available fits using the parameter p . The weight $e^{-\frac{1}{2}\text{AIC}_i}$ takes into account the goodness of a fit by incorporating the χ^2 . Furthermore, it penalizes fits with a great number of parameters and excluded data points. A lengthy discussion about the validity of model averaging with the AIC, and how it compares to other model-averaging procedures, can be found in [84]. In the generalized form of Eq. (C3) the single parameter p is replaced by an arbitrary function of the parameters $f(p)$. Using this generalization, we can combine the fit curves from the various fits into a single averaged curve. This is the curve we overlay on the data in Figs. 11–14.

As a specific example, we now provide additional details regarding the model-averaging procedure performed on the ratio data for operator V1 on the fine lattice. The ratio data and the outcome of the model-averaging procedure are shown on the bottom-left panel of Fig. 11. In this case we

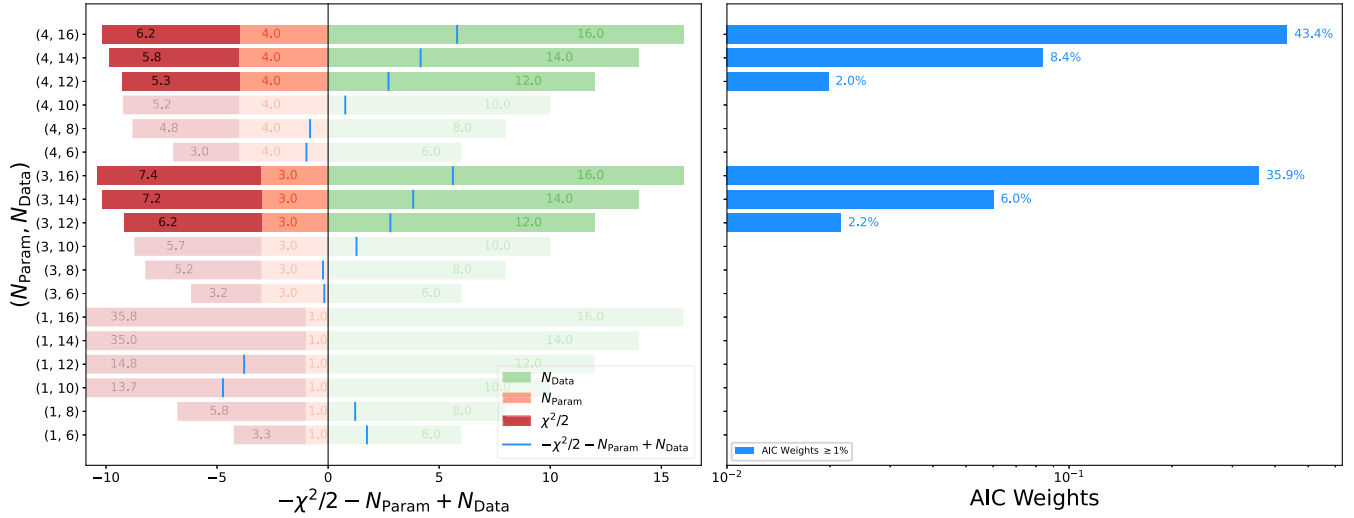


FIG. 18. Overview of the AIC weights for the model-averaging procedure applied to the fine lattice data for operator V1. Left: breakdown of the contributions to the AIC for each fit. The fits are ordered according to increasing number of parameters and included data points. The fits with 1, 3, and 4 parameters correspond to the functional forms (i), (ii), and (iii) of Eq. (C1), respectively. Fits with AIC weight smaller than 1% are shown in faint colors. Right: AIC weights exceeding or equal to 1%.

perform 6 fits for each functional form, for a total of 18 different fits. These fits differ in the number of parameters and in the number of data points employed. An overview of the AIC weight associated with each fit is given in Fig. 18. We find that the overall weight given to constant fits is completely negligible. This is to be expected, as in this case the ratio data are manifestly not compatible to a constant and require accounting for excited states. In contrast, ratio data such as that on the bottom-right panel of Fig. 11 are described well by a constant fit. This reflects on the distribution of the AIC weights being significantly different from the one shown in Fig. 18. The usefulness of the model averaging lies in the fact that we automatically take into account these differences. We perform exactly the same fits in each case, and let any difference in the data reflect in a difference in the AIC weights.

The model-averaging machinery that we just discussed has also been used for the two-point correlators and the summed ratios. In these cases, the discussion is completely analogous, though greatly simplified. For the two-point correlators, only two functional forms have been considered: a simple exponential, from which we extract only the ground-state energy, and the sum of two exponentials, from which we extract also the energy gap of the first excited state. Given that the data are one dimensional, the variation of the number of data points is straightforward. We fix the last time slice and start with a total of six points. We then increase the number of data points from below until we reach the first time slice. For the summed ratios, the only functional form considered is a linear function. The data are again one dimensional, and in this case multiple fits are performed by varying both the first and last value of t considered in the fit. This procedure differs from a simple

fit only when there are more than two source-sink separations available. Both for the two-point correlators and for the summed ratios, the estimates of the free parameters of the fits are combined into one single average using Eq. (C3), exactly as described above.

APPENDIX D: NONPERTURBATIVE RENORMALIZATION

Using mostly the same methods as our earlier work for operators with one derivative [41], we employ the non-perturbative Rome-Southampton method [118] to determine renormalization factors Z_{DDV}^ρ , Z_{DDA}^ρ , and Z_{DDT}^ρ for the two-derivative isovector vector, axial, and tensor operators. These depend on the irreducible representation ρ of the hypercubic group. As intermediate schemes, we use variants of both RI'-MOM [118,119] and RI-SMOM [120], which we then perturbatively convert and evolve to the $\overline{\text{MS}}$ scheme at scale 2 GeV.

In Landau gauge, we compute the quark propagator,

$$S(p) = \int d^4x e^{-ip \cdot x} \langle u(x) \bar{u}(0) \rangle, \quad (\text{D1})$$

and the Green's functions for operator $\mathcal{O}$,

$$G_{\mathcal{O}}(p', p) = \int d^4x' d^4x e^{-ip' \cdot x'} e^{ip \cdot x} \langle u(x') \mathcal{O}(0) \bar{u}(x) \rangle, \quad (\text{D2})$$

yielding the amputated Green's functions

$$\Lambda_{\mathcal{O}}(p', p) = S^{-1}(p') G_{\mathcal{O}}(p', p) S^{-1}(p). \quad (\text{D3})$$

To obtain a precise signal, we employ plane-wave sources to perform a full volume average. Provided that the operator renormalizes diagonally, so do the amputated Green's functions: $\Lambda_O^R = (Z_O/Z_\psi)\Lambda_O$. As in our previous work, we avoid an explicit determination of Z_ψ and instead obtain Z_O/Z_V from ratios, taking Z_V from the determination using pion three-point functions in Ref. [27].

One complication is that our operators do not renormalize diagonally: $\bar{q} \overleftrightarrow{D}_{\{\mu} \overleftrightarrow{D}_{\nu\}} \Gamma q$ can always mix with $\partial_\mu \partial_\nu (\bar{q} \Gamma q)$. We avoid this problem by choosing observables for which the mixing operator (a total derivative) vanishes. This is trivial for the nucleon forward matrix elements and for RI'-MOM kinematics; we will see below that it is also achievable for RI-SMOM.

1. Conditions and matching

Our strategy starts with the decomposition, in the continuum, of $\Lambda_{\mathcal{O}_{\mu\nu}^x}(p', p)$ into products of O(4)-invariant functions and kinematic tensors,

$$\Lambda_{\mathcal{O}_{\mu\nu}^x}(p', p) = \sum_i \Sigma_{\mathcal{O}^x}^{(i)}(p^2) \Lambda_{\mathcal{O}_{\mu\nu}^x}^{(i)}(p', p). \quad (\text{D4})$$

Taking into account the reduced symmetry of the lattice, we then decompose this into irreducible representations of the hypercubic group, replacing $\alpha\mu\nu$ with ρn , where n ranges from 1 to the dimension of ρ . To isolate the O(4)-invariant functions, we take the traces

$$\sum_n \text{Tr}[\Lambda_{\mathcal{O}_{\rho n}^x}^{(i)}(p', p) \Lambda_{\mathcal{O}_{\rho n}^x}(p', p)] = M_{\rho}^{ij}(p', p) \Sigma_{\mathcal{O}^x}^{(j)}(p^2), \quad (\text{D5})$$

where M is a computable kinematic matrix (see [41]). Our tensor decompositions below imply that at tree level, $\Sigma_{\mathcal{O}^x}^{(i)} = \delta^{i1}$, and our preferred renormalization conditions are $\Sigma_{\mathcal{O}_{R,\rho}^x}^{(1)}(\mu^2) = 1$. However, in some cases⁶ M is such that Eq. (D5) cannot be solved for $\Sigma^{(1)}$; when necessary, we add a linear combination of $\Sigma^{(j)}$, $j \neq 1$. For ratios of renormalization factors between two different lattice irreps of the same continuum operator, we take the same linear combination to ensure the ratio is scale and scheme invariant and is unity under restoration of O(4) symmetry.

We now provide the tensor decompositions. For conciseness, only the tensors that have possibly nonzero trace with the tree-level tensor are considered. The two-derivative vector and axial operators are

$$\mathcal{O}_{\mu\nu\rho}^V = -S\bar{\psi}\tau_3\gamma_\mu\overleftrightarrow{D}_\nu\overleftrightarrow{D}_\rho\psi, \quad (\text{D6})$$

⁶This might be avoided by not summing over n , which could yield a larger system of equations constraining $\Sigma^{(i)}$.

$$\mathcal{O}_{\mu\nu\rho}^A = -S\bar{\psi}\tau_3\gamma_\mu\gamma_5\overleftrightarrow{D}_\nu\overleftrightarrow{D}_\rho\psi, \quad (\text{D7})$$

where S takes the symmetric traceless part,

$$ST_{\mu\nu\rho} = \hat{T}_{\mu\nu\rho} - \frac{1}{2}\delta_{\{\mu\nu}\hat{T}_{\rho\}\alpha\alpha}, \quad \hat{T}_{\mu\nu\rho} = T_{\{\mu\nu\rho\}}. \quad (\text{D8})$$

Here we have elected to include a factor of $(-i)^2$ in the operator rather than a factor of i^2 in the tree-level tensor below.⁷ RI'-MOM kinematics correspond to $p' = p$ with scale $\mu^2 = p^2$; we obtain two tensors

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{(1)}(p, p) = S\gamma_\mu p_\nu p_\rho, \quad (\text{D9})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{(2)}(p, p) = \frac{\not{p}}{p^2} S p_\mu p_\nu p_\rho. \quad (\text{D10})$$

For RI-SMOM, $p^2 = (p')^2 = (p' - p)^2 = \mu^2$. Defining $q \equiv p' - p$ and $\bar{p} \equiv (p' + p)/2$, we get six tensors,

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{S(1)}(p', p) = S\gamma_\mu \bar{p}_\nu \bar{p}_\rho, \quad (\text{D11})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{S(2)}(p', p) = S\gamma_\mu q_\nu q_\rho, \quad (\text{D12})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{S(3)}(p', p) = \frac{\not{\bar{p}}}{\bar{p}^2} S \bar{p}_\mu \bar{p}_\nu \bar{p}_\rho, \quad (\text{D13})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{S(4)}(p', p) = \frac{\not{q}}{q^2} S q_\mu \bar{p}_\nu \bar{p}_\rho, \quad (\text{D14})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{S(5)}(p', p) = \frac{\not{\bar{p}}}{\bar{p}^2} S \bar{p}_\mu q_\nu q_\rho, \quad (\text{D15})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho}^V}^{S(6)}(p', p) = \frac{\not{q}}{q^2} S q_\mu q_\nu q_\rho. \quad (\text{D16})$$

Here, imposing C -symmetry results in considerably fewer tensors than Gracey [121]. Since the mixing operator is a second total derivative, its tensor structures must be of the form $Sq_\mu q_\nu \Lambda_\rho$, where Λ_ρ is a tensor of the zero-derivative operator; we therefore conclude that mixing can only occur in $\Sigma^{S(i)}$ for $i \in \{2, 5, 6\}$. For $\mathcal{O}_{\mu\nu\rho}^A$, the tensors contain an additional factor of γ_5 .

The two-derivative tensor operator is

$$\mathcal{O}_{\mu\nu\rho\sigma}^T = -S\bar{\psi}\tau_3\sigma_{\mu\nu}\overleftrightarrow{D}_\rho\overleftrightarrow{D}_\sigma\psi, \quad (\text{D17})$$

⁷The corresponding factor of $-i$ was also included in calculation of Ref. [41], although it was missing from the text of the paper.

where the symmetrization and trace subtraction is given by

$$ST_{\mu\nu\rho\sigma} = \hat{T}_{\mu\nu\rho\sigma} - \frac{5}{8}\hat{T}_{\mu\alpha\{\nu\delta_{\rho\sigma}\}} - \frac{1}{8}\delta_{\{\rho\sigma}\hat{T}_{\nu\}\mu\alpha\alpha} + \frac{6}{8}\delta_{\mu\{\nu\}\hat{T}_{\rho\sigma\}\alpha\alpha},$$

$$\hat{T}_{\mu\nu\rho\sigma} = \tilde{T}_{\mu\{\nu\rho\sigma\}}, \quad \tilde{T}_{\mu\nu\rho\sigma} = \frac{1}{2}(T_{\mu\nu\rho\sigma} - T_{\nu\mu\rho\sigma}). \quad (\text{D18})$$

In RI'-MOM kinematics, we again find two tensors,

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{(1)}(p, p) = \mathcal{S}\sigma_{\mu\nu}p_\rho p_\sigma, \quad (\text{D19})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{(2)}(p, p) = \frac{1}{p^2}\mathcal{S}\sigma_{\mu\alpha}p_\alpha p_\nu p_\rho p_\sigma. \quad (\text{D20})$$

As with the one-derivative case, we find that starting with the antisymmetrization of μ and ν reduces Gracey's three tensors [122] to two. For RI-SMOM, Ref. [123] has 31 tensors within the category we consider. The same antisymmetrization reduces the count to 18, then C -symmetry leaves us with the following ten:

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(1)}(p', p) = \mathcal{S}\sigma_{\mu\nu}\bar{p}_\rho\bar{p}_\sigma, \quad (\text{D21})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(2)}(p', p) = \mathcal{S}\sigma_{\mu\nu}q_\rho q_\sigma, \quad (\text{D22})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(3)}(p', p) = \frac{1}{\bar{p}^2}\mathcal{S}\sigma_{\mu\alpha}\bar{p}_\alpha\bar{p}_\nu\bar{p}_\rho\bar{p}_\sigma, \quad (\text{D23})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(4)}(p', p) = \frac{1}{q^2}\mathcal{S}\sigma_{\mu\alpha}q_\alpha q_\nu\bar{p}_\rho\bar{p}_\sigma, \quad (\text{D24})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(5)}(p', p) = \frac{1}{q^2}\mathcal{S}\sigma_{\mu\alpha}q_\alpha\bar{p}_\nu q_\rho\bar{p}_\sigma, \quad (\text{D25})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(6)}(p', p) = \frac{1}{q^2}\mathcal{S}\sigma_{\mu\alpha}\bar{p}_\alpha q_\nu q_\rho\bar{p}_\sigma, \quad (\text{D26})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(7)}(p', p) = \frac{1}{q^2}\mathcal{S}\sigma_{\mu\alpha}\bar{p}_\alpha\bar{p}_\nu q_\rho q_\sigma, \quad (\text{D27})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(8)}(p', p) = \frac{1}{q^2}\mathcal{S}\sigma_{\mu\alpha}q_\alpha q_\nu q_\rho q_\sigma, \quad (\text{D28})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(9)}(p', p) = \frac{1}{q^2\bar{p}^2}\sigma_{\alpha\beta}\bar{p}_\alpha q_\beta\mathcal{S}\bar{p}_\mu q_\nu\bar{p}_\rho\bar{p}_\sigma, \quad (\text{D29})$$

$$\Lambda_{\mathcal{O}_{\mu\nu\rho\sigma}^T}^{S(10)}(p', p) = \frac{1}{q^2\bar{p}^2}\sigma_{\alpha\beta}\bar{p}_\alpha q_\beta\mathcal{S}\bar{p}_\mu q_\nu q_\rho q_\sigma, \quad (\text{D30})$$

and mixing can only occur in $\Sigma^{S(i)}$ for $i \in \{2, 7, 8, 10\}$.

After converting to $\overline{\text{MS}}$, we evolve using the four-loop anomalous dimension for the vector and axial cases [124,125] and the three-loop anomalous dimension for the tensor case [122]. For RI'-MOM, we use three-loop matching [122], whereas for RI-SMOM, matching is done

at three-loop order for the vector and axial operators [126] and two-loop order for the tensor [123].

2. Calculation

We again follow Refs. [27,41]. Using periodic boundary conditions in space and time for the quarks (this is partially twisted, since the sea quarks are antiperiodic in time), we construct plane-wave sources with momenta either along the four-dimensional diagonal $p^{(i)} \in \{\frac{2\pi}{L}(k, k, k, k), \frac{2\pi}{L}(k, k, k, -k)\}$ or along the two-dimensional diagonal $p^{(i)} \in \{\frac{2\pi}{L}(k, k, 0, 0), \frac{2\pi}{L}(k, 0, k, 0)\}$, where $k \in \{2, 3, \dots, \frac{L}{4a}\}$. This allows both RI'-MOM and RI-SMOM kinematics for each of the diagonals. On the fine ensemble, we used 54 gauge configurations. Likewise, on the coarse ensemble, we initially chose 54 configurations; however, on one configuration, the twisted boundary condition made the Dirac operator near singular and the multigrid solver was unable to converge. Omitting this configuration, we used the remaining 53.

After perturbatively matching to $\overline{\text{MS}}$ and evolving to the scale 2 GeV, there remains residual dependence on the scale μ . This is caused by the window problem of being unable to neglect effects of both orders $a^2\mu^2$ and $\Lambda_{\text{QCD}}^2/\mu^2$. We first apply a tree-level correction factor⁸ $[(\sin \frac{2\pi a}{L}k)/(\frac{2\pi a}{L}k)]^2$. Then following Ref. [127], we fit the data using a polynomial in μ^2 plus sometimes a pole term, i.e., with the form $A + B\mu^2 + C\mu^4 + D/\mu^2$; the constant term A is our estimate of the ratio Z_O/Z_V .

Estimates of the ratio Z_O/Z_V for one irrep of the two-derivative vector, axial, and tensor operators are shown in Fig. 19. Systematic uncertainties are explored by performing three fits for each operator and renormalization scheme: (a) the 4D data in the range $\mu^2 \in [4, 20]$ GeV², (b) the 2D data in the range $[4, 15]$ GeV², and (c) setting $D = 0$, the 4D data in the range $[10, 30]$ GeV², which has limited sensitivity to a μ^{-1} term. The fit quality to these sometimes very precise data can be poor, so we scale the statistical uncertainty by $\sqrt{\chi^2/\text{degrees of freedom}}$ whenever this is greater than 1. The systematic uncertainty, which we estimate from the spread of results, is dominant, and we conservatively take the maximum of statistical uncertainties among the fits.

For the two-derivative tensor operator, we computed matrix elements belonging to three different irreps. The two relevant ratios of renormalization factors in different irreps, Z_{DDT}'/Z_{DDT}'' are shown in Fig. 20. We were only able to identify the same $O(4)$ -invariant function in two different irreps using RI'-MOM kinematics. As perturbation theory is not required here, we can use much smaller momenta, performing fits with $D = 0$ to (a) the 4D data in the range

⁸The square root of this was also used as a correction in Ref. [41], although not mentioned in the article.

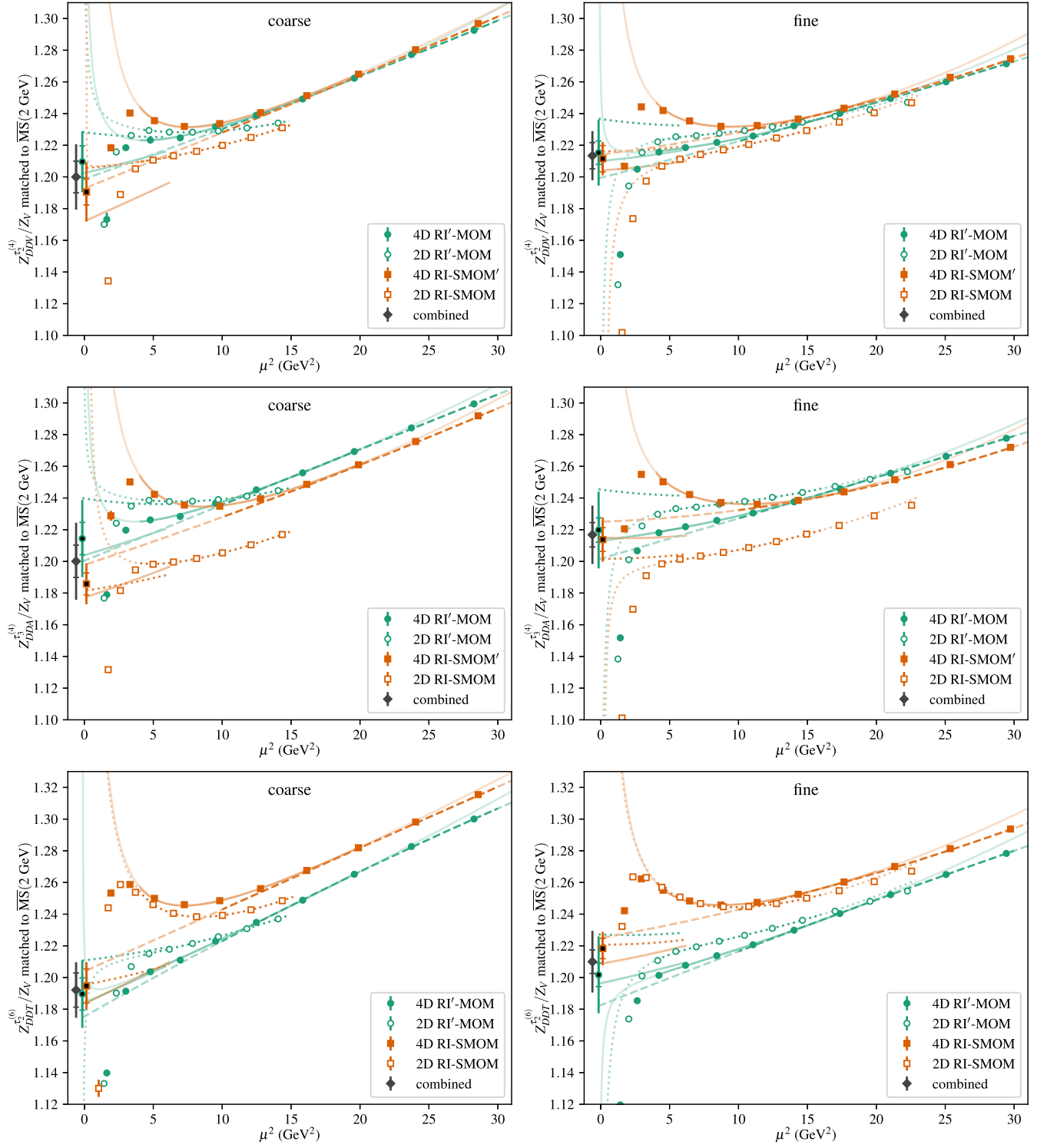


FIG. 19. Ratios of renormalization factors $Z_{DDV}^{\tau_2^{(4)}}/Z_V$ (top), $Z_{DDA}^{\tau_3^{(4)}}/Z_V$ (middle), and $Z_{DDT}^{\tau_5^{(6)}}/Z_V$ (bottom) on the coarse (left) and fine (right) ensembles, determined using RI'-MOM (green circles) and RI-SMOM (orange squares) kinematics and then matched to $\overline{\text{MS}}$ at scale 2 GeV. The open and filled symbols correspond to momenta along the two- and four-dimensional diagonals, respectively. For most points, the statistical error is smaller than the symbol. In most cases, the renormalization condition is $\Sigma^{(1)}(\mu^2) = 1$ or $\Sigma^{S(1)}(\mu^2) = 1$; RI-SMOM' indicates the condition $\Sigma^{S(1)}(\mu^2) + \Sigma^{S(3)}(\mu^2) = 1$; and the tensor RI-SMOM condition is $\Sigma^{S(1)}(\mu^2) + \frac{1}{2}\Sigma^{S(4)}(\mu^2) + \frac{1}{4}\Sigma^{S(5)}(\mu^2) = 1$. Fits (a) are shown with solid curves, (b) are shown with dotted curves, and (c) are shown with dashed curves; they are also shown with the pole term set to zero in the range $\mu^2 \in [0, 6]$ GeV². The points near $\mu^2 = 0$ show the combined estimates with statistical and systematic uncertainties.

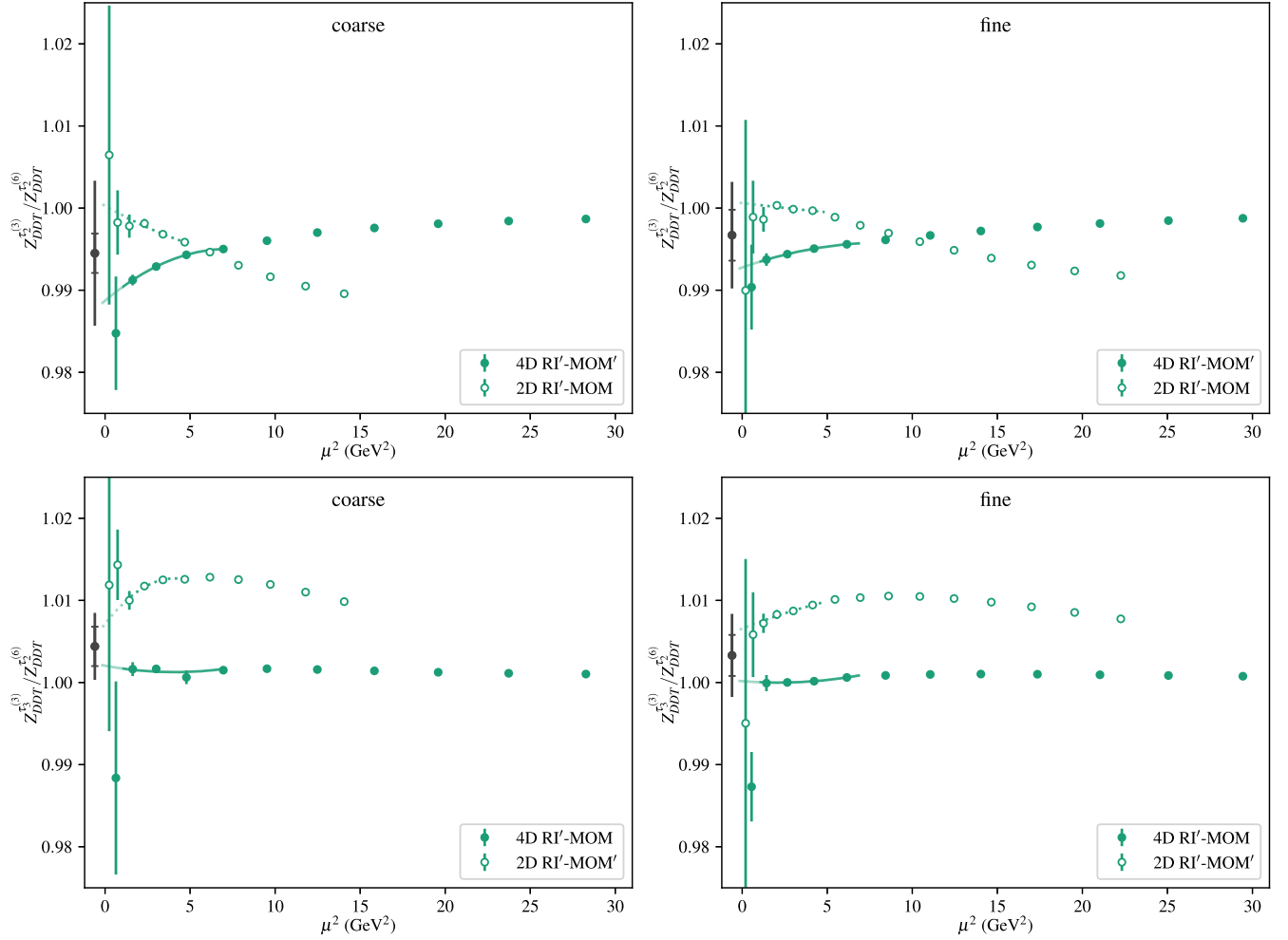


FIG. 20. Scale and scheme-invariant ratios of renormalization factors $Z_{DDT}^{\tau_3^{(3)}}/Z_{DDT}^{\tau_2^{(6)}}$ (top) and $Z_{DDT}^{\tau_3^{(3)}}/Z_{DDT}^{\tau_2^{(6)}}$ (bottom) on the coarse (left) and fine (right) ensembles, determined using the condition $\Sigma^{(1)}(\mu^2) = 1$ (RI'-MOM) or $\Sigma^{(1)}(\mu^2) + \frac{1}{2}\Sigma^{(2)}(\mu^2) = 1$ (RI'-MOM'). Fits (a) are shown with solid curves and fits (b) are shown with dotted curves.

$\mu^2 \in [1, 8] \text{ GeV}^2$ and (b) the 2D data in the range $[1, 5] \text{ GeV}^2$. These ratios are mostly within 1% of unity.

Our final ratios of renormalization factors are given in Table III.

APPENDIX E: CONTINUUM ESTIMATE

In this Appendix, we provide a functional-form and prior-width study motivating the choices we made for the continuum estimate in Sec. IV. For the continuum estimate, we tested the following *Ansätze*:

- (i) $\langle x^2 \rangle(a) = \langle x^2 \rangle_{\text{cont}}$,
 - (ii) $\langle x^2 \rangle(a) = \langle x^2 \rangle_{\text{cont}} \cdot (1 + m_1 \alpha_s a \Lambda_{\text{QCD}})$,
 - (iii) $\langle x^2 \rangle(a) = \langle x^2 \rangle_{\text{cont}} \cdot (1 + m_2 (a \Lambda_{\text{QCD}})^2)$,
 - (iv) $\langle x^2 \rangle(a) = \langle x^2 \rangle_{\text{cont}} \cdot (1 + m_1 (\alpha_s a \Lambda_{\text{QCD}}) + m_2 (a \Lambda_{\text{QCD}})^2)$.
- (E1)

The functional form (i) represents a fit to a constant. The functional forms (ii) and (iii) are two-parameter fits and are, respectively, linear and quadratic in the lattice spacing. The functional form (iv) is that of Eq. (18) and, as stated in Sec. IV, is the functional form we expect in our case. However, the functional form (iv) has three free parameters. Having only two lattice spacings, a fit to this functional form requires the use of priors. We constrained the parameters m_1 and m_2 with the Gaussian prior $\mathcal{N}(0, \sigma)$ and performed the fit to the form (iv) multiple times, varying σ from 0.5 to 32.

The results we obtain are presented in Fig. 21. In the figure, the continuum value $\langle x^2 \rangle_{\text{cont}}$ is plotted for each of the functional forms employed for the extrapolation and, in the case of form (iv), for each choice of prior width. The value that we choose as our final result is highlighted with a yellow star in the figure. As is evident, for each channel, our choice is completely compatible with the outcome of a constant fit, but it exhibits a larger

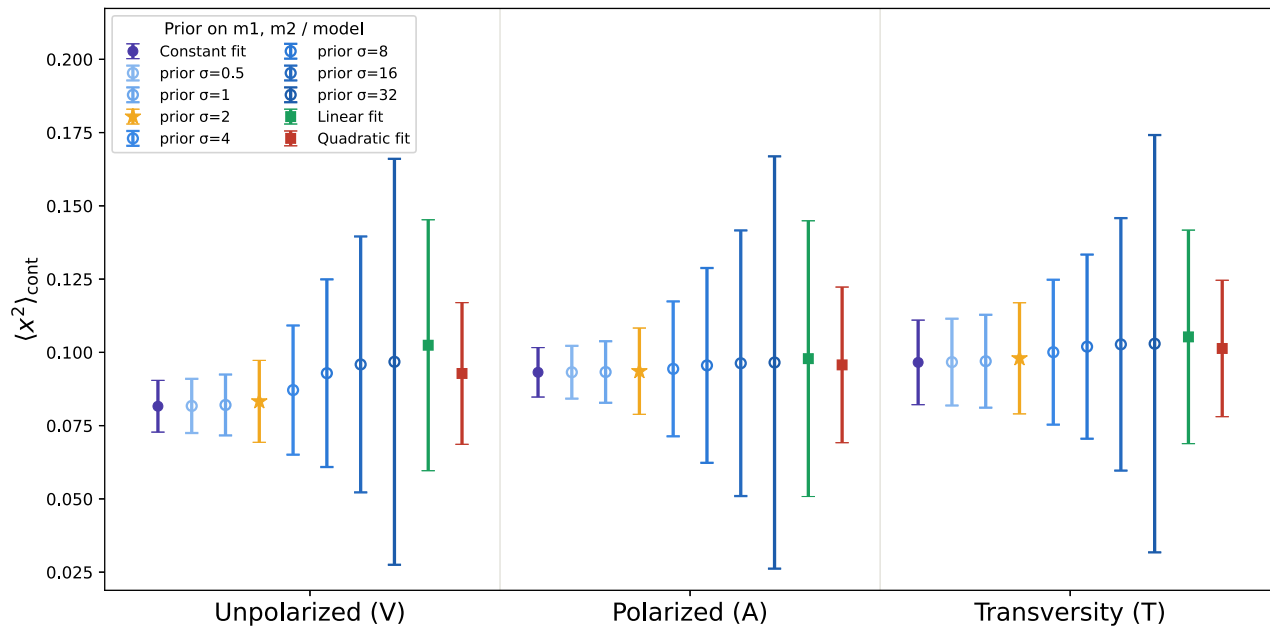


FIG. 21. Prior-width and functional-form study of the continuum estimate. For the three channels, the obtained value $\langle x^2 \rangle_{\text{cont}}$ is plotted for different choices of functional form and prior width on the parameters. A filled circle is used for the outcome of the fit to a constant. Empty circles are used for the three-parameter fits, where m_1 and m_2 are constrained by the Gaussian prior $\mathcal{N}(0, \sigma)$; from left to right in the plot, σ increases from 0.5 to 32. The value corresponding to $\sigma = 2$ is highlighted with a yellow star. The outcomes of the linear and quadratic two-parameter fits are plotted with a green and red square, respectively.

uncertainty. This fact justifies our preference for a prior-constrained estimate over a constant fit. In the case of functional form (iv), an increasing value of the prior width σ leads, as expected, to results characterized by an increasing uncertainty. More interestingly, the central values of the results remain stable; we observe a slight upward trend in central values for increasing values of σ , but these values are in any case compatible with ours. Analogously, the results of the linear and quadratic

two-parameter fits are compatible with our results, but they exhibit a larger uncertainty.

Given the functional-form and prior-width study presented here, we can conclude that our choice for the continuum estimates is the best one available with the given data. Although obtained from a prior-constrained extrapolation, our results show no significant difference in central values with respect to the results of a fit to a constant. Moreover, they exhibit a smaller uncertainty compared to that of the values obtained from the other models studied.

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