Nucleon and pion structure with lattice QCD simulations at physical value of the pion mass

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We present results on the nucleon scalar, axial and tensor charges as well as on the momentum fraction, and the helicity and transversity moments. The pion momentum fraction is also presented. The computation of these key observables is carried out using lattice QCD simulations at a physical value of the pion mass. The evaluation is based on gauge configurations generated with two degenerate sea quarks of twisted mass fermions with a clover term. We investigate excited states contributions with the nucleon quantum numbers by analyzing three sink-source time separations. We find that, for the scalar charge, excited states contribute significantly and to a less degree to the nucleon momentum fraction and helicity moment. Our result for the nucleon axial charge agrees with the experimental value. Furthermore, we predict a value of 1.027(62) in the MS scheme at 2 GeV for the isovector nucleon tensor charge directly at the physical point. The pion momentum fraction is found to be $\langle x \rangle_{u-d} = 0.214(15)(^{+12}_{-9})$ in the MS at 2 GeV.

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I. INTRODUCTION

The nucleon axial-vector coupling or nucleon axial charge $g_A$ is experimentally a well known quantity determined from the $\beta$-decay of the neutron. It is a key parameter for understanding the chiral structure of the nucleon and a quantity that has been studied extensively in chiral effective theories [1,2]. A description of baryon properties in chiral effective theory requires as an input $g_A$ and thus its value at the chiral limit and its dependence on the pion mass constitute important information that lattice QCD can provide. Its importance for phenomenology as well as the fact that it is rather straightforward to compute in lattice QCD have made it one of the most studied quantities within different fermion discretization schemes [3-9]. In lattice QCD, $g_A$ is determined directly from the zero momentum transfer nucleon matrix element of the axial-vector current without requiring any extrapolation from finite momentum transfer calculations as, for example, is required for the anomalous magnetic moment of the nucleon. In addition, being an isovector quantity, it does not receive any contributions from the coupling of the current to closed quark loops and thus one only needs to compute the connected contribution with well established lattice QCD techniques. Therefore, $g_A$ has come to be regarded as a prime benchmark quantity for the computation of lattice QCD matrix elements. Postdiction of the value of $g_A$ within lattice QCD is, therefore, regarded as an essential step before the reliable prediction of other couplings and form factors for which the same formalism is used.

Unlike $g_A$, the nucleon scalar and tensor charges are not well known. Limits on the value of the scalar and tensor coupling constants arise from $0^+ \rightarrow 0^+$ nuclear decays and the radiative pion decay $\pi \rightarrow e^+\nu\gamma$, respectively. They have become the focus of planned experiments to search for physics beyond the familiar weak interactions of the Standard Model sought in the decay of ultra-cold neutrons [10]. The computation of the tensor charge is particularly timely since new experiments using polarized $^3$He/Proton at Jefferson lab aim at increasing
the experimental accuracy of its measurement by an order of magnitude \cite{11}. In addition, experiments at LHC are expected to increase the limits to contributions arising from tensor and scalar interactions by an order of magnitude making these observables interesting probes of new physics originating at the TeV scale. Computing the scalar charge will also provide input for dark matter searches. Experiments, which aim at a direct detection of dark matter, are based on measuring the recoil energy of a nucleon hit by a dark matter candidate. In many supersymmetric scenarios \cite{12} and in some Kaluza-Klein extensions of the standard model \cite{13,14} the dark matter nucleon interaction is mediated through a Higgs boson. In such a case the theoretical expression of the spin independent scattering amplitude at zero momentum transfer involves the quark content of the nucleon or the nucleon sigma-term, which is closely related to the scalar charge. In fact, this contributes the largest uncertainty on the nucleon dark matter cross section. Therefore, computing the scalar $q_\delta$ and tensor $q_T$ charges of the nucleon within lattice QCD will provide useful input for the ongoing experimental searches for beyond the standard model physics.

Another experimental frontier that provides information on the quark and gluon structure of a hadron, is the measurement of parton distribution functions (PDFs) in a variety of high energy processes such as deep-inelastic lepton scattering and Drell-Yan in hadron-hadron collisions. PDFs give, to leading twist, the probability of finding a specific parton in the hadron carrying certain momentum and spin, in the infinite momentum frame. Their universal nature relies on factorization theorems that allow differential cross-sections to be written in terms of a convolution of certain process-dependent coefficients that encode the hard perturbative physics and process-independent PDFs that describe the soft, non-perturbative physics at a factorization energy scale $\mu$ \cite{13,14}. Because these PDFs are light-cone correlation functions it is not straightforward to calculate them directly in Euclidean space. Instead, one calculates Mellin moments of the PDFs expressed in terms of hadron matrix elements of local operators, which through the operator product expansion are related to the original light-cone correlation functions. Mellin moments are measured or extracted from phenomenological analyses in deep-inelastic scattering experiments and thus they can be directly compared to lattice results when converted to the same energy scale $\mu$.

In this work, we consider the three first moments that one can construct, namely the first moment of the spin-independent (or unpolarized) $q = q_l + q_T$, helicity (or polarized) $\Delta q = q_l - q_T$, and transversity $\delta q = q_T + q_L$ distributions, which are define as follows:

$$\langle x \rangle_q = \int_0^1 x [q(x) + \bar{q}(x)] \, dx \quad (1)$$

$$\langle x \rangle_{\Delta q} = \int_0^1 x [\Delta q(x) - \Delta \bar{q}(x)] \, dx \quad (2)$$

$$\langle x \rangle_{\delta q} = \int_0^1 x [\delta q(x) + \delta \bar{q}(x)] \, dx \quad (3)$$

where $q_l$ and $q_T$ correspond respectively, to quarks with helicity aligned and anti-aligned with that of a longitudinally polarized target, and $q_T$ and $q_L$ correspond to quarks with spin aligned and anti-aligned with that of a transversely polarized target. These moments, at leading twist, can be extracted from the hadron matrix elements of one-derivative vector, axial-vector and tensor operators at zero momentum transfer. Thus, they constitute the next level of observables in terms of complexity that can be computed in lattice QCD after the coupling constants that do not involve derivative operators. The unpolarized and polarized moments $\langle x \rangle_q$ and $\langle x \rangle_{\Delta q}$ of the nucleon are measured experimentally and thus lattice QCD provides a postdiction, while a computation of the nucleon transversity $\langle x \rangle_{\delta q}$ provides a prediction. It is worth mentioning a new approach proposed recently for measuring directly the PDFs within lattice QCD \cite{17,18}, which is currently under investigation \cite{19,20}.

In this paper, we extend the analysis of meson masses, the muon anomalous magnetic moment $g - 2$ and the meson decay constants considered in Ref. \cite{21}, to the nucleon matrix elements for the three first Mellin moments while for the pion we compute the momentum fraction. While the present paper builds on the methodology developed in Refs. \cite{22,26}, this work presents the first evaluation of these six quantities directly at the physical value of the pion mass. This is a substantial step forward since it avoids chiral extrapolations, which are often difficult and can lead to rather large systematic uncertainties.

The paper is organized as follows: In section II we define the nucleon and pion matrix elements, in section III we explain the lattice methodology, in section IV we give the simulation details and in section V our results. Section VI summarizes our findings and gives our conclusions.

II. MATRIX ELEMENTS

A. Nucleon

We are interested in extracting the forward nucleon matrix elements $\langle N(p)|O|N(p)\rangle$, with $p$ the nucleon initial and final momentum. We consider the complete set of local and one-derivative operators, yielding a non-zero result. The local scalar, axial-vector, and tensor operators are:
\[ \mathcal{O}_{S\alpha} = \bar{q} \frac{\tau^\alpha}{2} q, \quad \mathcal{O}_{A\mu}^\nu = \bar{q} \gamma_5 \gamma^\mu \frac{\tau^\alpha}{2} q, \quad \mathcal{O}_{T\mu}^\nu = \bar{q} \sigma^{\mu\nu} \frac{\tau^\alpha}{2} q. \]

We do not consider the vector operator \( \bar{\psi}(x) \gamma_m u(x) \psi(x) \) since this yields the renormalization constant \( Z_V \), which we calculate separately using our RI-MOM setup, as explained in section V. If one instead uses the lattice conserved Noether current, which we typically do in our computation of the nucleon electromagnetic form factors, we will need at least an order of magnitude more statistics than this work. The disconnected contributions receive disconnected contributions. Our high statistics study using an \( N_f = 2 + 1 + 1 \) ensemble of twisted mass fermions with pion mass of 373 MeV has shown that the disconnected contributions for the tensor isoscalar charge and the isoscalar first moments are very small compared to the connected. In the same study, the disconnected contributions to the isoscalar axial and scalar charge were found to be about (7-10)% of the connected. In this work, we will only compute the connected contributions. The disconnected contributions will need at least an order of magnitude more statistics and will be presented in a follow-up publication.

In what follows all expressions will be given in Euclidean time. For example, the one-derivative vector current that will be used in the computations of both nucleon and pion momentum fractions, in Euclidean time and setting \( \mu = \nu = 4 \), is given by:

\[ \mathcal{O}_{V\mu}^{4\mu} = \bar{q} \gamma_4 D^{4\mu} - \frac{1}{3} \sum_{k=1}^{3} \gamma^k \bar{D}^k \frac{\tau^\alpha}{2} q. \]

In this work, we consider the isovector quantities obtained from Eqs. (1) and (3) by using the Pauli matrix \( \tau^3 \). We also consider the isoscalar combination obtained by replacing \( \tau^\alpha \) with unity. The individual up- and down-quark combinations can be extracted form the isovector and isoscalar quantities which are equivalent to replacing \( \tau^\alpha \) with the projectors onto the up- or down- quarks. The isoscalar combination and the up- and down-quark contributions receive disconnected contributions. Our high statistics study using an \( N_f = 2 + 1 + 1 \) ensemble of twisted mass fermions with pion mass of 373 MeV has shown that the disconnected contributions for the tensor isoscalar charge and the isoscalar first moments are very small compared to the connected. In the same study, the disconnected contributions to the isoscalar axial and scalar charge were found to be about (7-10)% of the connected. In this work, we will only compute the connected contributions. The disconnected contributions will need at least an order of magnitude more statistics and will be presented in a follow-up publication.

For zero momentum transfer, the nucleon matrix elements of the local operators in Eq. (4) can be decomposed in the following form factors:

\[ \langle N(p, s') | \mathcal{O}_S | N(p, s) \rangle = \bar{u}_N(p, s') \left[ \frac{1}{2} G_S(0) \right] u_N(p, s), \]

\[ \langle N(p, s') | \mathcal{O}_A^\mu | N(p, s) \rangle = i \bar{u}_N(p, s') \left[ \frac{1}{2} G_A(0) \gamma^\mu \gamma_5 \right] u_N(p, s), \]

\[ \langle N(p, s') | \mathcal{O}_T^{\mu\nu} | N(p, s) \rangle = \bar{u}_N(p, s') \left[ \frac{1}{2} A_{T10}(0) \sigma^{\mu\nu} \right] u_N(p, s). \]

Thus, the scalar matrix element at zero momentum transfer yields the form factor \( G_S(0) \equiv g_S \), the local axial-vector \( G_A(0) \equiv g_A \) and the local tensor matrix element \( A_{T10}(0) \equiv g_T \). In all these quantities the operators are either the isovector or isoscalar combinations, or individual up- or down-quark contributions. At non-zero momentum, additional form-factors arise in the decomposition of Eqs. (6) and (7). Namely, the induced pseudo-scalar \( G_p(Q^2) \) appears as the second form factor in the decomposition of the matrix element of the axial-vector and the form factors \( B_{T10}(Q^2) \) and \( A_{T10}(Q^2) \) appear in the decomposition of the nucleon matrix element of the tensor operator, where \( Q^2 \) is the momentum transfer square in Euclidean time. These cannot be extracted at zero momentum transfer and will not be considered in this work.

The corresponding decomposition for the one-derivative operators in Eq. (5) is given by:
\[ \langle N(p, s')|\mathcal{O}^{\mu
u}_{b}\rangle|N(p, s)\rangle = \bar{u}_N(p, s') \left[ \frac{1}{2} A_{20}(0) \gamma^{[\mu} p^{\nu]} \right] u_N(p, s), \] \[ \langle N(p, s')|\mathcal{O}^{\alpha}_{a}\rangle|N(p, s)\rangle = i \bar{u}_N(p, s') \left[ \frac{1}{2} \tilde{A}_{20}(0) \gamma^{(\mu} p^{\nu)} \gamma^5 \right] u_N(p, s), \] \[ \langle N(p, s')|\mathcal{O}^{\mu
u}_{T}\rangle|N(p, s)\rangle = i \bar{u}_N(p, s') \left[ \frac{1}{2} A_{T20}(0) \sigma^{[\mu} p^{\nu]} \right] u_N(p, s). \]

The momentum fraction, helicity moment, and the transversity moment are obtained from the above forward matrix elements by \( \langle x \rangle_q = A^T_{20}(0), \langle x \rangle_{\Delta q} = \tilde{A}^q_{20}(0) \), and \( \langle x \rangle_{\delta q} = A^T_{T20}(0) \) respectively. Here we use the generic symbol \( q \) to denote the quark combination, where \( q = u + d \) will denote the isoscalar combination, \( q = u - d \) will denote the isovector combination and \( q = u \) or \( q = d \) denotes the individual up- and down-quark contributions. For instance, the isovector helicity moment will be denoted as \( \langle x \rangle_{\Delta u - \Delta d} = A^T_{A20}(0) \). For uniformity in our notation we will also write \( q^\mu_{A-d} \) for the nucleon axial charge, despite the fact that the measured axial charge is understood to be an isovector quantity.

**B. Pion**

The isovector momentum fraction of the pion \( \langle x \rangle^\pm_{u-d} \), can be extracted from the corresponding pion matrix element of the one-derivative vector operator. Specifically we use the following operator, sometimes also denoted as

\[ G^{\mu_1, \ldots, \mu_n}_{3pt}(\Gamma^\nu, p, t_s, t_{ins}) = \sum_{x_s, x_{ins}} e^{-i(x_s - x_0) \cdot p} \Gamma^\nu \beta_\alpha (J_{\alpha}(x_s, t_s) \mathcal{O}^{\mu_1, \ldots, \mu_n}_{\Gamma}(x_{ins}, t_{ins}) \tilde{J}_\beta(x_0, t_0)) \]

where \( x_0, x_{ins} \) and \( x_s \) are the source, insertion and sink coordinates respectively. In order to cancel unknown overlaps of the interpolating field with the nucleon state as well as the time evolution in Euclidean time we construct ratios of the three-point function with the two-point function, which is given by

\[ G_{2pt}(0, t_s) = \sum_{x_s} \Gamma^4 \beta_\alpha (J_{\alpha}(x_s, t_s) \tilde{J}_\beta(x_0, t_0)). \]

The projection matrices are

\[ \Gamma^4 = \frac{1}{4}(1 + \gamma_4), \quad \Gamma^k = \Gamma^4 i \gamma_5 \gamma_k. \]

We use the proton interpolating operators:

\[ J_{\alpha}(x) = \epsilon^{abc} u^a_\alpha(x) [u^\dagger b(x) C \gamma_\delta d^c(x)] \]

with \( a, b \) and \( c \) denoting color components. We employ Gaussian smeared quark fields \([29, 30]\) to increase the overlap with the proton state and decrease overlap with excited states. The smeared interpolating fields are given by

\[ q^{ab}_{\text{smeared}}(t, x) = \sum_y F^{ab}(x, y; U(t)) q^b(t, y), \]

\[ F = (I + a_G H)^{N_G}, \]

\[ H(x, y; U(t)) = \sum_{i=1}^3 [U_i(x) \delta_{x,y-i} + U_i^\dagger(x-i) \delta_{x,y+i}] \]

We apply APE-smearing to the gauge fields \( U_\mu \) entering the hopping matrix \( H \). The parameters for the Gaussian smearing \( a_G \) and \( N_G \) are optimized using the nucleon ground state \([31]\) such as to give a root mean square radius of about 0.5 fm. We use \( (N_G, a_G) = (50, 4) \) and \( (N_{APE}, a_{APE}) = (50, 0.5) \).
For the case of isovector quantities, the so-called disconnected contributions arising from the coupling of the nucleon interpolating operators with the nucleon spinors to nucleon three-point functions. FIG. 1: Connected (upper) and disconnected (lower) contributions to nucleon three-point functions.

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with
\[
G_{\text{Sp}}^{\lambda}(0, t_s, t_{\text{ins}}) = \sum_y \langle J_{\pi^\pm}(t_s) \, O_{\lambda}^{\lambda}(t_{\text{ins}}, y) \, J_{\pi^\pm}^+(t_0) \rangle.
\]

(23)

with \( J_{\pi^\pm}(x) = \bar{d}(x)\gamma_5 u(x) \) (\( J_{\pi^-}(x) = \bar{u}(x)\gamma_5 \bar{d}(x) \)) is the interpolating field of \( \pi^+ \) (\( \pi^- \)). As in the case of the nucleon, in the isovector combination up to lattice artifacts, the disconnected contributions vanish and will thus be dropped.

The pion two- and three-point correlators, unlike those of the nucleon, are evaluated by using a stochastic time-slice source (Z(2)-noise in both real and imaginary part) \([33,34]\) for all color, spin and spatial indices. This method, which is particularly suited for the pion, has been first applied to moments of parton distribution functions in Ref. \([36]\). The quark propagator \( S_{\lambda}^b(y) \) is obtained by solving

\[
\sum_y D_{\alpha\beta}^{ab}(z, y) \, S_{\beta}^b(y) = \xi(z)^{\alpha}_a \delta_{z_0, t_0} \quad \text{(source at } t_0) \quad (24)
\]

for \( S \). \( \xi(z)^{\alpha}_a \) is a \( Z(2) \) random source satisfying

\[
\begin{align*}
\langle \xi^*(x)^{\alpha}_a \xi(y)^{\beta}_b \rangle_r &= \delta_{xy} \delta_{ab} \delta_{\alpha\beta}, \\
\langle \xi(x)^{\alpha}_a \xi(y)^{\beta}_b \rangle_r &= 0,
\end{align*}
\]

(25)

where \( \langle \rangle_r \) denotes the average over many random sources. Using \( S \) we can define a so-called sequential or generalized propagator \( \Sigma_{\beta}^b(y) \) from \([37]\).

\[
\sum_y D_{\alpha\beta}^{ab}(z, y) \, \Sigma_{\beta}^b(y) = \gamma_5 \, S_{\alpha}^a(z) \delta_{z_0, t_s} \quad \text{(sink at } t_s). \quad (26)
\]

This method represents a generalization of the one-end-trick \([35]\) to moments of parton distribution functions. Its clear advantage is an increased signal to noise ratio at reduced computational costs at least when it is applied for meson observables. With a point source, 24 inversions per gauge configuration are needed: 12 (3 colors \( \times \) 4 spins) for the quark propagator and 12 for the generalized propagator. With the stochastic source discussed above, only two inversions are needed: one for the quark propagator and another one for the generalized propagator. For a comparison of stochastic versus point sources we refer to Ref. \([36]\).

The stochastic method described above can be adapted to work for other mesons. However, for moments of nucleon parton distribution functions we found no improvement in the signal to noise ratio for a comparable computational effort.

For \( \langle x \rangle_{u-d}^\pm \) it is sufficient to fix \( t_s - t_0 = T/2 \), where \( T \) is the temporal extent of the lattice. As in the case of the nucleon, the value of \( t_0 \) is chosen randomly on every gauge configuration in order to reduce autocorrelation.

### B. Ensuring ground state dominance

To extract the nucleon matrix element from the ratio defined in Eq. \([19]\) one needs to make sure that the contribution of the terms due to the excited states in numerator and denominator of Eq. \([21]\), the so-called contamination due to excited states, is negligible. We will employ three methods to check for ground state dominance, as described below.

In the first method, which we will refer to as the plateau method, one probes the region for which \( \Delta(t_s - t_{\text{ins}}) \gg 1 \) and \( \Delta(t_{\text{ins}} - t_0) \gg 1 \) such that excited state contributions are much smaller than the contribution of the ground state. Within this time interval the ratio becomes time independent and the time range where this happens is referred to as the plateau region. Fitting the ratio

\[
R(\Gamma^\lambda, t_s, t_{\text{ins}}) = \frac{\Delta(t_s - t_{\text{ins}}) \gg 1}{\Delta(t_{\text{ins}} - t_0) \gg 1} \quad \Pi(\Gamma^\lambda)
\]

(27)

over \( t_{\text{ins}} \) within this plateau region one obtains the plateau value, which is the desired matrix element \( \mathcal{M} \).

To ensure excited state suppression one repeats this procedure for multiple values of \( t_s \), checking that the plateau value does not change. However, the statistical errors grow exponentially with \( t_s \), which means that as the sink-source time separation increases the signal is lost as compared to the statistical noise making it difficult to detect any time-dependence. Increasing \( t_s \) therefore requires a corresponding increase in statistics if this check is to be useful \([25]\).

The second approach is to use the summation method proposed some time ago \([39]\) and recently applied to the study of the nucleon axial charge \([40]\). One sums the ratio over the time of the insertion,

\[
R^\text{sum}(\Gamma^\lambda) = \sum_{t_{\text{ins}}=t_0+\tau}^{t_s-\tau} R(\Gamma^\lambda, t_s, t_{\text{ins}}), \quad (28)
\]

with \( \tau \) selected such that contact terms are not included, i.e. \( \tau = 1 \) for local operators and \( \tau = 2 \) for derivative operators. The sum over the excited state contributions given in Eq. \([21]\) is a geometric series and can easily be summed to yield

\[
R^\text{sum}(\Gamma^\lambda) \propto C' + (t_s - t_0) \mathcal{M} + O(e^{-\Delta(t_s - t_0)})
\]

(29)

with \( C' \) a constant independent of \( t_s \). The advantage over the plateau method is that excited state contamination is suppressed by a larger factor \( \Delta(t_s - t_{\text{ins}}) \) as opposed to \( \Delta(t_s - t_{\text{ins}}) \) or \( \Delta(t_{\text{ins}} - t_0) \). However, the extraction of \( \mathcal{M} \) requires a fit to two parameters, resulting in general in larger statistical uncertainties. Nevertheless, this method provides a good consistency check of our results.

A third approach to extract the desired matrix element is to take into account in the fit the contribution of the first excited state in Eq. \([21]\). In this case, we simultaneously fit the two- and three-point correlation functions obtained from the lattice including the
ground state and the first excited state contributions. This is done by performing a combined fit to all sink-source separations and to both correlation functions with \( t_{\text{ins}} \) and \( t_s \) as independent variables. Like for the sum- 

mation method, we exclude the contact terms, i.e. for \( t_{\text{ins}} \in [t_0 + 1, t_s - 1] \) for the scalar, axial and tensor charges, and \( t_{\text{ins}} \in [t_0 + 2, t_s - 2] \) for the momentum fraction, polarized moment and trasversity moment, which include a derivative. We will refer to this method as the two-state fit method.

In this work, we consider agreement among the above three methods yielding the same value for \( \mathcal{M} \) as our criterion that excited states are sufficiently damped out.

If one has ground state dominance the nucleon matrix elements of the scalar, axial and tensor local operators, at zero momentum transfer and Euclidean time are related to the ratio as follows:

\[
\Pi^S(\Gamma^4) = \frac{gs}{2}
\]

\[
\Pi^A_k(\Gamma_k) = -i\delta_{jk}\frac{gA}{2}
\]

\[
\Pi^T_k(\Gamma_k) = \epsilon_{ijk}\frac{gT}{2}
\]

(30)

The corresponding expressions for the vector, axial and tensor one-derivative operators are:

\[
\Pi^V_{kk}(\Gamma^4) = -\frac{3m_N}{4}\langle x \rangle_{u \pm d}
\]

\[
\Pi^V_{kk}(\Gamma^4) = \frac{m_N}{4}\langle x \rangle_{u \pm d}
\]

\[
\Pi^A_{jk}(\Gamma_k) = -\frac{i}{2}\delta_{jk}m_N\langle x \rangle\Delta_{u\pm d}
\]

\[
\Pi^T_{jk}(\Gamma_k) = i\epsilon_{ijk}\frac{m_N}{8}(2\delta_{4p} - \delta_{4\mu} - \delta_{4\nu})\langle x \rangle_{s u \pm d}
\]

(31)

Note that after symmetrization and subtraction of the trace as indicated in Eq. 5, only one of the two expressions for \( \langle x \rangle_{u \pm d} \) is independent.

For the case of the pion we only present \( \langle x \rangle_{a \pm d} \). We consider the largest sink-source separation possible on each lattice, namely \( t_s - t_0 = T/2 \). This is possible for the pion since its two point function has constant signal to noise ratio independently of \( t_s - t_0 \). Therefore, we extract the pion momentum fraction using the plateau method at this single value of the sink-source separation:

\[
R^\pi(t_s, t_{\text{ins}}) = \frac{\Delta(t_s - t_{\text{ins}}) \geq 1}{\Delta(t_{\text{ins}} - t_0) \geq 1} \Pi^\pi
\]

(32)

where we use \( \Delta \) to generically denote the energy gap between the energy of the first excited state and the ground state of the hadron of interest in its rest frame. Given ground state dominance, the pion momentum fraction is at zero momentum transfer and Euclidean time obtained from the ratio via:

\[
\Pi^\pi = \frac{m_\pi}{2}(x)^{u \pm d}
\]

(33)

IV. SIMULATION DETAILS

We use the (maximally) twisted mass fermion (TMF) formulation of lattice QCD \[41], which is particularly suited for hadron structure calculations since it provides automatic \( \mathcal{O}(a) \) improvement requiring no operator modification \[42–45\]. Twisted mass ensembles with two degenerate flavors of light sea quarks (\( N_f = 2 \)) as well as ensembles including the strange and charm sea quarks (\( N_f = 2 + 1 + 1 \)) are produced by the European Twisted Mass Collaboration (ETMC) and technical details on the simulations can be found in Refs. \[46–48\] and \[49\] respectively. This work focuses on analysis of gauge configurations produced using two degenerate flavors of twisted mass light sea quarks (\( N_f = 2 \)) including a clover term. For the gauge action we use the Iwasaki action. The parameters of the four ensembles considered in this work are given in Table I. More details on the choice of action and the simulations are given in Refs. \[21\] \[50\] \[51\].

| \( \beta = 2.1 \), \( a = 0.093(1) \) fm, \( r_0/a = 5.32(5) \) | \( 24^3 \times 48 \), \( L = 2.23 \) fm | \( m_\mu \) (GeV) | 0.009006 | 0.003003 |
| \( 32^3 \times 64 \), \( L = 2.97 \) fm | \( m_\mu \) (GeV) | 0.338(9) | 0.244(8) |
| \( 48^3 \times 96 \), \( L = 4.46 \) fm | \( m_\mu \) (GeV) | 0.335(9) | 0.0009 |

For the nucleon structure observables, we analyze the ensemble with \( m_\mu = 0.0099 \). We will refer to this ensemble as the physical ensemble and speak in what follows of the physical point. For the case of the pion momentum fraction, we use all four ensembles of TMF with a clover term.

Although the observables of interest in this work are dimensionless and do not depend on the lattice spacing, it is useful to study their dependence on the pion mass, which is a dimensionfull quantity. In Ref. \[21\], the lattice spacing for the new \( N_f = 2 \) ensembles with the clover term was determined using gluonic quantities as well as the pion and kaon decay constants. Another determination of the lattice spacing mentioned in Ref. \[21\] is via the nucleon mass.

Table I: Input parameters of our new lattice ensembles used in this work. For each ensemble we give the lattice size, the bare quark mass (\( a\mu \)) and the corresponding pion mass (\( m_\pi \)). These ensembles use TMF at one value of \( \beta \) with a clover term with \( r_0/a = 1.57551 \). The lattice spacing given in the table is determined using the nucleon mass as explained in the text.
larger than physical light quark masses a chiral extrapolation was needed. We used the lowest order heavy baryon chiral perturbation theory expression, given by \[35\]

\[am_N = am_N^0 - 4(c_1/a)(am_\pi)^2 - \frac{3g_A^2}{16\pi(m_{f}/m_\pi)^2}(am_\pi)^3,\]

which is well-established within baryon chiral perturbation theory. \[m_N^0\] is the value of the nucleon mass in the chiral limit and \(-4c_1\) gives the \(\sigma\)-term written in units of the lattice spacing. The fit was constrained to reproduce the physical nucleon mass, by fixing the value of \(c_1\). Including an \(a^2\)-term in Eq. \[34\] had a negligible effect on the fit showing that indeed cut-off effects are small \[54\] for lattice spacings smaller than 0.1 fm. This justified the utilization of continuum chiral perturbation theory to determine the three lattice spacings for each \(N_f = 2\) or \(N_f = 2 + 1 + 1\) by simultaneously fitting each set of 17 \(N_f = 2 + 1 + 1\) or 11 \(N_f = 2\) ensembles. The values of the nucleon mass used are taken from Ref. \[54\] for the \(N_f = 2 + 1 + 1\) ensembles and from Ref. \[22\] for the \(N_f = 2\) ensembles. These values of the lattice spacings are used to obtain the pion mass for these ensembles.

For the physical ensemble using the values

\[am_\pi = 0.06196(9)\quad am_N = 0.440(4),\]

and assuming that we are exactly at the physical point we find \(a = 0.0925(8)\) fm where the average nucleon mass \(m_N = 0.939\) GeV is used as an input. With this lattice spacing we find \(m_\pi = 0.1323(12)\) MeV, where the largest part of the error comes from the error on the lattice spacing. This is about 5% less than the average physical pion mass. Using the values of Eq. \[35\] we find for the ratio \(m_N/m_{\pi^{-}} = 7.10(6)\) compared to the physical value of 0.939/0.138 = 6.8, which again differs by less than 5% from the physical value. In order to check what the effect of a possible small mismatch in the pion mass would be on the lattice spacing, we use the fit extracted from the \(N_f = 2 + 1 + 1\) ensembles to interpolate to the physical value of pion mass. This is done by making a combined fit of the 17 \(N_f = 2 + 1 + 1\) ensembles with their three lattice spacings and the lattice spacing for the physical ensemble as well as \(m_N^0\) as fit parameters. The fit yields \(\chi^2/d.o.f. = 1.6\) for d.o.f. = 12, which is a reasonable value. We find a value of \(a = 0.093(1)\) fm for the physical ensemble, consistent with the determination using Eq. \[35\], while the lattice spacings for the \(N_f = 2 + 1 + 1\) remain unchanged compared to the values obtained when the physical ensemble was not included. Using \(a = 0.093(1)\) we find \(m_{\pi^{-}} = 0.1312(13)\) GeV, which is consistent with the value extracted from Eq. \[35\]. Excluding from the fit pion masses larger than 300 MeV yields consistent results for the lattice spacings of the \(N_f = 2 + 1 + 1\) ensembles while it does not change the value of the lattice spacing at the physical point. We note that if we fit using the \(N_f = 2\) ensembles \[22\] \[53\] instead of the \(N_f = 2 + 1 + 1\) ensembles the value of \(a = 0.093(1)\) fm is unchanged. This indicates that the mild interpolation is very robust. In Fig. 2 we show the ratio of the nucleon to pion mass \(m_N/m_{\pi^{-}}\), which is a dimensionless observable determined purely from lattice quantities. We note that the values of the lattice spacings affect only the determination of the pion mass plotted as the x-axis. The curve shown in Fig. 2 is the fit to the ratio performed on the 17 \(N_f = 2 + 1 + 1\) ensembles alone. The resulting chiral fit using \(m_\pi < 500\) MeV yields \(\chi^2/d.o.f. = 1.4\) and describes

\[\chi^2/d.o.f. = 1.4\]

and describes

\[\chi^2/d.o.f. = 1.4\]
very well the data. In the figure we also include the values for the ratio for the $N_f = 2$ ensembles, which also fall on the same curve. This can be taken as an indication that indeed strange and charm sea quark effects are small for the nucleon sector. The consistency of our new result is demonstrated in Fig. 2 by the fact that the ratio $m_N/m_{\pi^\pm}$ for our physical ensemble falls on the curve determined from fitting the $N_f = 2 + 1 + 1$ alone. Fig. 2 provides a nice demonstration of the negligible effect of lattice artifacts on the $m_N/m_{\pi^\pm}$ ratio.

We note that the value of the lattice spacing determined from the nucleon mass analysis is fully consistent with the one determined from gluonic quantities such as the one related to the static quark-antiquark potential, $r_0$, and the ones related to the action density renormalised through the gradient flow. It is, however, larger by about 1% as compared to that extracted using $f_\pi$. This was also observed in our analysis of $N_f = 2$ and $N_f = 2 + 1 + 1$ TMF ensembles. In Table I we collect the lattice spacings for all the TMF ensembles determined using the nucleon mass and Eq. (34). We take as a systematic error due to the chiral extrapolation the shift in the mean value when discarding ensembles with pion mass greater than 300 MeV. For completeness we also give the values of $r_0$ determined from the nucleon mass in the same way as the lattice spacings, although they are not needed in this work. In what follows we use, for the physical ensemble, the value $a = 0.093(1)$. The lattice spacings given in Table I are used to convert the pion mass to physical units. No other physical quantity presented in this work is affected by the value of the lattice spacings.

V. RESULTS

For the nucleon observables we analyze 96 gauge field configurations with 16 randomly chosen positions for each configuration yielding a total of 1536 measurements. For the nucleon observables, we use three sink-source separations for both the plateau and the summation methods, namely $t_s/a = 10$, 12, and 14, corresponding to approximately 0.9 fm, 1.1 fm, and 1.3 fm. For all separations we have 1536 measurements, by computing the required two- and three-point correlation functions. First results on these quantities were presented in Refs. [57, 58]. For the pion we use the largest possible time separation namely $T/2$.

A. Renormalization

We determine the renormalization functions for the lattice matrix elements non-perturbatively, in the RI-MOM scheme employing a momentum source [59]. For the computation of the renormalization functions of the $N_f = 2 + 1 + 1$ ensembles we employed $N_f = 4$ simulations for at least three different values of the pion mass taking the chiral limit. A similar analysis was performed for the $N_f = 2$ TMF ensembles as well as for our new $N_f = 2$ TMF ensembles that include the clover term using the ensembles with $a\mu = 0.006, 0.003$ and 0.0009, the latter being at the physical pion point. In Refs. [60, 61] we carried out a perturbative subtraction of $O(a^2)$ terms that subtracts the leading cut-off effects yielding only a very weak dependence of the renormalization factors on $(ap)^2$ for which the $(ap)^2 \rightarrow 0$ limit can be reliably taken. In this work, we reduce even further the $O(a^2)$ contributions by subtracting lattice artifacts computed perturbatively to one-loop and to all orders in the lattice spacing, $O(g^2 a^\infty)$, so that we eliminate a large part of the cut-off effects. In fig. 3 we show the results on the axial and tensor renormalization functions after subtraction. As can be seen, lattice artifacts are practically removed allowing a robust extrapolation to $(ap)^2 = 0$. Due to the good quality of the plateaus after the subtraction of the $O(g^2 a^\infty)$ any choice for the fit within the non-perturbative region $(ap)^2 \in (2 - 7)$ yields consistent results. Details on this computation can be found in Ref. [62].

![FIG. 3: Results for the axial (upper) and tensor (lower) renormalization functions as a function of the momentum square in lattice units. The open (black) circles are the unsubtracted results while the filled triangles (magenta) show the data after subtracting lattice artifacts computed perturbatively to one-loop and to all orders in the lattice spacing, $O(g^2 a^\infty)$, so that we eliminate a large part of the cut-off effects. In fig. 3 we show the results on the axial and tensor renormalization functions after subtraction. As can be seen, lattice artifacts are practically removed allowing a robust extrapolation to $(ap)^2 = 0$. Due to the good quality of the plateaus after the subtraction of the $O(g^2 a^\infty)$ any choice for the fit within the non-perturbative region $(ap)^2 \in (2 - 7)$ yields consistent results. Details on this computation can be found in Ref. [62].](image)
functions in Table III, converting the scale dependent renormalization function in the \( \overline{\text{MS}} \) scheme at a scale \( \mu = 2 \, \text{GeV} \), which is applicable to all except \( Z_A \). The systematic error is computed by varying the interval for the continuum extrapolation \((ap)^2 \to 0\). The values of \( Z_P \) for the \( N_f = 2 + 1 + 1 \) ensembles are taken from Refs. [56, 63] where the pole subtraction was performed, while for the new ensembles with the clover term we use the result of this paper. The values given in Table III are used to renormalize the lattice matrix elements studied in this work. More details are reported in Ref. [62]. For the \( N_f = 2 \) TMF ensembles without the clover term we do not calculate the scalar charge and transversity and therefore the renormalization functions are not given.

![Table III: Renormalization functions for the ensembles used in this work. They are given in the twisted basis. They are the same in the physical basis except for \( Z_P \), which renormalizes the scalar operator in the physical basis. The renormalization functions for the local axial-vector, scalar and tensor operators are given in columns two, three and four, respectively. The last three columns give the renormalization functions for the derivative vector, axial vector and tensor operators. The first error is statistical and the second error systematic.](image)

The renormalization functions are given for the twisted basis. Going from the twisted to the physical basis affects only the renormalization function for the scalar charge, which, in the twisted basis, is renormalized with \( Z_P \). Furthermore, since disconnected contributions are neglected, the isovector and isoscalar are renormalized using the same renormalization functions. All our results on the scalar and tensor charges and on the moments of PDFs are given in the \( \overline{\text{MS}} \) scheme at an energy scale of 2 GeV.

### B. Nucleon scalar, axial and tensor charges

In what follows we will use the same format to present our results for a given observable in four plots unless otherwise mentioned. Our presentation is illustrated in Fig. 4. In the two upper panels we present the ratio of Eq. 19, as a function of the insertion time \((t_{\text{ins}})\), shifted by half the sink-source separation, i.e. \(t_{\text{ins}} - t_s/2\). This way, the midpoint time of the ratio coincides for all sink-source separations at \( t_{\text{ins}} - t_s/2 = 0 \). In what follows all times are measured relative to \( t_0 \) and thus we drop the reference to \( t_0 \). In the third panel we show the summed ratio as a function of the sink time, as obtained by Eq. 28 and in the bottom panel we compare results from the summation method and from the two-state fit method with those obtained by the plateau method.

Let us first discuss the results for the scalar charge shown in Fig. 4. In the two upper panels we show the ratio for the isoscalar and isovector scalar charges, for the three sink-source separations considered. As explained in the previous section, when the time separations \( \Delta t_{\text{ins}} \gg 1 \) and \( \Delta (t_s - t_{\text{ins}}) \gg 1 \), the ratio becomes time-independent. Fitting in the plateau region to a constant value, which we refer to as the plateau value, we obtain \( q_S \), as in Eq. 27. This is shown by the blue band in Fig. 4 for \( t_s = 14a \). One observes an increasing trend for the plateau value and a clear curvature, especially for the isoscalar, indicating dependence on excited states. Carrying out a two-state fit yields the dashed lines. As in the case of the summation method, the contact points \( t_{\text{ins}} = t_0 \) and \( t_{\text{ins}} = t_s \) are omitted. The value for \( q_S \) obtained by the two-state fit is given by the dashed line that spans the entire x-range of the figure, with the red band indicating the statistical error, while the result of the summation method is shown with the solid line and gray band indicating the error. As can be seen, within errors the two-state fit is consistent with the plateau fit, but
FIG. 4: Results for the isovector and isoscalar nucleon scalar charge: Upper two panels is the ratio from which $g_S$ is extracted as a function of $t_{ins} - t_s/2$ for the isoscalar (upper) and the isovector (lower). The blue bands spanning from $(-t_{ins} - t_s/2)/a = -4$ to 4 are fits to the ratio for $t_s/a = 14$. The dashed lines show the result of the two-state fit method. The dashed (solid) line spanning the entire x-range show the value obtained via the two-state (summation) method, with the band indicating the corresponding statistical error. In the third panel, the summed ratio is shown for the isovector (filled symbols) and isoscalar (open symbols) case. The line shows the result of a linear fit, while the bands show the statistical error based on the jackknife error of the fitted parameters. In the bottom panel, we show the result for $g_S$ when using the plateau method with $t_s/a = 10$, 12 and 14 (squares, circles, and rhombuses respectively), as well as when using the summation method denoted by “sm” (asterisks) and the two-state fit “2-st.” (triangles).

not with the value from the summation method, which, however, carries a very large error indicating the need to increase statistics in order to have a better assessment of the result of this method. In the third panel of Fig. 4 we show the summed ratio for the scalar charge as a function of the sink time, as obtained by Eq. (28), for the isovector and the isoscalar cases. Fitting to a linear dependence with respect to $t_s$, one extracts the desired matrix element from the slope (Eq. (29)), which is the result shown by the gray band in the two upper graphs of Fig. 4. The width of the bands is obtained by a jack-knife re-sampling of the summed ratio to obtain jack-knife errors for the slope, $M$, and intersection $C'$ of Eq. (29). The values for $g_S$ from the summation method and those obtained by the plateau method and the two-state fit method are shown in the bottom panel of the figure. One clearly observes the increasing trend
of the plateau values with increasing $t_s/a$ as well as the larger values of the summation method shown by the asterisks. This study shows that both larger sink-source time separations as well as larger statistics are needed in order to obtain a meaningful convergence of all methods. This corroborates our findings of our high statistics analysis of the $N_f = 2 + 1 + 1$ TMF ensemble with pion mass 373 MeV, referred to as B55.32 ensemble, where we showed that $t_s \sim 1.5$ fm is needed \cite{77}. Our current statistics do not allow to use such a large sink-source separation for the physical ensemble. We note that as a check of the robustness of the two-state fit, we omit more points besides the time slice of the source and the sink. In the case of the scalar charge, taking the fit range $t_{\text{ins}} \in [t_0 + 2, t_s - 2]$ and $t_{\text{ins}} \in [t_0 + 3, t_s - 3]$ we obtain: 2.18(34) and 2.22(33) respectively for the isovector case and 9.68(26) and 9.75(24) for the isoscalar, which are consistent with 2.16(34) and 9.62(27) extracted when just omitting the source and the sink. Thus for the scalar charge, the fluctuation of the central value when changing the fit-range is within the statistical error and of the order of 2%.

In Fig. 5 we show results for the axial charge following the same notation as that in Fig. 4. For the axial charge, one observes a milder dependence on $t_s$ showing that excited states contributions are suppressed for this observable. Because of this weaker dependence a two-state fit does not yield a meaningful result for these values of $t_s/a$, at least within the statistical accuracy of 1536 measurements. We therefore only show results for the plateau and summation methods. The values from the plateau method do not vary as a function of $t_s$ and are in agreement with the value extracted from the summation method, within the large statistical uncertainties of the latter.

Our results for the tensor charge ($g_T$) are shown in Fig. 6. The dependence of $g_T$ on $t_s$ is similar to that observed in the case of $g_A$ and thus a two-state fit fails to accurately resolve the excited states. Thus we only compare the results extracted using the summation and plateau methods in the bottom panel. As can be seen, $g_T$ exhibits no dependence on the sink-source separation within the current statistical uncertainties, evident by the same values extracted by fitting to the plateau for the three different sink-source separations. The value extracted from the summation method is in agreement but carries a much larger error and thus does not provide a stringent check.

C. Nucleon momentum fraction, helicity and transversity moments

The momentum fraction is shown in Fig. 7 for the connected isoscalar $(x)_{u+d}$ and isovector $(x)_{u-d}$ combinations. Both isoscalar and isovector channels exhibit excited state contributions, especially for the isoscalar channel. A two-state fit is performed using $t_{\text{ins}} \in [t_0 + 2, t_s - 2]$, which however yields too large errors to include in the plots (see Table IV). Using $t_{\text{ins}} \in [t_0 + 3, t_s - 3]$, we find a value of 0.48(19) for the isoscalar, which is consistent with the value given in Table IV. For the isovector both fit ranges yield consistent results albeit with a large error that does not allow to access the sensitivity on the fit range. Furthermore, as can be seen in the lowest panel of panel of Fig. 7 a decreasing trend is observed as the sink-source separation is increased from 10a to 14a, showing that elimination of excited state effects is responsible for reducing the value of this matrix element. The summation method yields a value that is even lower but with a large statistical uncertainty. Like for the case of the scalar charge a larger value of $t_s/a$ and increased statistics will be needed to reach consistency among the various methods with meaningful errors.
The helicity moment $\langle x \rangle_{\Delta u \pm \Delta d}$ and transversity moment $\langle x \rangle_{\delta u \pm \delta d}$ are shown in Figs. 8 and 9. For both isoscalar observables, a milder dependence on the sink-source separation is observed. This is also true for the isovector transversity moment. On the other hand, the isovector helicity moment shows a decreasing trend similar to that observed in the case of the isovector momentum fraction. The value obtained using the summation method is consistent in all cases with the plateau value when $t_s/a = 14$, albeit with a large statistical uncertainty.

The nucleon results presented in Figs. 4 to 6 and Figs. 7 to 9 are summarized in Table IV where we give the values obtained when using the plateau method and the summation method. Our results with sink-source time separation $12a$, $14a$, and the summation method agree within one to two standard deviations. The errors exhibited by the summation method, however, are still large, which is explained by the fact that this method relies on a two parameter fit, contrary to the plateau method which is a fit to a constant. Nevertheless, within our current statistics, the summation method can provide an additional check of excited state effects.

We observe that the scalar charge $g_S$ and momentum fraction $\langle x \rangle_q$ exhibit non-negligible excited state effects.
when increasing the sink-source separation. For these cases we show in Table V the results when employing the two-state fit method. For both observables, the two-state fit result agrees with the plateau method for $t_s/a = 14$.

In Table VI we give our results for the isovector quantities as determined from the plateau method using $t_s \sim 1.3 \, \text{fm}$, as well as for the up- and down-quark contributions neglecting disconnected diagrams. We note that for the up- and down-quark contributions of these quantities we carry out the complete analysis with jack-knife resampling starting from three-point correlation functions with only an up- or down-quark insertion. Alternatively one can form linear combinations of the final isovector and isoscalar results of Table V which will give consistent up- and down-quark contributions within statistical errors. Except for the scalar and the momentum fraction, the results of Table VI are in agreement with the value obtained using the summation method. For the scalar and the momentum fraction they are consistent with the result extracted using the two-state fit albeit with large statistical error especially for the momentum fraction. Since for the scalar there are large differences still between the results at different values of $t_s$ as well as from the value extracted using the summation method we do not include a single value in the table.

Our TMF results for the three isovector charges $g_{A,x}^{u-d}$, $g_{A,x}^{a-d}$ and $g_{T,x}^{u-d}$ and moments $\langle x \rangle_{u-d}$, $\langle x \rangle_{\Delta u-\Delta d}$ and $\langle x \rangle_{\delta u-\delta d}$ are collected in Figs. 10 and 11. In the Appendix we give our updated results for our high statistics analysis of the $B55.32$ ensemble for several sink-source separations in Tables VIII and IX as well as for one $N_f = 2 + 1 + 1$ ensemble at a finer lattice spacing $\Delta t_s$ in Table X. These results use the new renormalization functions given in Table III. For $g_{A,x}^{u-d}$, $\langle x \rangle_{u-d}$
and $\langle x \rangle_{\Delta u - \Delta d}$ we include results using $N_f = 2$ at three lattice spacings and, for one mass, at two different volumes [22 23]. These are given with the new renormalization functions in Table [X] of the Appendix. These results show that cut-off effects are small for lattice spacings smaller than 0.1 fm. Finite volume effects are not visible within our statistical accuracy when comparing results for two ensembles simulated at a pion mass of about 300 MeV and $Lm_\pi = 3.3$ and $Lm_\pi = 4.6$. For the physical ensemble we show results for $t_s = 12a \simeq 1.1$ fm and $t_s = 14a \simeq 1.3$ fm and from using the summation method. We expect $\langle x \rangle_{u - d}$ to have moderate excited states contamination as revealed by our high-statistics investigation of $\langle x \rangle_{u - d}$ for the $N_f = 2 + 1 + 1$ ensemble with $m_\pi = 373$ MeV that showed that its value decreases with increasing $t_s$ [25]. Our current results at the physical point with 1536 statistics have much larger errors as compared to what was achieved in Ref. [24] but there is a clear decreasing trend as we increase $t_s$. For the scalar charge the excited state contributions are large, as can be seen both from the results obtained with the $N_f = 2 + 1 + 1$ ensemble with 373 MeV where a high statistics analysis is carried out but also for the physical ensemble where no convergence is achieved with the summation method. We expect $\langle x \rangle_{u - d}$ and $\langle x \rangle_{\Delta u - \Delta d}$ our results from the summation method are in agreement with the experimental values, the errors are still too large and must be reduced by a factor of at least two to draw a safe conclusion. How-

FIG. 10: Isovector nucleon scalar charge $g_A^{u - d}$ (upper), axial charge $g_A^{u - d}$ (middle), and tensor charge $g_A^{u - d}$ (lower) using the values of Table [X]. Twisted mass fermion (TMF) results are shown for i) $N_f = 2$, $a = 0.089$ fm (open green squares), $a = 0.07$ fm (open blue diamonds) and $a = 0.056$ fm (open magenta circles); ii) $N_f = 2 + 1 + 1$, $a = 0.082$ fm (filled green squares), $a = 0.064$ fm (filled blue diamonds) and iii) $N_f = 2$ TMF clover-improved $a = 0.093$ fm (physical ensemble), $t_s/a = 12$ (filled red triangle), $t_s/a = 14$ (open red triangle), summation method (open right triangle). The physical value is shown with the black asterisk. For the scalar charge we show with the open yellow square the value when $t_s \sim 1.5$ fm.

FIG. 11: Isovector nucleon momentum fraction $\langle x \rangle_u$ (upper), helicity $\langle x \rangle_{\Delta u}$ (middle), and transversity $\langle x \rangle_{\delta q}$ (lower). The notation is the same as that in Fig. 10.
ever, we stress that our value for $g_4^{-u-d}$ from the plateau method using $t_s \sim 1.3$ fm agrees with the experimental value. To our knowledge, this is the first computation for the axial charge is reproduced from the plateau fit as compared to the case of the nucleon.

### D. Pion momentum fraction

In this section we present results on the isovector pion momentum fraction. Three $N_f = 2$ TMF ensembles with the clover term are analyzed with heavier than physical pion masses, two of which with spatial lattice size 2.23 fm and one with spatial lattice size 2.98 fm. A fourth ensemble that includes the clover term is simulated using the physical value of the pion mass and spatial lattice extent of 4.46 fm. This is the ensemble used for the nucleon observables and the ensemble details can be found in Table I. The number of measurements, which are well separated in the number of HMC trajectories, is given in Table VII.

In Fig. 12 we show the ratio Eq. (22) as a function of $t_{\text{ins}}/a$ for the physical ensemble. The black horizontal line represents the value quoted in Table VII. The statistical accuracy of the pion correlation functions allows for a more careful assessment of systematic uncertainties in the plateau fit as compared to the case of the nucleon. Namely, we obtain the plateau value by performing constant fits to the data with all possible fit ranges with degrees of freedom larger than 5. For each of these fits a weight factor

$$w = \left( \frac{1 - 2|p - 0.5|}{W} \right)^2 \left( \frac{1 - 2|p_{m_n} - 0.5|}{W_{m_n}} \right)^2$$

is computed, where $p$ ($p_{m_n}$) is the p-value of the fit and $W$ ($W_{m_n}$) the statistical error of the fit parameter (of $m_n$) determined using 1500 bootstrap samples. The pion mass itself is also determined for a large number of fit-ranges. The final result is determined as the weighted median over all combinations of fit-ranges. The 68.54% confidence interval of the weighted distribution is quoted as the systematic uncertainty.

For the twisted mass value $a\mu = 0.006$ we have two spatial lattice sizes available, namely $L/a = 24$ and $L/a = 32$. Within errors, the result for $\langle x \rangle_{u-d}^{\pi}$ agrees between these two ensembles. We show the $\langle x \rangle_{u-d}^{\pi}$ results for $L/a = 24$ and $L/a = 32$ in Fig. 13 as a function of $t_{\text{ins}}/a$.

We compare our $N_f = 2$ clover-improved results with results obtained for $N_f = 2$ twisted mass ensembles without the clover term published in Ref. [36]. These ensembles were simulated using $\beta = 3.90$ with four values of the bare quark mass: $a\mu = 0.004, 0.0064, 0.0085$ and 0.0100. The lattice spacing for these ensembles is 0.089(1) fm, which is similar to the clover-improved ensembles. For $a\mu = 0.004$ we have again two spatial lattice extents $L/a = 24$ and $L/a = 32$ available. As for the clover-improved ensembles the results for $\langle x \rangle_{u-d}^{\pi}$ agree between the two volumes.
FIG. 14: The renormalised momentum fraction of the pion \( \langle x \rangle_{u-d}^\pi \) as a function of the squared pion mass at renormalization scale \( \mu = 2 \text{ GeV} \) in the \( \overline{\text{MS}} \) scheme. The results of this work (red symbols) are shown together with previous results obtained using \( N_f = 2 \) ensembles (green symbols) compared to the phenomenological value (black star) from Ref. [64]. Results at two values of the pion mass but different lattice volumes are shown by the open squares (24\(^3 \times 48\)) and diamonds (32\(^3 \times 64\)).

From the comparison of the different available spatial lattice sizes we conclude that within the current statistical uncertainties we cannot detect significant finite volume effects for \( m_\pi L \leq 3.2 \) realized for the \( \beta = 3.90, a \mu = 0.004, L/a = 24 \) ensemble. The physical ensemble has slightly smaller \( m_\pi L = 2.97 \), and the clover ensemble with \( a \mu = 0.003 \) has \( m_\pi L = 2.77 \). Therefore, we cannot completely exclude finite size effects for these two ensembles. All other ensembles have \( m_\pi L > 3.2 \). Note that we are currently generating a physical ensemble with \( L/a = 64 \), which will allow us to check for finite size effects. We expect pion observables to be more sensitive to finite size effects than nucleon observables; having a larger volume will enable us to confirm this expectation.

The results for the renormalized isovector momentum fraction of the pion \( \langle x \rangle_{u-d}^\pi \) are summarized in Table VII. The renormalization factors used are given in Table III at 2 GeV in the \( \overline{\text{MS}} \) scheme. The results are also displayed in Fig. 14 as a function of the squared pion mass. In Fig. 14 one observes that there is agreement between the clover-improved and non-clover improved ensembles within errors. Note that systematic uncertainties are not displayed.

In Fig. 14 we compare with the latest phenomenological value for \( \langle x \rangle_{u-d}^\pi \) which can be found in Ref. [64] and reads

\[
\langle x \rangle_{u-d}^\pi = 0.256(13).
\]

Note that the result given in Ref. [64] is at \( \mu = 5.2 \text{ GeV} \) renormalization scale and we have translated it to \( \mu = 2 \text{ GeV} \) using three loop perturbation theory. The phenomenological value is compatible with the value of 0.214(15)\( \pm (12) \) computed for the physical ensemble.

The results presented here can be compared to Ref. [8], where \( N_f = 2 \) non-perturbatively clover improved Wilson fermions have been used, including two ensembles with pion mass values around 150 MeV. Two values of the lattice spacing are investigated, \( a = 0.06 \) and \( a = 0.07 \) fm, respectively. In that reference a bending of the momentum fraction values towards small pion mass values is observed, while the agreement at \( m_\pi > 300 \text{ MeV} \) to the results presented here is reasonable.

E. Comparison of nucleon observables with different fermion actions

In this section we compare our results on nucleon observables with other recent results obtained using simulations with similar parameters.

FIG. 15: Results for the nucleon axial charge for different fermion actions. Twisted mass fermion results are shown with open green squares for \( N_f = 2 \) ensembles [22], with filled blue squares for \( N_f = 2 + 1 + 1 \) [26] and with the open red triangle for the physical ensemble using the plateau value at \( t_s/a = 14 \) (see Table VI). Results are also shown using \( N_f = 2 \) clover fermions (filled purple diamonds) [65]; \( N_f = 2 + 1 + 1 \) staggered sea and clover valence quarks (filled light blue inverted triangles) [65]; \( N_f = 2 + 1 \) with DWF on a staggered sea (filled yellow circles) [67]; and \( N_f = 2 + 1 \) clover (black x-symbols) [65].

A number of lattice QCD collaborations are investigating \( g_A \) since, as emphasized already, this is considered a benchmark quantity for lattice QCD. In Fig. 15 we show results for \( N_f = 2 \) [22] and \( N_f = 2 + 1 + 1 \) [26] twisted mass fermions obtained in previous analyses using simulations with pion masses in the range of 450 MeV to 210 MeV for various volumes always satisfying the condition \( Lm_\pi > 3 \). For \( N_f = 2 \) ensembles, three values of the lattice spacing were analyzed, namely \( a = 0.089, 0.07 \) and 0.056 fm and, at one pion mass of about 300 MeV, for two different volumes. As already pointed
out, the consistency among these results indicates small cut-off and finite volume effects. The $N_f = 2$ values are consistent with the values extracted using two $N_f = 2 + 1 + 1$ ensembles with lattice spacing $a = 0.082$ fm and $a = 0.064$ fm, showing that there are no visible strange and charm sea quark effects on these quantities at least to the accuracy we now have. This allows a comparison with results using different fermion discretization schemes even before the continuum extrapolation is performed. In Fig. 13 we include results obtained using clover improved fermions from two collaborations: In Ref. [68] results were obtained using $N_f = 2$ clover fermions with smallest pion mass of 150 MeV and three lattice spacings $a = 0.08$ fm, 0.07 fm and 0.06 fm as well as several volumes. These results are in agreement with ours. The LHPC analyzed $N_f = 2 + 1$ tree-level clover-improved Wilson fermions with 2-HEX stout smeared gauge links provided by the BMW collaboration using smallest pion mass of 149 MeV at one lattice spacing $a = 0.116$ fm [68]. These tend in general to have lower values. This is particularly severe close to the physical pion mass. LHPC also computed the axial charge in a mixed action approach that uses DWF on staggered sea
quarks by LHPC [67] with \( a = 0.124 \) fm where high accuracy results were produced for heavier pion masses. These results are in good agreement with ours. We note that both TMF and clover-improved results are extracted using the plateau method with sink-source time separation of about 1 fm to 1.2 fm with the exception of our result for the physical ensemble where we used time separations of up to 1.3 fm. In addition, results at two pion masses using a hybrid action with clover valence on \( N_f = 2 + 1 + 1 \) staggered fermions and are included here for comparison. They tend to be higher than other results although they are compatible with our \( N_f = 2 + 1 + 1 \) value at pion mass of about 210 MeV, which albeit carries a large error. The general conclusion is that the lattice results for pion mass higher than about 300 MeV, which are more accurate as compared to those at smaller pion masses, are in agreement. This is an indication that lattice systematics are under control in this pion mass range. Results for pion masses smaller than about 300 MeV, in general, have larger statistical errors and agreement among them is harder to assess. They clearly indicate the need for more precise values and a reliable assessment of systematic uncertainties. This is particularly relevant for the results close to the physical point where we observe a disagreement between clover results from LHPC at pion mass of 149 MeV and from Ref. [65] at similar pion mass. This discrepancy was claimed to be due to excited states, which were shown to be suppressed with improved smearing in Ref. [65]. This needs to be further investigated with a dedicated precision calculation with a complete assessment of systematic uncertainties. Other results using clover-improved fermions not shown here are those by the CLS collaboration [10], which extracted their values from the summation method. A complete set of the results on \( g_A \) can be found in Ref. [6]. The result of this work is shown with the open triangle obtained for \( t_s = 1.3 \) fm. This value is in agreement with the experimental value with, however admittedly a rather large error.

The calculation of the scalar and tensor charges has received more attention recently due to their relevance for searches of new scalar and tensor couplings beyond the familiar weak interactions of the Standard Model in the decay of ultra-cold neutrons. We compare our TMF results in Fig. 16 with those obtained by three groups whose results on the nucleon axial charge were also included in Fig. 15. The first set of results are from Ref. [65] using \( N_f = 2 \) clover fermions at three lattice spacings. The second set is from the LHPC group which in Ref. [71] used \( N_f = 2 + 1 \) clover with 2-HEX stout smeared gauge links at lattice spacings \( a = 0.116 \) fm and \( a = 0.09 \) fm, \( N_f = 2 + 1 \) DWF with \( a = 0.084 \) fm and a hybrid action of DWF on staggered sea with \( a = 0.124 \) fm. Both these groups used the plateau method and sink-source time separation within 1 to 1.2 fm. The third set of results are from Ref. [66] at one lattice spacing for the scalar and from Ref. [70] at three lattice spacings for the tensor obtained using a hybrid action of DWF on \( N_f = 2 + 1 + 1 \) staggered fermions and employing a two-state fit. For the case of the scalar charge shown in the upper panel of Fig. 16 we observe overall a good agreement among all lattice results obtained with similar sink-source separation. However, our high-statistics analysis using \( N_f = 2 + 1 + 1 \) TMF at pion mass 373 MeV revealed excited states contamination, which only become negligible when \( t_s \approx 1.5 \) fm, increasing the value of \( g_A \). The value extracted when \( t_s = 1.48 \) fm is shown in Fig. 15 by the open green square. A similar analysis for the physical ensemble also reveals large contributions from excited states for \( g_A^{s-d} \). Comparing results obtained for \( t_s \approx 1.1 \) fm and 1.3 fm we confirm an increasing value as we increase \( t_s \). However, the statistical error is large despite the fact that we have 1536 measurements as compared to 1200 used for the ensemble at \( m_\pi = 373 \) MeV. This demonstrates that, obtaining the same accuracy at the physical point for \( t_s \approx 1.5 \) fm, which may be needed to suppress excited states, requires more than an order of magnitude increase in statistics.

Results on the isovector tensor charge are compared in the lower panel of Fig. 16. Our TMF results shown in Fig. 16 show that excited state contributions are less severe for \( g_A^{s-d} \) and that the values at \( t_s/a = 12 \) and \( t_s/a = 14 \) are consistent. Indeed our value at the physical point obtained using \( t_s \approx 1.3 \) fm is in very good agreement with other lattice results providing a prediction for this important quantity directly at the physical point.

Recent lattice QCD results have also been obtained for the isovector momentum fraction and helicity. A comparison of our results for \( \langle x \rangle_{u-d} \) and \( \langle x \rangle_{\Delta u-\Delta d} \) with other collaborations is shown in Fig. 17. We only show results extracted using the plateau method. Most of the analyses employed a sink-source separation of 1 to 1.2 fm including our TMF \( N_f = 2 \) ensembles. As shown in Ref. [25] where \( \langle x \rangle_{u-d} \) was computed using our \( N_f = 2 + 1 + 1 \) ensemble at pion mass of 373 MeV and high-statistics, excited states may not be negligible for this observable. Indeed, this is confirmed by our current analysis for the physical ensemble where there is a decreasing trend as \( t_s \) increases. Our value at the physical point is in agreement with the other lattice values extracted close to the physical point. These are from Ref. [74], which is an update of Ref. [74] for \( m_\pi \approx 160 \) MeV and from LHPC at \( m_\pi \approx 150 \) MeV using \( N_f = 2 + 1 \) clover fermions with 2-HEX smeared gauge action [68]. Our value at \( t_s \approx 1.3 \) fm is still larger than the experimental value. We are currently performing a high statistics analysis for our physical ensemble using larger values of \( t_s \) to investigate contamination due to excited states, which tend to decrease the value of \( \langle x \rangle_{u-d} \). For larger pion masses we show results using \( N_f = 2 + 1 \) DWF from the RBC-UKQCD collaborations [72], from LHPC [67] using DWF on \( N_f = 2 + 1 \) staggered sea and from the QCDSF collaboration using \( N_f = 2 \) clover fermions [73]. Results from LHPC used perturbative renormalization which could explain the fact that these are in general lower than other
lattice results. For the case of \( \langle x \rangle_{\Delta u - \Delta d} \) the situation is similar and our value using the physical ensemble is still larger than its experimental value. As for the momentum fraction there is a decreasing trend as \( t_s \) increases. In fact the summation method yields a value that is consistent with the experimental value as can be seen in Fig. 11. However, the error is too large and our goal in a future analysis is to reduce it by a factor of two so as to confirm agreement with the experimental value. Resolving these discrepancies will give more confidence on our prediction for the transversity moment.

VI. CONCLUSIONS

In this work we present results on the pion momentum fraction and key nucleon observables using lattice QCD simulations at the physical value of the up and down quarks. Our analysis of the isovector pion momentum fraction uses \( N_f = 2 \) ensembles with the clover term simulated at three different values of the light quark mass. We find a value of \( \langle x \rangle_{u - d} = 0.214(15)(\pm 0.12) \) in the MS at 2 GeV at the physical point.

For the nucleon system, we compute the three local and three one-derivative isovector and isoscalar matrix elements at zero momentum transfer. In our calculation we analyze three sink-source time separations, which allows us to investigate excited state effects by observing the dependence of the extracted nucleon matrix elements on this separation. For all observables we compare the plateau method with the summation method. In some cases the sensitivity on the sink time \( t_s \) is good enough so that a two-state fit can also be applied as a third method to detect excited state contaminations. Employing these different methods to ensure that contamination from excited states is suppressed is crucial in obtaining reliable results. However, for this study to be meaningful one needs larger statistics in particular for large sink-source time separations and for the summation method. For the pion momentum fraction where statistical errors are smaller one extracts the relevant matrix element using the largest possible time separation ensuring ground state dominance. Our results for the nucleon axial charge and isovector pion momentum fraction are in agreement with their experimental values, which constitutes a very important conclusion of this study. Since the tensor charge is found to behave similarly to the axial charge as far as ground state dominance is concerned we can predict its value at the physical point to be \( g_T^{u - d} = 1.027(62) \) in the MS scheme at 2 GeV. Assuming that disconnected contributions remain as small at the physical point as they were found at a pion mass of 373 MeV where they were shown to be negligible \[27\] \[28\], we can give a direct prediction for the individual up- and down-quark tensor charges. We find \( g_T^u = 0.791(53) \) and \( g_T^d = -0.236(33) \) (see Table VII).

Thus, this first lattice study of nucleon and pion structure at the physical values of the light quark masses is very promising for future precision calculations of these key quantities directly at the physical point. Ongoing plans include an analysis with increased statistics for general momentum transfer and new \( N_f = 2 + 1 + 1 \) simulations with their mass fixed to physical values, combined with larger volumes and improved algorithms for noise reduction such as multiple right-hand-side solvers. After reproduction of benchmark quantities such as \( g_A \) for the nucleon and the pion, lattice QCD is in a position to turn to quantities more difficult to obtain experimentally such as the scalar and tensor charges \( g_S \) and \( g_T \). Such charges are of high interest in phenomenology and experiments since these enter in couplings of protons to super-symmetric candidate particles. Their precise determination can therefore be used to exclude regions in dark matter searches and influence future experimental set-ups for new physics searches.

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Appendix

In this Appendix we give the ETMC results for the \( N_f = 2 \) and the \( N_f = 2 + 1 + 1 \) ensembles published in Refs. \[22\] \[26\] respectively. These results are updated using the new renormalization functions given in Table III. In Tables VIII and IX we collect the results for the \( f = 2 + 1 + 1 \) simulations published in \[27\] \[28\]. We show the ratios from which the isovector and isoscalar
connected charges and first moments of PDFs are extracted. The ratios are computed for a total of five sink-source time separations spanning a time range of about 0.8 fm to 1.5 fm enabling us to apply the summation method as check for. This high statistics analysis allows us to perform a two-state fit for all quantities except the axial charge where the excited state contamination is the mildest. As our final values we take the plateau value that is in agreement with the value extracted from the summation method and two-state fit when possible. Finally in Tables VIII and IX we give the results for all our other ensembles where only one sink-source separation was employed.

TABLE VIII: Updated results for the $N_f = 2 + 1 + 1$ B55.32 ensemble for the nucleon charges and first moments of parton distribution functions. For the isoscalar combination we give only the connected contribution.

| $t_s/a$  | Plateau method | summation two-state |
|----------|----------------|---------------------|
|          | $g_s$          | method              |
|          |                | fit                 |
| isovector| 1.08(3)        | 1.12(3)             |
|          | 1.16(4)        | 1.08(10)            |
|          | 1.46(20)       | 1.19(10)            |
| isoscalar| 5.07(4)        | 5.45(4)             |
|          | 5.74(6)        | 5.95(13)            |
|          | 6.33(28)       | 6.46(15)            |
| stat.    | 2429           | 4396                |
|          | 4396           | 2018                |
|          | 1200           |                     |
| $g_A$    | 1.143(4)       | 1.152(5)            |
|          | 1.155(8)       | 1.174(20)           |
|          | 1.184(19)      |                     |
| isoscalar| 0.596(3)       | 0.591(4)            |
|          | 0.589(7)       | 0.605(16)           |
|          | 0.583(16)      |                     |
| stat.    | 2429           | 4396                |
|          | 4396           | 2018                |
| $g_T$    | 1.119(6)       | 1.087(7)            |
|          | 1.058(11)      | 1.080(30)           |
|          | 1.023(27)      | 1.053(21)           |
| isoscalar| 0.680(5)       | 0.666(6)            |
|          | 0.660(9)       | 0.663(21)           |
|          | 0.624(22)      | 0.646(9)            |
| stat.    | 2278           | 4040                |
|          | 4040           | 1762                |

TABLE IX: Updated results for the $N_f = 2 + 1 + 1$ B55.32 ensemble for the nucleon first moments of parton distributions. For the isoscalar combination we give only the connected contribution.

| $t_s/a$  | Plateau method | summation two-state |
|----------|----------------|---------------------|
|          | $\langle x \rangle_q$ | method |
|          |                | fit |
| isovector| 0.290(4)       | 0.270(3) |
|          | 0.252(4)       | 0.233(9) |
|          | 0.252(19)      | 0.223(9) |
| isoscalar| 0.720(8)       | 0.677(5) |
|          | 0.639(6)       | 0.607(11) |
|          | 0.663(21)      | 0.554(15) |
| stat.    | 2429           | 4396 |
|          | 4396           | 2018 |
|          | 1200           |     |
| $\langle x \rangle_{\Delta q}$ | 0.328(3) | 0.312(3) |
|          | 0.297(3)       | 0.298(8) |
|          | 0.270(8)       | 0.286(9) |
| isoscalar| 0.207(3)       | 0.198(2) |
|          | 0.189(3)       | 0.193(8) |
|          | 0.172(7)       | 0.184(7) |
| stat.    | 2429           | 4396 |
|          | 4396           | 2018 |
| $\langle x \rangle_{bq}$ | 0.372(5) | 0.349(4) |
|          | 0.322(5)       | 0.316(12) |
|          | 0.283(14)      | 0.284(17) |
| isoscalar| 0.254(4)       | 0.239(4) |
|          | 0.219(6)       | 0.215(15) |
|          | 0.178(14)      | 0.183(21) |
| stat.    | 2278           | 4041 |
|          | 4041           | 1763 |
FIG. 18: The ratios from which the isovector charges (left) and the first moments of PDFs (right) are extracted as a function of the insertion-source time separation for the B55.32 ensemble. The statistics used are given in Tables [VIII and IX].
FIG. 19: The ratios from which the isoscalar charges (left) and the first moments (right) are extracted as a function of the insertion-source time separation for the B55.32 ensemble. Only connected contributions are included. The statistics used are given in Tables VIII and IX.
TABLE X: Updated results for the $N_f = 2 + 1 + 1$ TMF ensemble with $m_\pi = 213$ MeV and $a = 0.064$ fm. In the last column we give the number of measurements for all observables.

| $\beta$ ($L^3 \times T$) | $m_\pi$ (GeV) | $g_\Lambda^{u-d}$ | $g_2^{u-d}$ | $g_T^{u-d}$ | $\langle x \rangle_{u-d}$ | $\langle x \rangle_{u-d} - \langle x \rangle_{d-d}$ | $\delta u - \delta d$ | $t_s/a$ | Statistics |
|-------------------------|--------------|------------------|-------------|-------------|-----------------|------------------------|--------------|--------|-----------|
| 2.10 ($48^3$ x 96)      | 0.2134(6)    | 1.185(61)        | 1.024(368)  | 1.110(61)   | 0.241(19)       | 0.276(21)              | 0.275(26)   | 18     | 900       |

TABLE XI: Updated results for the $N_f = 2$ TMF ensembles.

| $\beta$ ($L^3 \times T$) | $m_\pi$ (GeV) | $g_\Lambda^{u-d}$ | $\langle x \rangle_{u-d}$ | $\langle x \rangle_{u-d} - \langle x \rangle_{d-d}$ | $t_s/a$ | Statistics |
|-------------------------|--------------|------------------|-------------------------|------------------------|--------|-----------|
| 3.90 ($48^3$ x 96)      | 0.3032(16)   | 1.129(34)        | 0.270(17)               | 0.291(10)              | 12     | 943       |
| 3.90 ($32^3$ x 64)      | 0.2600(9)    | 1.174(48)        | 0.279(13)               | 0.282(14)              | 667    | 351       |
| 4.05 ($32^3$ x 64)      | 0.2925(18)   | 1.211(67)        | 0.241(25)               | 0.317(24)              | 16     | 447       |
| 4.20 ($32^3$ x 64)      | 0.4698(18)   | 1.138(25)        | 0.250(13)               | 0.294(9)               | 18     | 357       |
| 4.20 ($48^3$ x 96)      | 0.2622(11)   | 1.142(44)        | 0.274(20)               | 0.290(15)              | 245    |           |

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