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Axial, Scalar and Tensor Charges of the Nucleon from 2+1+1-flavor Lattice QCD

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We present results for the isovector axial, scalar and tensor charges $g_A^{u-d}$, $g_S^{u-d}$ and $g_T^{u-d}$ of the nucleon needed to probe the Standard Model and novel physics. The axial charge is a fundamental parameter describing the weak interactions of nucleons. The scalar and tensor charges probe novel interactions at the TeV scale in neutron and nuclear β-decays, and the flavor-diagonal tensor charges $g_T^d$, $g_T^s$ and $g_T^n$ are needed to quantify the contribution of the quark electric dipole moment (EDM) to the neutron EDM. The lattice-QCD calculations were done using nine ensembles of gauge configurations generated by the MILC Collaboration using the HISQ action with 2+1+1 dynamical flavors. These ensembles span three lattice spacings $a \approx 0.06, 0.09$ and $0.12$ fm and light-quark masses corresponding to the pion masses $M_\pi \approx 2761 \pm 14 \pm 17$ MeV. High-statistics estimates on five ensembles using the all-mode-averaging method allow us to quantify all systematic uncertainties and perform a simultaneous extrapolation in the lattice spacing, lattice volume and light-quark masses for the connected contributions. Our final estimates, in the MS scheme at 2 GeV, of the isovector charges are $g_A^{u-d} = 1.195(33)(20)$, $g_S^{u-d} = 0.971(12)(6)$ and $g_T^{u-d} = 0.987(51)(20)$. The first error includes statistical and all systematic uncertainties except that due to the extrapolation Ansatz, which is given by the second error estimate. Combining our estimate for $g_A^{d-u}$ with the difference of light quarks masses $(m_d - m_u)^{\text{QCD}} = 2.670(35)$ MeV given by the Flavor Lattice Average Group (FLAG), we obtain $(M_N - M_P)^{\text{QCD}} = 2.590(49)$ MeV. Estimates of the connected part of the flavor-diagonal tensor charges of the proton are $g_T^p = 0.792(42)$ and $g_T^n = -0.194(14)$. Combining our new estimates with precision low-energy experiments, we present updated constraints on novel scalar and tensor interactions, $\epsilon_{S,T}$, at the TeV scale.

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I. INTRODUCTION

The nucleon axial charge $g_A^{u-d}$ is an important parameter that encapsulates the strength of weak interactions of nucleons. It enters in many analyses of nucleon structure and of the Standard Model (SM) and Beyond-the-SM (BSM) physics. For example, the rate of proton-proton fusion, which is the first step in the thermonuclear reaction chains that power low-mass hydrogen-burning stars like the Sun, is sensitive to it. It impacts the extraction of $V_{ud}$ and tests of the unitarity of the CKM matrix, and the analysis of neutrinoless double-beta decay. At present, the ratio of the axial to the vector charge, $g_A/g_V$, is best determined from the experimental measurement of neutron beta decay using polarized ultracold neutrons by the UCNA Collaboration, 1.2756(30) [1], and by PERKEO II, 1.2761±14 [2]. Note that, in the SM, $g_V = 1$ up to second order corrections in isospin breaking [3, 4] as a result of the conservation of the vector current. Using $V_{ud}$ determined from superallowed nuclear beta decay or pion decay in combination with the average neutron lifetime measurement also gives a consistent value for $g_A^{u-d}$ [5, 6]. Given the important role $g_A^{u-d}$ plays in parametrizing the structure and weak interactions of nucleons, and probing signatures of new physics, it is important to calculate it directly with O(1%) accuracy using lattice QCD and eventually confront the theoretical prediction with experimental measurements.

The isovector scalar and tensor charges of the nucleon, combined with the helicity-flip parameters $b$ and $b_v$ in the neutron decay distribution, probe novel scalar and tensor interactions at the TeV scale [7]. To optimally bound such scalar and tensor interactions using planned measurements of these $b$ and $b_v$ parameters at the $10^{-3}$ precision level [8–10], requires the matrix elements of the local scalar and tensor quark bilinear operators within the nucleon state to be calculated with a precision of 10–15% [7]. Future higher-precision measurements of $b$ and $b_v$ would require correspondingly higher-precision calculations of the matrix elements to place even more stringent bounds on TeV-scale couplings. In a recent work [11], we showed that lattice-QCD calculations have reached a level of control over all sources of systematic errors needed to yield the tensor charge with the required precision. The data for the scalar 3-point func-

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tions is about a factor of five more noisy. In this paper we show that by using the all-mode-averaging (AMA) error-reduction technique [12, 13] on the same set of ensembles used in Ref. [11], we can increase the statistics significantly and extract the scalar charge with $O(15\%)$ uncertainty. These higher-statistics results also improve upon our previous estimates of the tensor charges.

In addition to probing novel scalar and tensor interactions at the TeV scale, precise estimates of the matrix elements of the flavor-diagonal tensor operators are needed to quantify the contributions of the $u$, $d$, $s$, $c$ quark electric dipole moments (EDM) to the neutron electric dipole moment (nEDM) [11, 14]. Most extensions of the Standard Model designed to explain nature at the TeV scale have new sources of CP violation, and the nEDM is a very sensitive probe of these. Thus, planned experiments aiming to reduce the current bound on the nEDM is a very sensitive probe of these. Thus, planned experiments aiming to reduce the current bound on the nEDM [11, 14] will put stringent constraints on many BSM theories, provided the matrix elements of novel CP-violating interactions, of which the quark EDM is one, are calculated with the required precision.

The tensor charges are also given by the zeroth moment of the transversity distributions that are measured in many experiments including Drell-Yan and Semi-Inclusive Deep Inelastic Scattering (SIDIS). Transversity distributions describe the net transverse polarization of quarks in a transversely polarized nucleon, and there exists an active program at Jefferson Lab (JLab) to measure them [16]. The extraction of the transversity distributions from the data taken over a limited range of $Q^2$ and Bjorken $x$ is, however, not straightforward and requires additional phenomenological modeling. As discussed in Sec. VIII, lattice-QCD estimates of $g_{T}^{u-d}$ are the most accurate at present. Future experiments will significantly improve the extraction of the transversity distributions. Thus, accurate calculations of the tensor charges using lattice QCD will continue to help elucidate the structure of the nucleon in terms of quarks and gluons and provide a benchmark against which phenomenological estimates utilizing measurements at JLab and other experimental facilities worldwide can be compared.

The methodology for calculating the isovector charges in an isospin symmetric theory, that is, measuring the contribution to the matrix elements of the insertion of the zero-momentum bilinear quark operators in one of the three valence quarks in the nucleon, is well developed [17–19]. Calculation of the flavor-diagonal charges is similar except that it gets additional contributions from contractions of the operator as a vacuum quark loop that interacts with the nucleon propagator through the exchange of gluons. Our estimates of disconnected contributions to $g_{T}^{u,d,s}$ were given in Ref. [11], where we showed that these contributions are small, $O(0.01)$, and in most cases consistent with zero within errors.\footnote{The five ensembles analyzed were $a12m310$, $a12m220$, $a09m310$, $a09m220$ and $a06m310$. Analysis of the physical mass ensemble $a09m130$ is ongoing.}

In this paper we show that by using the all-mode-averaging (AMA) error-reduction technique [12, 13] on the same set of ensembles used in Ref. [11], we can increase the statistics significantly and extract the scalar charge with $O(15\%)$ uncertainty. These higher-statistics results also improve upon our previous estimates of the tensor charges.

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The HP calculation on the simulated, the number of configurations analyzed, and the number of measurements made using the HP and AMA methods.

For each ensemble, we also give the values of the source-sink separation $t_{\text{sep}}/a$.

### Table I. Parameters, including the Goldstone pion mass $M_\pi^{\text{sea}}$, of the 2+1+1-flavor HISQ lattices generated by the MILC Collaboration and analyzed in this study are quoted from Ref. [22]. The lattice scale is determined using $r_1$ [22]. Symbols used in the plots are defined along with the ensemble ID. All fits are made versus $M_\pi^{\text{val}}$ and finite-size effects are analyzed in terms of $M_\pi^{\text{val}}L$. Estimates of $M_\pi^{\text{val}}$, the clover-on-HISQ pion mass, are the same as given in Ref. [11] and the error is governed mainly by the uncertainty in the lattice scale. For each ensemble, we also give the values of the source-sink separation $t_{\text{sep}}$ simulatated, the number of configurations analyzed, and the number of measurements made using the HP and AMA methods.

The HP calculation on the $a12m220L$ ensemble has been done with a single $t_{\text{sep}} = 10$ while the LP analysis has been done with $t_{\text{sep}} = \{8, 10, 12, 14\}$.

| Ensemble ID | $a$ (fm) | $M_\pi^{\text{sea}}$ (MeV) | $M_\pi^{\text{val}}$ (MeV) | $L^3 \times T$ | $M_\pi^{\text{val}}L$ | $t_{\text{sep}}/a$ | $N_{\text{conf}}$ | $N_{\text{meas}}^{\text{HP}}$ | $N_{\text{meas}}^{\text{AMA}}$ |
|------------|---------|----------------|----------------|----------------|----------------|----------------|--------------|----------------|----------------|
| a12m310 $\triangle$ | 0.1207(11) | 305.3(4) | 310.2(2.8) | 24$^3 \times 64$ | 4.55 | $\{8, 10, 11, 12\}$ | $\{8, 10, 12\}$ | 1013 | 8104 | 64832 |
| a12m220S $\triangleleft$ | 0.1202(12) | 218.1(4) | 225.0(2.3) | 24$^3 \times 64$ | 3.29 | | | 1000 | 24000 |
| a12m220 $\triangledown$ | 0.1184(10) | 216.9(2) | 227.9(1.9) | 32$^3 \times 64$ | 4.38 | | | 958 | 7664 |
| a12m220L $\triangledown$ | 0.1189(09) | 217.0(2) | 227.6(1.7) | 40$^3 \times 64$ | 5.49 | | | 1010 | 8080 | 68680 |
| a00m310 $\triangledown$ | 0.0888(08) | 312.7(6) | 313.0(2.8) | 32$^3 \times 96$ | 4.51 | | | 881 | 7048 |
| a00m220 $\star$ | 0.0872(07) | 220.3(2) | 225.9(1.8) | 48$^3 \times 96$ | 4.79 | | | 890 | 7120 |
| a00m130 | 0.0871(06) | 128.2(1) | 138.1(1.0) | 64$^3 \times 96$ | 3.90 | | | 883 | 7064 | 84768 |
| a00m320 $\square$ | 0.0582(04) | 319.3(5) | 319.6(2.2) | 48$^3 \times 144$ | 4.52 | | | 1000 | 8000 | 64000 |
| a00m220 $\diamond$ | 0.0578(04) | 229.2(4) | 235.2(1.7) | 64$^3 \times 144$ | 4.41 | | | 650 | 2600 | 41600 |

by the MILC Collaboration [22]. These are the same ensembles as used in Ref. [11], where we presented an analysis of the tensor charge. Their parameters are summarized in Table I.

The correlation functions needed to calculate the matrix elements are constructed using Wilson-clover fermions on these HISQ ensembles. This mixed-action, clover-on-HISQ approach, leads to a non-unitary formulation that at small, but a priori unknown, quark masses suffers from the problem of exceptional configurations. In Ref. [11], we described the tests performed to show the absence of any such exceptional configurations in our statistical samples. The mixed-action approach also introduces additional corrections to the leading chiral and continuum extrapolation Ansatz. In Sec. V, we analyze the observed dependence of the charges on $M_\pi$ over the range $135 \lesssim M_\pi \lesssim 320$ MeV with and without the chiral logarithm corrections in the fit Ansatz. It turns out that with our current data, the observed dependence on the lattice spacing $a$ and the quark masses is accounted for by the lowest-order correction terms.

The parameters used in the analysis of 2- and 3-point functions with clover fermions are given in Table II. The Sheikholeslami-Wohlert coefficient [24] used in the clover action is fixed to its tree-level value with tadpole improvement, $\epsilon_{\text{sw}} = 1/u_0^4$, where $u_0$ is the fourth root of the plaquette expectation value calculated on the hypercubic (HYP) smeared [25] HISQ lattices.

The masses of light clover quarks were tuned so that the clover-on-HISQ pion masses, $M_\pi^{\text{val}}$, match the HISQ-on-HISQ Goldstone ones, $M_\pi^{\text{sea}}$. Both estimates are given in Table I. All fits in $M_\pi^2$ to study the chiral behavior are made using the clover-on-HISQ $M_\pi^{\text{val}}$ since the correlation functions, and thus the chiral behavior of the charges, have a greater sensitivity to it. Henceforth, for brevity, we drop the superscript and denote the clover-on-HISQ pion mass as $M_\pi$.

Performing fits using the HISQ-on-HISQ values, $M_\pi^{\text{sea}}$, did not change the estimates significantly.

Most of the details of the methodology, the calculation strategy and the analysis are the same as described in Ref. [11]. The new feature in the current work is the use of the AMA method [12, 13] to recalculate all quantities on the five ensembles that had the largest uncertainty: $a12m310, a12m220L, a00m130, a06m310$ and $a06m220$. These new estimates have significantly smaller statistical errors, and this improvement allows us to better understand and quantify the excited-state contamination. Using these more precise estimates improves our final combined extrapolation in the lattice volume, $M_\pi L \to \infty$, lattice spacing, $a \to 0$, and the light-quark mass, $M_{\pi 0} \to 135$ MeV.

### A. Correlation Functions

The interpolating operator $\chi$ used to create/annihilate the nucleon state is

$$\chi(x) = \epsilon^{abc} \left[ q_1^T(x) C \gamma_5 \left( \frac{1 + \gamma_4}{2} q_2(x) \right) \right] q_1(x) \quad (1)$$

with color indices $\{a, b, c\}$, charge conjugation matrix $C = \gamma_0 \gamma_2$, and $q_1$ and $q_2$ denote the two different flavors of light quarks. At zero momentum, this operator couples only to the spin-$\frac{1}{2}$ state. The non-relativistic projection $(1 \pm \gamma_4)/2$ is inserted to improve the signal, with the plus and minus sign applied to the forward and backward propagation in Euclidean time, respectively [27].

The 2-point and 3-point nucleon correlation functions
at zero momentum are defined as
\[
C_{\alpha\beta}^{2pt}(t) = \sum_{x} \langle 0| \chi_{\alpha}(t, x) \chi_{\beta}(0, 0)|0\rangle, \tag{2}
\]
\[
C_{\Gamma}^{3pt}(t, \tau) = \sum_{x, x'} \langle 0| \chi_{\alpha}(t, x) \mathcal{O}_{\Gamma}(\tau, x') \chi_{\beta}(0, 0)|0\rangle, \tag{3}
\]
where \(\alpha\) and \(\beta\) are spinor indices. The source is placed at timeslice 0, \(t\) is the sink timeslice, and \(\tau\) is an intermediate timeslice at which the local quark bilinear operator \(\mathcal{O}_{\Gamma}(x) = \bar{q}(x) \Gamma q(x)\) is inserted. The Dirac matrix \(\Gamma\) is 1, \(\gamma_{4}\), \(\gamma_{5}\gamma_{5}\) and \(\gamma_{i}\gamma_{j}\) for scalar (S), vector (V), axial (A) and tensor (T) operators, respectively. In this work, subscripts \(i\) and \(j\) are defined in Eqs. (6) and (7) are discussed in Sec. III.

The nucleon charges \(g_{i}^{N}\) are obtained from the matrix element
\[
\langle N(p, s)| \mathcal{O}_{\Gamma}^{\dagger}(N(p, s)) = g_{i}^{N} \bar{u}_{s}(p) \Gamma u_{s}(p) \tag{4}
\]
with spinors satisfying
\[
\sum_{s} u_{s}(p) \bar{u}_{s}(p) = \bar{p} + m_{N}. \tag{5}
\]

To extract the charges, we first construct the projected 2- and 3-point correlation functions
\[
C_{\Gamma}^{2pt}(t) = \langle \text{Tr} | \mathcal{P}_{2pt} C_{\Gamma}^{2pt}(t) \rangle \tag{6}
\]
\[
C_{\Gamma}^{3pt}(t, \tau) = \langle \text{Tr} | \mathcal{P}_{3pt} C_{\Gamma}^{3pt}(t, \tau) \rangle. \tag{7}
\]
The operator \(\mathcal{P}_{2pt} = (1 + \gamma_{4})/2\) is used to project on to the positive parity contribution for the nucleon propagating in the forward direction. For the connected 3-point contributions, \(\mathcal{P}_{3pt} = \mathcal{P}_{2pt}(1 + i \gamma_{5} \gamma_{3})\) is used. Note that the \(C_{\Gamma}^{3pt}(t, \tau)\) defined in Eq. (7) becomes zero if \(\Gamma\) anticommutes with \(\gamma_{4}\), so only \(\Gamma = 1, \gamma_{4}, \gamma_{5}\gamma_{5}\) and \(\gamma_{i}\gamma_{j}\) elements of the Clifford algebra survive. The fits used to extract the charges from the 2- and 3-point functions defined in Eqs. (6) and (7) are discussed in Sec. III.

| ID     | \(m_{i}\) | \(\text{csw}\) | Smearing Parameters |
|--------|----------|----------------|---------------------|
| a12m310 | −0.0695  | 1.05094       | \{5.5, 70\}        |
| a12m220S| −0.075   | 1.05091       | \{5.5, 70\}        |
| a12m220 | −0.075   | 1.05091       | \{5.5, 70\}        |
| a12m220L| −0.075   | 1.05091       | \{5.5, 70\}        |
| a09m310 | −0.05138 | 1.04243       | \{5.5, 70\}        |
| a09m220 | −0.0554  | 1.04239       | \{5.5, 70\}        |
| a09m130 | −0.058   | 1.04239       | \{5.5, 70\}        |
| a06m310 | −0.0398  | 1.03493       | \{6.5, 70\}        |
| a06m220 | −0.04222 | 1.03493       | \{5.5, 70\}        |

TABLE II. The parameters used in the calculation of clover propagators. The hopping parameter \(a\) in the clover action is given by \(2m_{i} = 1/(m_{i} + 4)\). The Gaussian smearing parameters are defined by \(N_{GS} = \sigma N_{GS}\), both in Chroma convention [26]. The parameter \(N_{GS}\) is the number of applications of the Laplacian operator and the width of the smearing is controlled by \(\sigma\). \(m_{i}\) is tuned to achieve \(M_{\sigma}^{\text{val}} \approx M_{\sigma}^{\text{sea}}\).

B. The AMA Method

The high-statistics calculation using the all-mode-averaging (AMA) technique [12, 13] was carried out on five ensembles. To implement the AMA method, we choose four different source timeslices separated by \(T/4\) on each configuration. Starting from each of these timeslices we calculate the 2- and 3-point correlators by choosing \(N_{LP} = 16\) source locations from which low-precision (LP) evaluation of the quark propagator is carried out. The resulting LP estimates for 2- and 3-point functions from these \(4 \times 16 = 64\) sources may be biased due to incomplete inversion of the Dirac matrix. To remove this bias, we place an additional high-precision (HP) source on each of the four timeslices from which we calculate both LP and HP correlation functions. Thus, in our implementation of the AMA method, \(64 + 4\) LP and HP calculations are done on each configuration. These \(4\) HP calculations are the same as used in the full HP study presented in Ref. [11] and, therefore, needed no additional calculations. In total, the new simulations generated \(4 \times 16 + 4 = 68\) LP 2- and 3-point correlation functions per configuration.

Using four HP and \(64 + 4\) LP correlators on each configuration, the bias corrected 2- and 3-point functions are given by
\[
C_{\text{imp}} = \frac{1}{N_{LP}} \sum_{i=1}^{N_{LP}} C_{LP}(x_{i}^{LP})
\]
\[
+ \frac{1}{N_{HP}} \sum_{i=1}^{N_{HP}} [C_{HP}(x_{i}^{HP}) - C_{LP}(x_{i}^{HP})], \tag{8}
\]
where \(C_{LP}\) and \(C_{HP}\) are the 2- and 3-point correlation functions calculated in LP and HP, respectively, and \(x_{i}^{LP}\) and \(x_{i}^{HP}\) are the two kinds of source positions.

The basic idea of AMA is that, in the low-precision evaluation, the LP average, first term in Eq. (8), may be biased. The bias is corrected by the second low-statistics term without significantly increasing the overall statistical errors. To determine the LP stopping criteria, we compared LP and AMA results using 50 configurations from the \(a12n310\) ensemble with \(r_{LP} \equiv |\text{residue}_{LP}/|\text{source}| = 10^{-2}, 5 \times 10^{-3}, 10^{-3}\) and \(10^{-4}\). All four LP estimates agreed with the AMA estimate within \(\sigma\). To reduce computational cost and yet be conservative, we selected \(r_{LP} = 10^{-3}\) for all calculations presented in this work.

In our current implementation, 17 LP measurements cost the same as one HP when using the multigrid algorithm for inverting the Dirac matrix [28]. Adding \(64 + 4\) LP measurements doubled the cost compared to 4 HP measurements, whereas the increase in statistics is by a factor of 16 in the AMA analysis with bias correction. Note that only four of the existing eight HP source positions were used for bias correction as these were found to be sufficient. Also, on the \(a06m220\) ensemble, only four HP measurements were made on each configuration.
FIG. 1. Comparison of the unrenormalized $g_{u-d}$ data obtained using all HP measurements (left) with the AMA method (right). The parameters for these five ensembles are given in Table I. The increase in statistics with the AMA method significantly improves the resolution of the data at the various source-sink separations, $t_{sep}$. In each case, the solid line within the grey error band is the $t_{sep} \rightarrow \infty$ result given by the 2-state fit using Eqs. (9) and (10) and the colored lines are its value for different $t_{sep}$ plotted in the same color as the data. On the $a12m220L$ ensemble, the HP data was generated only with $t_{sep} = 10$. 
FIG. 2. Comparison of the unrenormalized $g_{S}^{u-d}$ data obtained using all HP measurements (left) with the AMA method (right). The rest is the same as in Fig. 1.
FIG. 3. Comparison of the unrenormalized $g_{\tau u-d}$ data obtained using all HP measurements (left) with the AMA method (right). The rest is the same as in Fig. 1.
FIG. 4. Comparison of the unrenormalized $g_V^{u-d}$ data obtained using all HP measurements (left) with the AMA method (right). The rest is the same as in Fig. 1.
To test how the errors change with the bias correction, we compare the results for the charges on the five ensembles analyzed using both HP and AMA methods. We compared both HP versus AMA and AMA versus LP estimates. A comparison of the HP versus the AMA data for the masses and amplitudes extracted from the nucleon 2-point function is shown in Tables III and IV. Comparison of the isovector charges $g_{\Lambda}^{u-d}$, $g_{S}^{u-d}$, $g_{T}^{u-d}$ and $g_{T}^{d}$ is shown in Figs. 1, 2, 3 and 4, respectively. The increase in statistics with the AMA method (see Table I) significantly improves the precision of the data at the various source-sink separations, $t_{\text{sep}}$. We have used in the analysis of the 3-point functions. In each panel of the four figures, the grey error band and the solid line within it gives the $t_{\text{sep}} \to \infty$ value obtained from the 2-state fit using Eqs. (9) and (10). The two estimates are, in most cases, consistent and in the rest the difference is less than $2\sigma$. The AMA data at each $t_{\text{sep}}$ has much smaller errors, consequently, the $t_{\text{sep}} \to \infty$ estimates from the 2-state fit to the AMA data are more precise.

Comparing the AMA with the LP data, we find that in each case the difference is a tiny fraction of the statistical error in the AMA calculation; that is, the bias correction term is negligible. This is shown in Tables III and IV for the 2-point data and in Tables VI, VII and VIII for the matrix elements extracted from the 3-point data. Thus, our conclusion is that using the multi-grid solver [28, 29] with a low-accuracy stopping criterion $r_{\text{LP}} = |\text{residue}||_{\text{LP}}/|\text{source}| \approx 10^{-3}$, is as good as the HP inversion with $r_{\text{HP}} = 10^{-8}$--$10^{-12}$ for the calculation of the nucleon charges at the level of statistical precision achieved in this work.

Our final errors are obtained using a single elimination Jackknife analysis over the configurations; that is, we first construct the average defined in Eq. (8) on each configuration. Because of this “binning” of the data, we do not need to correct the Jackknife estimate of the error for correlations between the 64 LP measurements per configuration. It is, however, useful to determine the number of source positions one can place on each configuration beyond which the additional computational cost offsets the gain in statistics. The following tests indicate that the correlations between estimates from various sources are reasonably small with up to $O(100)$ sources per configuration on lattices with $M_{\pi}L \gtrsim 4$ and $M_{\pi}T \gtrsim 8$.

- Comparing the errors in the estimates for masses and amplitudes given in Tables III and IV, we find that the AMA errors are a factor of 2–4 smaller than those in the all HP analysis. (In the limit of no correlations, the scaling factor should be $\sqrt{64/8} = 2.83$.) A similar improvement is seen in the matrix elements as shown in Tables VI, VII and VIII. In most cases, the improvement is observed to become better with decreasing quark mass and lattice spacing.

- Figure 5 illustrates that the errors decrease by a factor of about 3.7 when the number of LP sources are increased from 4 to 64 on the $a_06m220$ lattices. The gain is similar in both the 2- and 3-point functions.

- On the $a_06m310$ ensemble, we compared estimates of the 2- and 3-point correlation functions using 64 and 128 LP sources during the study of the disconnected diagram contribution reported in Ref. [11]. We found that the errors are reduced by only a factor of 1.2. A similar comparison of 2- and 3-point functions obtained using 64 and 128 LP sources in the $a_06m310$ AMA2 study discussed in Sec. VI shows that errors reduce by only a factor of 1.15. Thus, both tests indicate that the gain in statistics becomes small when more the 64 LP sources per configuration are used on lattices with $M_{\pi}L \sim 4$.

A second technique used to reduce correlations in the AMA calculations is to choose the 64 LP source points randomly within and between configurations. On each configuration, the four source timeslices are chosen randomly to be $r+\alpha T/4$ with $r$ a random integer $\in \{1, T/4\}$ and $\alpha \in \{0, 1, 2, 3\}$. On the $a_06m220$ ensemble, each of these four timeslices is then divided into 16 boxes of size $L/2 \times L/2 \times L/4$ and a random source point is chosen within each of these boxes. On the rest of the ensembles, the 16 source points on each of the 4 timeslices are chosen randomly. In the HP calculation, the 8 source points were taken to be the same on all the configurations. A statistical analysis comparing the HP and AMA data shows that choosing the source points randomly reduces the final errors. For example, the standard error in the mean constructed by choosing a single source point per configuration is smaller for the LP data with randomly selected source point versus the HP data in which the source point was fixed to be the same on all the configurations.

To reduce computational cost, we have used the coherent sequential source method [30]. Four sequential sources on the four sink timeslices were calculated and held in computer memory. These were added and a single inversion performed to construct the coherent sequential propagator. Details of the method are given in Ref. [31], where we also showed that this method does not increase the bias or the errors.

To estimate errors, we performed both correlated and uncorrelated fits to the nucleon 2- and 3-point functions data. The final statistical errors were calculated using a single elimination jackknife method with uncorrelated fits to both the 2- and 3-point functions since correlated fits were not stable for the 3-point functions in all cases. In all cases in which the correlated fits to the 3-point functions were stable under changes in the fit ranges and had $\chi^2 \lesssim 1$, the correlated and uncorrelated fits gave overlapping estimates.

Having high-statistics data with the AMA method significantly improves the analysis. For example, the plateaus in the effective-mass plots extend to larger Euclidian time as discussed in Sec. III. This allowed fits to
TABLE III. Estimates of the masses $M_0$ and $M_1$ and the amplitudes $A_0$ and $A_1$ extracted from the fits to the 2-point correlation functions using the 2-state Ansatz given in Eqs. (9) and (10). We give the results of fits to both the HP and the AMA data for the five ensembles $a12m310$, $a12m220L$, $a09m130$, $a06m310$ and $a06m220$. The Gaussian smearing parameters, $\{\sigma, N_{GS}\}$, used in the calculation of the 2- and 3-point connected correlation functions are given in Table II. The fit range used is listed as case 1 in Table V.

| ID   | Type | Fit Range | $aM_0$ | $aM_1$ | $A_0^2 \times 10^{11}$ | $A_1^2 \times 10^{11}$ | $A_0^2/A_1^2$ |
|------|------|-----------|--------|--------|----------------------|----------------------|-------------|
| $a12m310$ | HP   | 2–15      | 0.6669(53) | 1.36(11) | 6.57(27) | 6.28(61) | 0.96(7) |
| $a12m310$ | AMA  | 3–15      | 0.6722(22) | 1.64(16) | 6.95(12) | 9.5(3.4) | 1.36(47) |
| $a12m220S$ | HP    | 2–15      | 0.6233(55) | 1.42(13) | 6.58(26) | 6.94(93) | 1.05(11) |
| $a12m220$ | HP    | 2–15      | 0.6232(49) | 1.45(15) | 6.58(24) | 6.8(1.1) | 1.03(14) |
| $a12m220L$ | HP    | 2–15      | 0.6046(71) | 1.16(12) | 5.68(37) | 5.63(51) | 0.99(6) |
| $a12m220L$ | LP    | 3–15      | 0.6118(26) | 1.18(7) | 5.99(15) | 4.64(50) | 0.78(7) |
| $a09m310$ | HP    | 4–20      | 0.4943(62) | 0.87(9) | 13.6(1.1) | 14.4(1.7) | 1.05(8) |
| $a09m220$ | HP    | 4–20      | 0.4553(58) | 0.86(8) | 11.8(9) | 15.2(2.1) | 1.29(11) |
| $a09m130$ | HP    | 3–20      | 0.4186(76) | 0.83(6) | 9.74(89) | 17.2(1.0) | 1.76(10) |
| $a09m130$ | AMA   | 5–20      | 0.4150(45) | 0.73(5) | 8.70(59) | 11.7(8) | 1.34(6) |
| $a06m310$ | HP    | 5–30      | 0.3219(37) | 0.58(2) | 0.53(4) | 1.26(6) | 2.35(12) |
| $a06m310$ | HP    | 7–30      | 0.3277(18) | 0.59(2) | 0.59(2) | 1.10(8) | 1.86(8) |
| $a06m220$ | HP    | 5–30      | 0.3166(17) | 0.64(5) | 13.0(1.5) | 38.5(5.4) | 2.96(20) |
| $a06m220$ | AMA   | 7–30      | 0.3068(17) | 0.63(2) | 11.3(3) | 38.5(3.0) | 3.41(18) |

TABLE IV. Same as Table III except that the fit range used is listed as case 3 in Table V.

| ID   | Type | Fit Range | $aM_0$ | $aM_1$ | $A_0^2 \times 10^{11}$ | $A_1^2 \times 10^{11}$ | $A_0^2/A_1^2$ |
|------|------|-----------|--------|--------|----------------------|----------------------|-------------|
| $a12m310$ | HP   | 3–15      | 0.6641(76) | 1.20(17) | 6.38(46) | 4.5(9) | 0.70(11) |
| $a12m310$ | AMA  | 3–15      | 0.6722(22) | 1.64(16) | 6.95(12) | 9.5(3.4) | 1.36(47) |
| $a12m220S$ | HP    | 3–15      | 0.6202(94) | 1.20(27) | 6.37(54) | 4.3(1.5) | 0.67(18) |
| $a12m220$ | HP    | 3–15      | 0.6216(73) | 1.27(30) | 6.47(42) | 4.5(2.2) | 0.69(30) |
| $a12m220L$ | HP    | 3–15      | 0.597(14) | 0.96(17) | 5.16(87) | 4.19(33) | 0.81(14) |
| $a12m220L$ | LP    | 4–15      | 0.6109(35) | 1.11(13) | 5.92(22) | 3.78(98) | 0.64(15) |
| $a09m310$ | HP    | 5–20      | 0.4933(78) | 0.84(12) | 13.4(1.5) | 13.0(2.9) | 0.97(15) |
| $a09m220$ | HP    | 5–20      | 0.4529(68) | 0.84(12) | 11.7(1.1) | 14.1(3.8) | 1.21(24) |
| $a09m130$ | HP    | 4–20      | 0.413(12) | 0.75(10) | 8.9(1.6) | 14.0(1.4) | 1.56(18) |
| $a09m130$ | AMA   | 6–20      | 0.4137(60) | 0.71(7) | 8.50(85) | 10.8(1.5) | 1.27(9) |
| $a06m310$ | HP    | 6–30      | 0.3190(47) | 0.54(3) | 0.50(5) | 1.08(6) | 2.17(16) |
| $a06m310$ | AMA   | 8–30      | 0.3268(23) | 0.56(3) | 0.58(3) | 0.95(10) | 1.66(11) |
| $a06m220$ | HP    | 6–30      | 0.3149(84) | 0.61(8) | 12.5(2.0) | 32.3(7.3) | 2.59(28) |
| $a06m220$ | AMA   | 8–30      | 0.3069(18) | 0.63(2) | 11.3(4) | 39.2(5.0) | 3.47(35) |

To summarize, we find that the AMA method with $O(100)$ randomly selected source positions on each configuration is a very cost-effective way to increase the statistics significantly and consequently improve the quality of the fits used to extract the estimates for the charges on each ensemble. Having these estimates with small errors improves the quality of the final fits made to obtain results in the continuum limit and at the physical light-quark mass as discussed in Sec. V.

III. EXCITED-STATE CONTAMINATION

Nucleon charges are given by the matrix elements of the bilinear quark operators between ground-state nucleons. The lattice operator $\chi$ given in Eq. (1), however, couples to the nucleon, its excitations and multiparticle states with the same quantum numbers. We incorporate three strategies to reduce excited-state contamination:

- The overlap between the nucleon operator and the excited states is reduced by using tuned smeared sources when calculating the quark propagators. We construct gauge-invariant Gaussian smeared sources by applying the three-dimensional Laplacian operator $\nabla^2$ a fixed number of times $N_{GS}$, $(1 - \sigma^2 \nabla^2/(4N_{GS}))^{N_{GS}}$. The smearing parameters $\{\sigma, N_{GS}\}$ for each ensemble are given in Table II and are the same as in Ref. [11] in order to avoid...
TABLE V. The fit parameters $t_{\text{min}}$ and $\tau_{\text{skip}}$ defining the four cases used to analyze the 2- and 3-point functions data. The parameter $t_{\text{min}}$ is the starting value of time used in the 2-point fit and $\tau_{\text{skip}}$ is the number of point skipped adjacent to the source and sink in the fit to the 3-point data. The triplets of numbers correspond to the three lattice spacings $a = \{0.12, 0.09, 0.06\}$ fm, respectively. The three exceptions to these fit ranges are specified in Tables III and IV. The ending timeslices in the 2-point fits, were chosen to be $t_{\text{max}} = \{15, 20, 30\}$ in all cases.

| Case | $t_{\text{min}}$ (2pt HP) | $t_{\text{min}}$ (2ptAMA) | $\tau_{\text{skip}}$ (3pt) |
|------|-----------------|-----------------|-----------------|
| 1    | $\{2.4, 5\}$   | $\{3.5, 7\}$   | $\{2.3, 4\}$   |
| 2    | $\{2.4, 5\}$   | $\{3.5, 7\}$   | $\{3.4, 6\}$   |
| 3    | $\{3.5, 6\}$   | $\{4.6, 8\}$   | $\{2.3, 4\}$   |
| 4    | $\{3.5, 6\}$   | $\{4.6, 8\}$   | $\{3.4, 6\}$   |

repeating the expensive HP calculation needed for the AMA analysis. Also, the same smearing is used at the source and sink points to construct the smeared-smeared 2- and 3-point correlation functions.

- We calculate the 3-point correlation functions for a number of values of the source-sink separation $t_{\text{sep}}$ given in Table I. We fit the data at all $t_{\text{sep}}$ simultaneously using the 2-state Ansatz given in Eq. (10) to estimate the $t_{\text{sep}} \to \infty$ value.

- We include one excited state in the analysis of the 2-point and 3-point functions as given in Eqs. (9) and (10). We find that this Ansatz has enough free parameters to fit the data and the additional five parameters needed to include a second excited state would be very poorly determined.

The 2-state Ansatz used to fit the 2- and 3-point functions is,

$$C^{2\text{pt}}(t_f, t_i) = |A_0|^2 e^{-M_0(t_f-t_i)} + |A_1|^2 e^{-M_1(t_f-t_i)},$$  \hspace{1cm} (9)

$$C^{3\text{pt}}(t_f, \tau, t_i) = |A_0|^2 \langle 0|O|0\rangle e^{-M_0(t_f-t_i)} +$$

$$|A_1|^2 \langle 1|O|1\rangle e^{-M_1(t_f-t_i)} +$$

$$A_0^* A_1^* \langle 0|O|1\rangle e^{-M_0(\tau-t_i)} e^{-M_1(t_f-\tau)} +$$

$$A_0^* A_1 \langle 1|O|0\rangle e^{-M_1(\tau-t_i)} e^{-M_0(t_f-\tau)},$$  \hspace{1cm} (10)

where $\tau$ is the time at which the operator is inserted and $t_f - t_i = t_{\text{sep}}$ in the 3-point function calculation. The states $\langle 0 \rangle$ and $\langle 1 \rangle$ represent the ground and “first excited” nucleon states, respectively. To extract the charges $g_{\Lambda, S}^{u-d}$, $g_{\Lambda, T}^{u-d}$ and $g_{\Gamma}^{u-d}$, we only need to examine the real part of the correlation functions with the operator insertion at zero momentum, in which case $A_0$ and $A_1$ are real and the matrix element $\langle 0|O|1\rangle = \langle 1|O|0\rangle$. Thus, we need to extract seven parameters from fits to the 2- and 3-point functions. The four parameters, $M_0$, $M_1$, $A_0$ and $A_1$ are estimated first from the 2-point data and are then used as inputs in the extraction of matrix elements from fits to the 3-point data. Fits to both 2- and 3-point data are done within the same Jackknife process to take into account correlations.

Five of the seven parameters, $M_0$, $M_1$ and the three matrix elements $\langle 0|O|0\rangle$, $\langle 0|O|1\rangle$ and $\langle 1|O|1\rangle$ are physical once the discretization errors and higher excited-state contaminations have been removed from them. The amplitudes $A_0$ and $A_1$ depend on the choice of the interpolating nucleon operator and the smearing parameters used to generate the smeared sources. It is clear from Eqs. (9) and (10) that the ratio of the amplitudes, $A_1/A_0$, is the quantity to minimize in order to reduce excited-state contamination since it determines the relative strength of the overlap of the nucleon operator with the first excited-state. Estimates of $\langle 0|O|1\rangle$, $\langle 1|O|1\rangle$, $\langle 0|O|0\rangle$...
the mass gap $M_1 - M_0$, and the ratio $A_1/A_0$ can be used, post facto, to bound the size of the excited-state contamination for a given source-sink separation $t_{\text{sep}}$.

Results of the 2-state fits to the 2-point functions needed to extract $M_0$, $M_1$, $A_0$ and $A_1$ are consistent within errors for two sets of starting timeslices $t_{\text{min}}$ as shown in Tables III and IV. The $\chi^2$/d.o.f. of the correlated fits are also similar for the two fit ranges. These fit ranges are specified in Table V.

Higher statistics with the AMA method allow us to fit the data with larger $t_{\text{min}}$. The HP and AMA estimates for $M_0$ and $A_0$ with different fit range are consistent for all the ensembles and are independent of $t_{\text{min}}$. This is expected since these ground-state estimates are sensitive only to the data at large $t$ and that is the same in both choices of the fit ranges. We also note that the scaling of the errors is consistent with the naive expectation, $\sqrt{N_{\text{HP}}/N_{\text{LP}}}$.

We illustrate the improvement with the AMA method compared to just the HP analysis in Fig. 6 using the $a09m130$ data fit with $t_{\text{min}} = 6$. The plateau in the effective-mass $M_{\text{eff}}(t+0.5) = -\log\{C_{2pt}(t+1)/C_{2pt}(t)\}$, where $C_{2pt}(t)$ is the 2-point nucleon correlation function at time separation $t$, extends about four timeslices further with the AMA data. In the limit $t \to \infty$, $M_{\text{eff}}(t)$ converges to the ground-state mass $M_0$. A comparison of the error estimates in both the data points and in the result of the fit shows that the extraction of the masses and the amplitudes improves very significantly with the AMA method.

The data in Tables III and IV show a $2\sigma$ difference in the extraction of $M_0$ from the four ensembles $a12m220S$, $a12m220L$ and $a12m220L$ with AMA$^2$. The effective-mass data for the four calculations is shown in Fig. 7. The errors in the $a12m220S$, $a12m220L$ data are large and the data show a noisy plateau over the range $7 \leq t \leq 10$. As a result, the 2-state fit is sensitive to the choice of $t_{\text{min}}$. The higher statistics and larger volume $a12m220L$ AMA data show a plateau over the interval $9 \leq t \leq 15$ and the fit is stable under changes in $t_{\text{min}}$. Because of this difference in the quality of the data, it is difficult to assess if the $t \to \infty$ estimates have been obtained in the $a12m220S$ and $a12m220L$ data. As a result, we are not able to determine what fraction of the difference in $M_0$ is due to finite-volume effects and how much is due to statistics.

The quantities that are harder to extract and are sensitive to the choice of $t_{\text{min}}$ are $M_1$ and $A_1$. In most cases, results of fits with larger $t_{\text{min}}$ (Case 3 versus Case 1 in Table V) yield smaller values for $M_1$ and $A_1$. This is expected since, within a 2-state fit Ansatz, these parameters effectively capture the contributions of all the higher states and fitting with larger $t_{\text{min}}$ uses data with relatively less higher-states contamination. In practice, one has to compromise between using data with smaller errors at smaller $t_{\text{min}}$ and picking a large $t_{\text{min}}$ to reduce higher excited-state contamination. We have picked the second set with the larger $t_{\text{min}}$ for presenting our final

$^2$ We checked for bias in the $a12m220L$ data using the $t_{\text{sep}} = 10$ HP data and found it to be negligible as in the other four AMA studies. Assuming that this is true at other values of $t_{\text{sep}}$, we include the $a12m220L$ LP data as part of the AMA discussion.
results. Note that the error estimates are slightly larger with this choice.

As discussed above, we need to minimize the ratio of the amplitudes, \( A_1/A_0 \), to reduce the overlap of the nucleon operator with the first excited-state by tuning the smearing parameters. (In general, all the \( A_n/A_0 \) when up to \( n \) excited states are included in the fit Ansatz). Our additional tests on the \( a_{06} \) ensembles discussed in Sec. VI show that increasing the smearing size \( \sigma \) over the range simulated reduces \( A_1/A_0 \) and the excited-state contamination, most notably in the axial and scalar charges. On the other hand, beyond a certain size \( \sigma \), the statistical errors based on a given number of gauge configurations start to increase. Also, when calculating the form factors, one expects the optimal \( \sigma \) to decrease with increasing momentum. Thus, one has to compromise between obtaining a good statistical signal and reducing excited-state contamination in both the charges and the form factors, when all these quantities are being calculated with a single choice of the smearing parameters.

The data in Tables III and IV show an increase in the ratio \( A_1/A_0 \) as the lattice spacing is decreased. This suggests that the smearing parameter \( \sigma \) should have been scaled with the lattice spacing \( a \). The dependence of the ratio on the two choices of \( t_{\text{min}} \) used in the fits (estimates in Table III versus Table IV) and between the HP and AMA estimates for each choice is much smaller. Based on these trends and additional tests discussed in Sec. VI, a better choice for the smearing parameters when calculating the matrix elements at zero-momentum transfer is estimated to be \( \{5,70\} \), \( \{7,120\} \) and \( \{9,200\} \) for the \( a = 0.12, 0.09 \) and 0.06 \( fm \) ensembles, respectively. In physical units, a rule-of-thumb estimate for tuning the smearing size is \( \sigma a \approx 0.55 \text{ fm} \).

To extract the three matrix elements \( \langle 0 | O_T | 0 \rangle \), \( \langle 1 | O_T | 0 \rangle \) and \( \langle 1 | O_T | 1 \rangle \), for each operator \( O_T = O_{A,S,T,V} \), from the 3-point functions, we make one overall fit using the data at all values of the operator insertion time \( \tau \) and the various source-sink separations \( t_{\text{sep}} \) using Eq. (10). From such fits we extract the \( t_{\text{sep}} \rightarrow \infty \) estimates under the assumption that the contribution of all higher states is isolated by the 2-state Ansatz given in Eqs. (9) and (10).

In Figs. 8, 9 and 10, we show the data for the unrenormalized isovector charges \( g_{A}^{u-d} \), \( g_{S}^{u-d} \) and \( g_{T}^{u-d} \) for the seven ensembles at different values of \( a \) and \( M_{\pi} \) used in the final analysis. The other two ensembles, \( a_{12m220S} \) and \( a_{12m220T} \) at \( a = 0.114 \text{ fm} \) and \( M_{\pi} = 227 \text{ MeV} \), allow us to study the finite-volume effect. The data at central values of \( \tau \approx t_{\text{sep}}/2 \) show significant, about 15\%, dependence of \( g_{A}^{u-d} \) on \( t_{\text{sep}} \) between 1 and 1.5 \( fm \) for the \( a = 0.09 \) and 0.06 \( fm \) ensembles. In \( g_{T}^{u-d} \), this effect is less than 5\%. The size of the effect in \( g_{S}^{u-d} \) is not clear due to the much larger errors. Based on these data and additional tests discussed in Sec. VI, the two key observations are: (i) the 2-state Ansatz given in Eqs. (9) and (10) fits the data at multiple values of \( t_{\text{sep}} \) and gives a reliable estimate of the \( t_{\text{sep}} \rightarrow \infty \) value, and (ii) the behavior of the unrenormalized data versus \( \tau \) and \( t_{\text{sep}} \) are less sensitive to the value of \( M_{\pi} \) for fixed \( a \) compared to versus \( a \) for fixed \( M_{\pi} \). The behavior of the renormalized charges is discussed in Sec. V.

The estimates of the matrix elements obtained from the fits to the 3-point correlation functions for the unrenormalized charges are given in Tables VI, VII and VIII for the nine ensembles. Again, for the case of the five ensembles analyzed using the AMA method, we give the HP and the AMA estimates. For each of the two choices of fit ranges for the 2-point functions, listed in Tables III and IV, we determined the three matrix elements for two different choices of the number of time-slices, \( \tau_{\text{skip}} \), skipped on either end of the 3-point correlation functions. These two choices are \( \tau_{\text{skip}} = \{2, 3, 4\} \) and \( \{3, 4, 6\} \) for the three lattice spacings \( a = \{0.12, 0.09, 0.06\} \) \text{ fm} \), respectively. The four cases of fit parameters used in the analysis are summarized in Table V.

The results for \( \langle 0 | O_T | 0 \rangle \) for all four cases (two fit ranges for the 2-point functions and two choices of \( \tau_{\text{skip}} \) for the 3-point functions) are consistent as shown in Tables VI, VII and VIII. Estimates of \( \langle 0 | O_T | 1 \rangle \) and \( \langle 1 | O_T | 1 \rangle \) are also similar between Case 1 and Case 3, especially for the data with the AMA method. We choose Case 3 for our final estimates as it has (i) the larger \( t_{\text{min}} \) corresponding to a larger suppression of excited-states in the 2-point fits; and (ii) the smaller value for \( \tau_{\text{skip}} \) whereby more points at each \( t_{\text{sep}} \) are included in the 3-point fits to give a better determination of \( \langle 0 | O_T | 1 \rangle \).

The consistency between the four estimates of the matrix elements allows us to draw the following qualitative conclusions regarding excited-state contamination in \( u-d \) and \( a-d \) for the nine ensembles discussed in Sec. VI:

- Estimates of \( \langle 1 | O_T | 1 \rangle \) given in Tables VI, VII and VIII are poorly determined. Within the 2-state approximation, the effect of a nonzero \( \langle 1 | O_T | 1 \rangle \) is to change the data at all \( \tau \), for fixed \( t_{\text{sep}} \), by a constant amount. For \( g_{A}^{u-d} \), \( \langle 1 | O_T | 1 \rangle \) is large on the \( a = 0.09 \) and 0.06 \( fm \) ensembles and has the same sign as \( \langle 0 | O_T | 1 \rangle \). The two contributions, therefore, add to give a large excited-state contribution. For \( g_{T}^{u-d} \), the data in Fig. 10 show less than 5\% dependence on \( t_{\text{sep}} \) in the central regions (values of operator insertion time \( \tau \) at which the contribution of a nonzero \( \langle 0 | O_T | 1 \rangle \) is the smallest) and the contribution of \( \langle 1 | O_T | 1 \rangle \) is small. For \( g_{S}^{u-d} \), the data in Fig. 10 show a significant excited-state effect only for the \( a = 0.06 \) \( fm \) ensembles that is largely accounted for by the contribution of the \( \langle 0 | O_S | 1 \rangle \) term.

- Estimates of \( \langle 0 | O_S | 1 \rangle \) vary between \(-0.05 \) and \(-0.41 \) for \( g_{S}^{u-d} \). This matrix element gives the negative curvature observed in Fig. 9, and the ground-state estimate of \( g_{S}^{u-d} \) converges from below.
Data for $g_A^{u-d}$ show excited-state contamination on the two $a = 0.06$ fm ensembles $a06m310$ and $a06m220$. The 2-state fit gives reliable $t_{\text{sep}} \rightarrow \infty$ estimates as shown in Fig. 9. In Sec. VI, we present data from additional simulations on the $a06m310$ and $a06m220$ ensembles and discuss the limitations of the 2-state fit when the errors are large and the data at different $t_{\text{sep}}$ overlap as a result.

Estimates of $\langle 0 \vert O_T \vert 1 \rangle$ vary between 0.1 and 0.26 for $g_T^{u-d}$ and give rise to the positive curvature evident in Fig. 10. The ground-state estimate of $g_T^{u-d}$ converges from above.

There is evidence for excited-state contamination in $g_T^{u-d}$ on the $a12m310$, $a12m220L$ and $a09m130$ ensembles with AMA as shown in Fig. 10. This 5% effect can be accounted for by the larger value of $\langle 1 \vert O_T \vert 1 \rangle$ that has the same sign as the $\langle 0 \vert O_T \vert 1 \rangle$ contribution as shown in Table VIII. In all three cases, the 2-state Ansatz fits the data at multiple values of $t_{\text{sep}}$ covering the range 1.0–1.4 fm, and gives stable $t_{\text{sep}} \rightarrow \infty$ estimates under changes in $\tau_{\text{skip}}$ and $t_{\text{sep}}$.

In all cases, the data with the largest $t_{\text{sep}}$ are noisy and do not contribute significantly to the fit. Much higher-statistics are needed for fits to be sensitive to data with $t_{\text{sep}} \gtrsim 1.5$ fm.

Our conclusion is that the 2-state fit reduces the uncertainty due to the excited-state contamination in $g_A^{u-d}$, $g_T^{u-d}$ and $g_T^{d-d}$ to within a few percent (size of the statistical errors) with the smearing parameters and values of $t_{\text{sep}}$ we have used. Also, the data in Tables VI, VII and VIII indicate that the variation in the determination of $A_1/A_0$ and $M_1 - M_0$ with different choices of the fit ranges does not have a significant effect on the final
$t_{\text{sep}} \to \infty$ estimates of the charges obtained from the 2-state fits.

**IV. RENORMALIZATION OF OPERATORS**

The calculation of the renormalization constants $Z_A$, $Z_V$, $Z_S$ and $Z_T$ of the quark bilinear operators in the RI-sMOM scheme [32, 33] has been done on six ensembles: $a12m310$, $a12m220$, $a09m310$, $a09m220$, $a06m310$ and $a06m220$. The method and the details of this calculation have been given in Ref. [11] and here we briefly describe new aspects of the calculations and state the results.

To derive $Z_A$, $Z_S$, $Z_T$ and $Z_V$ in the continuum $\overline{\text{MS}}$ scheme at $\mu = 2\text{ GeV}$, starting with the lattice results obtained in the RI-sMOM scheme, we proceed as follows. The RI-sMOM estimate obtained at a given lattice squared four-momentum $q^2$ is first converted to the $\overline{\text{MS}}$ scheme at the same scale (horizontal matching) using two-loop perturbative relations expressed in terms of the coupling constant $\alpha_{\text{MS}}(q^2)$ [34]. This estimate at $\mu = q^2$, is then run in the continuum in the $\overline{\text{MS}}$ scheme to 2 GeV using the 3-loop anomalous dimension relations for the scalar and tensor bilinears [5, 35]. The result is a set of data points as a function of $q^2$ that are shown in Figs. 11 and 12. The mass-independent renormalization factors are extracted from these as discussed below.

In calculations at sufficiently small values of the lattice spacing $a$, one expects a window, $\eta \Lambda_{\text{QCD}} \ll q \ll \xi \pi/a$, in which the data for the $Z$'s, shown in Figs. 11 and 12, are independent of $q$; that is, the data should show a plateau versus $q$. The lower cutoff $\eta \Lambda_{\text{QCD}}$ is dictated by nonperturbative effects and the upper cutoff $\xi \pi/a$ by discretization effects. Here $\eta$ and $\xi$ are, a priori, unknown dimensionless numbers of $O(1)$ that depend on the lattice action and the link smearing procedure. The main systematics contributing to the lack of such a window and the resulting uncertainty in the extraction of the renormalization constants are (i) breaking of the Euclidean $O(4)$ rotational symmetry to the hypercubic group, because of which different combinations of $q$, with the same $q^2$ give different results in the RI-sMOM scheme; (ii)
nonperturbative effects at small $q^2$; (iii) discretization errors at large $q^2$ other than the $O(4)$ breaking effects listed above; and (iv) truncation errors in the perturbative matching to the $\overline{\text{MS}}$ scheme and running to 2 GeV. These systematics are discussed below.

To assess the truncation errors, we compare the conversion factor using 2-loop matching and 3-loop running versus 1-loop matching and 2-loop running. The 2-loop series for the matching of $Z_T$ is poorly behaved. For example, the 2-loop series for $Z_T$ when using horizontal matching between the RI-sMOM and $\overline{\text{MS}}$ scheme is $1 + 0.0052 + 0.0159$ at $q^2 = 4$ GeV$^2$ and is $1 + 0.0037 + 0.0078$ at $q^2 = 25$ GeV$^2$. In obtaining these estimates we used the 4-flavor $\alpha_s(\overline{\text{MS}}, 2$ GeV) = 0.3051 and $\alpha_s(\overline{\text{MS}}, 5$ GeV) = 0.2138. On the other hand, the 2-loop series for $Z_S$ at $q^2 = 4$ GeV$^2$, $1 - 0.0157 - 0.0039$, is much better behaved. The poor convergence of the 2-loop matching factor suggests a systematic uncertainty of $O(2\%)$ for $Z_T$. Our final error estimates given in Table X are larger than this. The series for the factor describing the running in the continuum is better behaved and the difference between the 2- and 3-loop estimate between the values of $q^2$ used in the analysis and 4 GeV$^2$ is less than 20% of the quoted errors and starts to become significant only for $q^2 < 1$ GeV$^2$ where $\alpha_s$ is large. Consequently, we use data with $q^2 > 4$ GeV$^2$ when obtaining our final estimates given in Tables IX and XII.

The lattice data in the RI-sMOM scheme have significant $O(4)$ breaking effects. The size of the spread in $Z_A$, $Z_S$, $Z_T$ and $Z_V$ and in the ratios $Z_A/Z_V$, $Z_S/Z_V$, and $Z_T/Z_V$ is illustrated in Fig. 13 using the a06m220 ensemble by plotting all the data using green circles. From this full data set, we pick the points with the smallest value of $\sum_{\mu}(p_1)_\mu^2/(p_1^2)^2 + \sum_{\mu}(p_2)_\mu^2/(p_2^2)^2$, where $(p_1)_\mu$ and $(p_2)_\mu$ are the momenta in the two external fermion legs, $q_\mu = (p_1)_\mu - (p_2)_\mu$, and $(p_i)^2 = \sum_{\mu}(p_i)_\mu^2$. These points, shown as red diamonds, are expected to have smaller $O(4)$ breaking effects. Of these red points, the data between 9.2–11.2 GeV$^2$ is less than 25% of the quoted errors and starts to become significant only for $q^2 < 1$ GeV$^2$ where $\alpha_s$ is large. Consequently, we use data with $q^2 > 4$ GeV$^2$ when obtaining our final estimates given in Tables IX and XII.

FIG. 10. The 2-state fit results for the unrenormalized tensor charge $g_T^{u-d}$ data. The rest is the same as in Fig. 8.
TABLE VI. Estimates of the matrix element $\langle 0|O_A|0\rangle$ for the isovector axial operators for four cases of the fit ranges defined in Table V. We also give estimates of the matrix elements $\langle 0|O_A|1\rangle$ and $\langle 1|O_A|1\rangle$ for Case 1 and Case 3. For the four ensembles, $a12m310$, $a9m130$, $a06m310$ and $a06m22$, we give both the AMA and LP estimates. We find that the bias correction term is negligible in all cases.

| ID   | Type | Case 1  | Case 2  | Case 3  | Case 4  | Case 1  | Case 3  |
|------|------|---------|---------|---------|---------|---------|---------|
|      |      | $\langle 0|O_A|0\rangle$ |         |         |         | $\langle 0|O_A|1\rangle$ |         | $\langle 0|O_A|1\rangle$ |         |
|      |      |         |         |         |         |         |         |         |
| a12m310 | HP  | 1.249(22) | 1.246(26) | 1.248(26) | 1.243(33) | 0.019(12) | (2.42) | (2.42) | 0.016(46) | 0.42(8) |
| a12m310 | AMA | 1.252(9)  | 1.251(11) | 1.252(9)  | 1.251(11) | 0.006(24) | (2.28) | (2.28) | 0.060(24) | (2.28) |
| a12m310 | LP  | 1.252(9)  | 1.251(11) | 1.252(9)  | 1.251(11) | 0.060(24) | (2.28) | (2.28) | 0.060(24) | (2.28) |
| a12m220S | HP  | 1.275(32) | 1.287(39) | 1.283(39) | 1.295(48) | 0.187(64) | (7.18) | (7.18) | 0.199(69) | 0.62(6) |
| a12m220 | HP  | 1.271(27) | 1.265(33) | 1.273(30) | 1.263(39) | 0.068(58) | (16.0) | (16.0) | 0.063(63) | (5.15) |
| a12m220L | HP  | 1.285(22) | 1.291(25) | 1.337(83) | 1.346(89) | 0.125(47) | (14.50) | (14.50) | 0.156(40) | (14.50) |
| a12m220L | LP  | 1.276(10) | 1.275(14) | 1.279(12) | 1.276(16) | 0.084(22) | (0.818) | (0.818) | 0.087(25) | (0.017) |
| a9m310  | HP  | 1.255(21) | 1.255(25) | 1.262(30) | 1.262(30) | 0.118(35) | (0.718) | (0.718) | 0.123(38) | (0.319) |
| a9m310  | AM  | 1.267(22) | 1.277(25) | 1.272(30) | 1.283(33) | 0.135(34) | (2.025) | (2.025) | 0.138(37) | (1.729) |
| a9m310  | LP  | 1.172(39) | 1.164(46) | 1.177(44) | 1.163(55) | 0.129(14) | (0.143) | (0.143) | 0.102(49) | (0.847) |
| a9m310  | AM  | 1.247(16) | 1.258(19) | 1.255(24) | 1.266(27) | 0.126(19) | 0.64(35) | 0.64(35) | 0.122(18) | (6.328) |
| a9m310  | LP  | 1.247(16) | 1.257(19) | 1.255(24) | 1.265(26) | 0.126(19) | 0.60(36) | 0.60(36) | 0.100(23) | (6.938) |
| a6m310  | HP  | 1.167(22) | 1.156(26) | 1.172(24) | 1.157(29) | 0.022(20) | (0.030) | (0.030) | 0.019(24) | (0.450) |
| a6m310  | AM  | 1.209(14) | 1.209(15) | 1.212(14) | 1.212(16) | 0.058(16) | 0.23(16) | 0.23(16) | 0.060(17) | (2.142) |
| a6m310  | LP  | 1.210(13) | 1.210(15) | 1.213(14) | 1.213(16) | 0.058(16) | 0.24(17) | 0.24(17) | 0.061(17) | (2.142) |
| a6m310  | LP  | 1.227(50) | 1.238(57) | 1.234(51) | 1.244(60) | 0.182(61) | 0.2(31) | 0.2(31) | 0.186(62) | (6.232) |
| a6m310  | AM  | 1.234(17) | 1.241(19) | 1.243(17) | 1.241(19) | 0.122(18) | 0.60(32) | 0.60(32) | 0.121(18) | (6.328) |
| a6m310  | LP  | 1.234(17) | 1.241(18) | 1.234(17) | 1.241(18) | 0.117(18) | 0.70(34) | 0.70(34) | 0.116(18) | (7.539) |

TABLE VII. Estimates of the matrix elements for the isovector scalar operator. The rest is the same as in Table VI.

The data for $Z_{q_{1}}$, $Z_{q_{2}}$, and $Z_{T}$ show much smaller $O(4)$ breaking, presumably because some of the systematics cancel. Our final estimates of the renormalized charges are, therefore, obtained using these ratios as discussed below. Overall, a better understanding and control over the artifacts due to $O(4)$ symmetry breaking in the RI-MOM scheme is needed as the contribution of the uncertainty in the renormalization constants to the errors in the charges is now larger than the statistical errors and the excited-state contamination.

After conversion to the $\overline{MS}$ scheme at 2 GeV, the selected data points that minimize $\sum_{\mu} (p_{1})^{\mu}/((p_{1})^{2})^{2} + \sum_{\mu} (p_{2})^{\mu}/((p_{2})^{2})^{2}$ for each $q^{2}$ are plotted in Fig. 11 for the six ensembles as a function of $q^{2}$. The data for $Z_{T}$ and $Z_{T}/Z_{S}$ show nonperturbative effects at low $|q|$ values followed by an approximate plateau for $Z_{A}$, $Z_{T}$, and $Z_{T}$, whereas the data for $Z_{S}$ continue to show a large $q$ dependence.

From these data in the $\overline{MS}$ scheme at 2 GeV, we extract the estimates in two ways [11]:
Method A: We fit the data with \( q^2 > 0.8 \text{ GeV}^2 \) using the Ansatz \( c/q^2 + Z + dq \), where the first term \( c/q^2 \) is used to account for nonperturbative artifacts and the third, \( dq \), for the discretization errors. The errors in the \( Z \)'s are obtained by using 100 bootstrap samples.

Method B: The estimate for \( Z \) is taken to be an average over the data points in an interval about \( q^2 = \Lambda/a \), where the scale \( \Lambda = 3 \text{ GeV} \) is chosen to be large enough to avoid non-perturbative effects and above which perturbation theory is expected to be reasonably well-behaved. This choice satisfies both \( qa \to 0 \) and \( \Lambda/q \to 0 \) in the continuum limit as desired, and \( q_a a - \sin(q_a a) < 0.05 \) to bound discretization effects. In our simulations, this choice corresponds to \( q^2 = 5, 6.8 \) and \( 10.2 \text{ GeV}^2 \) for the \( a = 0.12, 0.09 \) and \( 0.06 \) fm ensembles, respectively. To estimate the value and the error, we further choose an interval of 2 \( \text{GeV}^2 \) about these \( q^2 \), i.e., we take the mean and the standard deviation of the data over the ranges 4–6, 5.8–7.8 and 9.2–11.2 \( \text{GeV}^2 \).

The interval of \( q^2 \) that contributes to both methods is consistent with the general requirement that \( \eta A_{QCD} \ll q \ll \pi/\eta \), with \( \eta \) and \( \xi \) of \( O(1) \), to avoid both nonperturbative and discretization artifacts.

The estimates using method B for all four \( Z \)'s and at all three values of the lattice spacing are found to overlap for the two values of \( M_\pi \). As a result, in Ref. [11] we had neglected possible mass dependence in implementing Method A and made a fit using the Ansatz \( c/q^2 + Z + dq \) to the combined data. In this work, we analyze the 6 ensembles separately and present the estimates from both methods in Table IX.

The estimates from Method A show significant dependence on \( M_\pi \) in some cases even though the data at the two values of \( M_\pi \) overlap. We do not find a uniform trend with \( M_\pi \) at the three different values of \( a \), and given the size of the errors in the data at the two values of \( M_\pi \) we are not able to make a reliable extrapolation in \( M_\pi \). So we ignore possible dependence on \( M_\pi \) in the data and average the estimates from the two methods at the two values of \( M_\pi \) given in Table IX to obtain a “mass-independent” estimate. For the error estimate we take the larger of the two: half the spread or the largest statistical error.

The data for the ratios \( Z_T/Z_V \) are shown in Fig. 12. As highlighted above, we find that the systematic effects due to \( O(4) \) breaking are smaller in the ratios. The data again show a rough plateau in \( Z_A/Z_V \) and \( Z_T/Z_V \) but not in \( Z_S/Z_V \). We also find a significant variation with \( M_\pi \) and between the two methods in some cases, which we include in our error estimates as explained above. The final mass-independent renormalization constants \( Z_T \) and \( Z_T/Z_V \) at the three lattice spacings are given in Table X. The errors in these renormalization constants are added in quadrature to those in the extraction of the bare nucleon charges \( g_{A,S,T} \) and \( g_{A,S,T}^{bare} \) given in Table XI to obtain the renormalized charges in two ways:

- Using the product of the ratios, \( Z_T/Z_V \times (g_T/g_v)^{a_d} \), along with the identity \( Z_V g_v^{a_d} = 1 \). These are given in Table XII.
- Using the product \( Z_T g_T \). These estimates are given in Table XIII for the isovector charges.

The two estimates differ by 1–3%. Most of this difference correlates with the deviation of \( Z_V g_v^{a_d} \) from unity as shown in Table XIII. The deviation is about 1 O: approximately 3%, 3% and 2% at the three lattice spacings,

| ID       | Type | Case 1       | Case 2       | Case 3       | Case 4       |
|----------|------|--------------|--------------|--------------|--------------|
| a12m310  | HP   | 1.096(21)    | 1.092(21)    | 1.084(31)    | 1.081(33)    |
| a12m310  | AMA  | 1.087(10)    | 1.082(10)    | 1.087(10)    | 1.082(10)    |
| a12m310  | LP   | 1.087(10)    | 1.082(10)    | 1.087(10)    | 1.082(10)    |
| a12m220S | HP   | 1.086(26)    | 1.079(31)    | 1.067(46)    | 1.060(51)    |
| a12m220  | HP   | 1.111(24)    | 1.107(28)    | 1.105(32)    | 1.102(36)    |
| a12m220L | LP   | 1.058(19)    | 1.059(20)    | 1.043(29)    | 1.050(29)    |
| a12m220L | LP   | 1.063(12)    | 1.063(13)    | 1.056(19)    | 1.058(18)    |
| a9m310   | HP   | 1.025(24)    | 1.027(26)    | 1.021(31)    | 1.023(31)    |
| a9m220   | HP   | 1.030(20)    | 1.030(21)    | 1.029(22)    | 1.030(22)    |
| a9m310   | HP   | 0.993(33)    | 1.001(36)    | 0.980(45)    | 0.993(47)    |
| a9m130   | AMA  | 0.974(20)    | 0.981(20)    | 0.967(28)    | 0.975(26)    |
| a9m130   | LP   | 0.973(19)    | 0.979(19)    | 0.966(28)    | 0.974(26)    |
| a6m310   | HP   | 0.961(20)    | 0.958(22)    | 0.951(24)    | 0.950(26)    |
| a6m310   | AMA  | 0.976(10)    | 0.981(10)    | 0.972(12)    | 0.978(12)    |
| a6m310   | LP   | 0.976(10)    | 0.981(10)    | 0.972(12)    | 0.978(12)    |
| a6m220   | HP   | 0.995(43)    | 1.002(47)    | 0.990(48)    | 1.000(51)    |
| a6m220   | AMA  | 0.984(10)    | 0.986(10)    | 0.984(10)    | 0.986(10)    |
| a6m220   | LP   | 0.984(9)     | 0.985(10)    | 0.984(9)     | 0.986(10)    |

TABLE VIII. Estimates of the matrix elements for the isovector tensor operator. The rest is the same as in Table VI.
$a = 0.12, 0.09$ and $0.06$ fm, respectively. The magnitude of these deviations is consistent with our estimates of errors in the renormalization constants given in Table X, which are now larger than the statistical errors. A more detailed discussion of the error budget and the final error estimates are given in Sec. VII.

The discretization errors in the two estimates of the renormalized charges are different, so one should only compare the results after extrapolation. In Sec. V, we show that even though the estimates on individual ensembles differ by 1–3%, the value of the charges after extrapolation to the continuum limit and the physical pion mass are consistent. The errors in the data $Z_T g_T$ and in the extrapolated value obtained from them are larger. This is because the data for both, $Z_T / Z_V$ and $g_T / g_V^{u-d}$, have smaller errors, presumably because some of the systematics cancel in the ratios. Our final estimates are, therefore, obtained using $(Z_T / Z_V) \times (g_T / g_V^{u-d})$ with the relation $Z_V g_V^{u-d} = 1$. 

FIG. 11. Data for the four renormalization constants $Z_A$, $Z_S$, $Z_T$ and $Z_V$ in the $\overline{\text{MS}}$ scheme at $\mu = 2$ GeV as a function of the lattice momenta $|q|$ used in the RI-sMOM scheme. The data are organized as follows: (left column) $a = 0.12$ fm, (middle column) $a = 0.09$ fm and (right column) $a = 0.06$ fm ensembles. In each panel, we show the data at the two values of $M_x$ analyzed and use blue squares to label the $M_x \approx 310$ MeV and red diamonds for the $M_x \approx 220$ MeV ensembles. The dashed line is the linear part of the fit $c / q^2 + Z + dq$ used in method A to extract the $Z$’s. Data in the region of $q^2$ used to extract the $Z$’s using Method B are shown using green ($M_x \approx 310$ MeV) and orange ($M_x \approx 220$ MeV) symbols.
FIG. 12. Data for the ratios of renormalization constants $Z_A/Z_V$, $Z_S/Z_V$, $Z_T/Z_V$ in the $\overline{MS}$ scheme at $\mu = 2$ GeV as a function of the lattice momenta $|q|$ used in the RI-sMOM scheme. The rest is the same as in Fig. 11.

| ID         | $Z_A$   | $Z_S$  | $Z_T$   | $Z_V$  | $Z_A/Z_V$ | $Z_S/Z_V$ | $Z_T/Z_V$ |
|------------|---------|--------|---------|--------|-----------|-----------|-----------|
| a12m310    | 0.929(5)| 0.912(06)| 0.899(4)| 0.904(4)| 1.035(3)  | 0.975(04) | 1.000(2)  |
| a12m220    | 0.926(7)| 0.852(20)| 0.901(6)| 0.890(6)| 1.045(4)  | 0.984(13) | 1.012(3)  |
| a09m310    | 0.951(4)| 0.868(45)| 0.945(5)| 0.912(7)| 1.037(6)  | 0.909(54) | 1.031(4)  |
| a09m220    | 0.899(9)| 0.867(22)| 0.931(9)| 0.889(8)| 1.018(5)  | 1.007(20) | 1.050(7)  |
| a06m310    | 0.948(5)| 0.863(11)| 1.005(6)| 0.934(4)| 1.014(3)  | 0.922(10) | 1.068(5)  |
| a06m220    | 0.979(4)| 0.901(10)| 1.043(5)| 0.951(3)| 1.032(2)  | 0.952(09) | 1.103(5)  |
| a12m310    | 0.979(1)| 0.925(17)| 0.989(14)| 0.933(14)| 1.0472(21)| 0.991(17) | 1.058(2)  |
| a12m220    | 0.970(9)| 0.914(11)| 0.984(9)| 0.921(10)| 1.0526(35)| 0.994(14) | 1.068(4)  |
| a09m310    | 0.975(10)| 0.901(13)| 1.013(11)| 0.937(11)| 1.0411(22)| 0.962(5)  | 1.081(2)  |
| a09m220    | 0.972(7)| 0.878(6)| 1.018(6)| 0.934(7)| 1.0407(14)| 0.941(8)  | 1.090(3)  |
| a06m310    | 0.980(8)| 0.840(9)| 1.064(8)| 0.951(8)| 1.0300(6)| 0.883(4)  | 1.118(2)  |
| a06m220    | 0.981(7)| 0.835(3)| 1.060(5)| 0.957(6)| 1.0255(8)| 0.873(4)  | 1.109(3)  |

TABLE IX. The renormalization constants $Z_A$, $Z_S$, $Z_T$, $Z_V$ and the ratios $Z_A/Z_V$, $Z_S/Z_V$ and $Z_T/Z_V$ in the $\overline{MS}$ scheme at 2 GeV obtained on six ensembles at the three values of the lattice spacings. (Top) Estimates are from method A using the fit $1/q^2 + Z + dq$. (Bottom) Estimates from method B obtained by averaging the data over an interval in $q^2$ as described in the text.

V. RESULTS FOR THE CHARGES $g_A$, $g_S$, $g_T$

To extrapolate the estimates of the renormalized charges given in Table XII to the continuum limit ($a \to 0$), the physical pion mass ($M_{\pi^0} = 135$ MeV) and the infinite volume limit ($L \to \infty$), we need to use an appropriate fit Ansatz, motivated by chiral perturbation theory, for the nine data points. For discussions on predictions of chiral perturbation we direct the reader to Refs. [36–41]. To test these predictions, one ideally requires data at many lattice spacings and small pion masses. Also,
the analysis is simplest if one can hold two of the three variables constant to study the variation with the third. Our nine data points do not allow such a study. For example, estimates at the three different volume points, $a_{12}m220S$, $a_{12}m220$ and $a_{12}m220L$, at fixed $M_\pi$ and $a$ are consistent within errors for all the three charges. In fact, the spread in the data in most cases is small enough that they can be fit with a linear Ansatz in each variable. Our goal, given the limited number of data points and the small variations in each of the three variables, is to make a simultaneous fit keeping the minimum number of parameters corresponding to the leading terms in the chiral expansion.

Keeping only the leading corrections in $a$ and $M_\pi L$, we have studied the following Ansatz motivated by chiral perturbation theory [36–42]:

$$
g_{A,T}(a, M_\pi, L) = c_1 + c_2 a + c_3 M_\pi^2 + c_3 \log M_\pi^2 \ln \left( \frac{M_\pi}{M_\rho} \right)^2 + c_4 M_\pi^2 e^{-M_\pi L} \frac{X(M_\rho L)}{X(M_\rho L)},$$

$$
g_S(a, M_\pi, L) = c_1 + c_2 a + c_3^2 M_\pi + c_3 M_\pi^2 + c_4^2 \log M_\pi^2 \ln \left( \frac{M_\pi}{M_\rho} \right)^2 + c_4 M_\pi e^{-M_\pi L} \frac{Y(M_\rho L)}{Y(M_\rho L)},$$

where $M_\rho$ is the chiral renormalization scale. Note that the leading discretization errors are linear in $a$ for our clover-on-HISQ formalism with unimproved operators, and the leading chiral correction to $g_S^{u-d}$ starts at $O(M_\pi)$ [36]. The finite-volume correction, in general, consists of a number of terms, each with different powers of $M_\pi L$ in the denominator and depend on several low-energy constants (LEC) [39]. These powers of $M_\pi L$ are symbolically represented by $X(M_\pi L)$ and $Y(M_\rho L)$. Since the variation of these factors is small compared to the exponential over the range of $M_\pi L$ investigated, we

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**FIG. 13.** Data for the renormalization constants in the $\overline{\text{MS}}$ scheme at $\mu = 2$ GeV as a function of the lattice momenta $|q|$ used in the RI-MOM scheme. (Top) The data for $Z_A$, $Z_S$ and $Z_T$ for all combinations of $(p_1)_\mu$ and $(p_2)_\mu$ calculated using green circles. The subset of points that minimize $\sum_{\mu} (p_1)_\mu / (p_2)_\mu + \sum_{\mu} (p_2)_\mu / (p_1)_\mu$ for each $q^2$ are shown using red diamonds. The value and error using method B discussed in the text is given by the average and variance of the points shown in black over the range 9.2–11.2 GeV$^2$. (Bottom) The data for the ratios $Z_A/Z_V$, $Z_S/Z_V$ and $Z_T/Z_V$ using the same symbols.

**TABLE X.** The final mass-independent renormalization constants $Z_A$, $Z_S$, $Z_T$, $Z_V$ and the ratios $Z_A/Z_V$, $Z_S/Z_V$ and $Z_T/Z_V$ in the $\overline{\text{MS}}$ scheme at 2 GeV at the three values of the lattice spacings used in our analysis. The central value is the average of estimates from the two methods and at the two pion masses given in Table IX and the errors are taken to be half the spread.
TABLE XI. Estimates of the bare connected charges using the fit ranges defined under Case 3 in Table V. The isovector charges $g_u^{u-d} = (0)_{O_T^{(0)}}$ are the same as Case 3 in Tables VI, VII and VIII. Ensembles marked with an asterisk denote results obtained with the AMA method.

| ID     | $g_A^{d}$ | $g_A^{u}$ | $g_u^{u-d}$ | $g_{V}^{d}$ | $g_{V}^{u}$ | $g_{u-d}$ |
|--------|-----------|-----------|-------------|-------------|-------------|-----------|
| a12m310 | 0.932(9)  | -0.320(5) | 1.252(9)    | 3.31(6)     | 2.40(4)     | 0.91(4)   |
| a12m310*| 0.932(9)  | -0.320(5) | 1.252(9)    | 3.31(6)     | 2.40(4)     | 0.91(4)   |
| a12m220S| 0.969(37) | -0.313(21)| 1.283(39)   | 4.49(52)    | 3.45(37)    | 1.03(32)  |
| a12m220  | 0.942(29) | -0.332(15)| 1.273(30)   | 3.87(27)    | 3.21(21)    | 0.67(18)  |
| a12m220L | 1.015(75) | -0.322(22)| 1.337(83)   | 4.74(72)    | 3.67(63)    | 1.10(17)  |
| a12m220L*| 0.949(11)| -0.332(6) | 1.279(12)   | 4.10(18)    | 3.27(14)    | 0.83(66)  |

TABLE XII. Results for the renormalized charges using the fit ranges defined under Case 3 in Table V. Estimates of the flavor diagonal charges include only the connected contribution. The final errors are obtained by adding in quadrature the errors in estimates of the ratios $g_u^{bare}/g_u^{true}$ to the errors in the ratios of the renormalization constants, $Z_T/Z_V$ given in Table X. Estimates for $g_u^{u-d}$ neglect the disconnected contributions that were shown to be tiny in Ref. [11]. Rest is the same as in Table XI.

| ID     | $g_A^{d}$ | $g_A^{u}$ | $g_u^{u-d}$ | $g_{V}^{d}$ | $g_{V}^{u}$ | $g_{u-d}$ |
|--------|-----------|-----------|-------------|-------------|-------------|-----------|
| a12m310 | 0.908(26) | -0.319(14)| 1.221(28)   | 3.16(18)    | 2.41(14)    | 0.73(92)  |
| a12m310*| 0.944(11) | -1.3145(55)| 1.299(14)   | 3.066(62)   | 2.226(39)   | 0.840(36) |
| a12m220S| 0.960(38) | -0.310(22)| 1.270(42)   | 4.19(48)    | 3.23(34)    | 0.96(30)  |
| a12m220  | 0.917(30) | -0.326(16)| 1.240(32)   | 3.56(25)    | 2.95(20)    | 0.62(16)  |
| a12m220L | 0.975(48) | -0.309(19)| 1.284(46)   | 4.29(52)    | 3.32(47)    | 1.00(13)  |
| a12m220L*| 0.931(13)| -0.3524(69)| 1.255(16)   | 3.79(16)    | 3.03(14)    | 0.77(50)  |

The dependence of the data on the lattice spacing, pion mass and the lattice volume is small. We, therefore, investigated fits with the Ansatz given in Eqs. (11) and (12) and, in addition, a number of Ansätze with various subsets of terms. In each case, the parameters $c_3^{log}$ and $c_4$ (or $c_5$) are poorly determined and consistent with zero, reflective of the small range and small variation in the data with the pion mass and the lattice volume. Also, $\lambda_{A,T}^{2,\text{f.o.}} < 1$ in all cases, so it does not provide a good criterion for deciding the best fit Ansatz. We, therefore, considered the Ansatz with just the leading term in each of the three variables:

$$g_{A,T}(a, M_\pi, L) = c_1 + c_2 a + c_3 M_\pi^2 + c_4 M_\pi^2 e^{-M_\pi L},$$

(13)

$$g_{S}(a, M_\pi, L) = c_1 + c_2 a + c_3 M_\pi + c_4 M_\pi e^{-M_\pi L}.$$  

(14)

Using these Ansätze, the 9-point fits (9-pt) to the data for the isovector charges, renormalized using $g_{V}^{bare}/g_{V}^{true}$, are shown in fig. 14. The fits to $g_{u-d}^{u-d}$ and $g_{u-d}^{u-d}$ show a sizeable variation with $a$. We show the same 9-point fit in Fig. 15 using the renormalised charges obtained using $Z_T \times Z_V$ and find that the variation of $g_{A,T}^{u-d}$ with $a$ is smaller. The systematics in the two ways of obtaining the renormalized charges are different but removed by the extrapolation to the continuum limit as suggested by the agreement between the results
TABLE XIII. Estimates of the renormalized isovector charges obtained using $Z_V$ with $Z_T$ given in Table X and $g_T^\text{bare}$ in Table XI. All estimates are obtained using the fit ranges defined under Case 3 in Table V. We also give results for the bare and renormalized $g_V^{u-d}$ in columns five and six. Estimates in the sixth column differ from $Z_V g_V^{u-d} = 1$, predicted by the conservation of the vector charge, by 2–3%. Ensembles marked with an asterisk denote results obtained with the AMA method.

| ID          | $g_A^{u-d}$ | $g_S^{u-d}$ | $g_T^{u-d}$ | $g_V^{u-d}$ | $Z_V g_V^{u-d}$ |
|-------------|-------------|-------------|-------------|-------------|-----------------|
| a12m310*    | 1.185(45)   | 0.738(97)   | 1.019(52)   | 1.068(10)   | 0.972(23)       |
| a12m310     | 1.189(39)   | 0.817(50)   | 1.022(44)   | 1.065(4)    | 0.969(22)       |
| a12m220S    | 1.219(53)   | 0.93(29)    | 1.003(61)   | 1.055(14)   | 0.960(25)       |
| a12m220     | 1.209(48)   | 0.61(16)    | 1.038(54)   | 1.073(12)   | 0.977(24)       |
| a12m220L    | 1.270(88)   | 0.99(16)    | 0.981(50)   | 1.088(36)   | 0.990(39)       |
| a12m220L*   | 1.215(40)   | 0.749(62)   | 0.993(46)   | 1.065(3)    | 0.969(21)       |

| Method | $g_A^{u-d}$ | $g_S^{u-d}$ | $g_T^{u-d}$ |
|--------|-------------|-------------|-------------|
| $g_T^\text{bare} / g_T^\text{bare} \times Z_T / Z_V$ | 1.195(33) | 0.97(12) | 0.987(51) |
| $\chi^2$/d.o.f. | 0.28 | 0.67 | 0.44 |

TABLE XIV. Results of the 9-point fit to the data for the isovector charges renormalized in two ways: using $g_T^\text{bare} / g_T^\text{bare} \times Z_T / Z_V$ with $g_T^\text{bare} / Z_V = 1$ given in Table XII and $g_T^\text{bare} \times Z_T$ given in Table XIII.

We find that the smallest volume point, a12m220S, provides a large lever arm in the determination of the shape of the finite-volume correction, as can be seen by comparing the 9-pt (Fig. 14) versus the 8-pt (Fig. 17) fits. Nevertheless, the fits do not show a significant difference for $M_L \lesssim 4$.

To further explore the sensitivity of the data for the isovector charges $g_V^{u-d}$ to chiral logarithms, we make 8-point fits (neglecting the a12m220S point and assuming that the finite-volume corrections can be ignored for $M_L \lesssim 4$) with and without a chiral logarithm term:

$$g_{A,T}(a, M_\pi) = c_1 + c_2 a + c_3 M^2_\pi + c_4 \log M^2_\rho \ln \frac{M^2_\pi}{M^2_\rho}.$$  \hspace{1cm} (15)

The chiral renormalization scale is taken to be $M_\rho = 0.775$ GeV. Results for the parameters $c_i$ are summarized in Table XVI with and without the $c_3^\log$ term. The parameter $c_4$ (or $c_4^\log$) is again poorly constrained by the data since the variation in the estimates between $M_\pi = 135$ and 320 MeV is comparable to the errors in the individual points for all three charges as can be seen in Figs. 14, 16 and 17. The main effect of adding the $c_3^\log$ term is an adjustment with $c_3$: there is a large cancellation between the contributions of these two terms. Also, the errors in both $c_3$ and $c_4^\log$ are O(1) in all three charges. To test whether the chiral logarithm term improves the predictive power of the fit, we again use the Akaike Information Criterion [43]. The $\chi^2$ changes by much less than two units, indicating that adding the chiral logarithm is not justified. Also, for the scalar charge, we find little difference in the fits between using $c_3 M^2_\rho$ versus $c_3^\log M_\rho$ as the leading chiral term.

The bottom line is that changing the fit Ansatz from Eqs. (11) and (12) to Eqs. (13) and (14) to that given in Eq. (15) does not significantly change the estimates for the charges as can be seen by comparing the last column of Tables XV and XVI.

Our final results for the isovector charges using the 9-point fit are presented in Table XXII in Sec. VII after we revisit our error analysis and assign an additional systematic error to account for the uncertainty due to the various fit Ansatz discussed above.

To obtain the flavor-diagonal charges $g_T^u$ and $g_T^d$ and the isoscalar combination $g_T^{u+d}$ requires calculation of the disconnected contributions. We have not carried out any new simulations to update estimates of the disconnected contributions to the tensor charges that were shown to be $O(1\%)$ of the connected contribution and consistent with zero in Ref. [11]. We, therefore, consider the connected part to be a good approximation to the full result and present updated results for $g_T^u, g_T^d$ and $g_T^{u+d}$ in Table XVII. The disconnected contributions to the axial and scalar charges are larger, about 0.1 and $O(1)$, re-
FIG. 14. The 9-point fit using Eqs. (13) and (14) to the data for the renormalized isovector charges, $g_A^{u-d}$, $g_S^{u-d}$ and $g_{T}^{u-d}$, in the $\overline{\text{MS}}$ scheme at 2 GeV. The result of the simultaneous extrapolation to the physical point defined by $a \to 0$, $M_\pi \to M_{\pi}^{\text{phys}} = 135$ MeV and $L \to \infty$ are marked by a red star. The error bands in each panel show the simultaneous fit as a function of a given variable holding the other two at their physical value. The data are shown projected on to each of the three planes. The overlay in the middle figures with the dashed line within the grey band, is the fit to the data versus $M_\pi^2$ neglecting dependence on the other two variables. The symbols used for data points from the various ensembles are defined in Table I.

spectively, and we are working on a more detailed analysis of these. We, therefore, do not present results for the isoscalar combinations $g_A^{u+d}$ and $g_S^{u+d}$ but give only the connected contributions to the flavor-diagonal charges $g_A^{u,d}$ using the same three fits, 9-point, 9-point with log and the 8-point, in Table XVII.

We show the behavior of the connected parts of the flavor-diagonal charges $g_{A,S,T}^{u,d}$ versus the lattice spacing and the pion mass in Figs. 18, 19 and 20 using 9-point fits with $c_3^{\log} = 0$ in the Ansatz given in Eq. 15. The plots show that estimates of $g_T^u$ are about four times larger than of $g_T^d$, and both are essentially flat with respect to the pion mass, the lattice spacing and the lattice volume. The behavior of $g_A^{u,d}$, shown in Fig. 19, is similar in magnitude and sign to that in $g_T^{u,d}$. Again, data show little dependence on the pion mass, however, there is a notable increase of $g_A^u$ with $a$ that carries over to $g_A^{u-d}$ plotted in Fig. 14. The 9-point fits with the $c'_3$ term for $g_S^u$ and $g_S^d$ are shown in Fig. 20. These data are much larger in magnitude and show a significant dependence on the quark mass.

The final results for the connected parts of the flavor-diagonal charges $g_A^u$ and $g_A^d$ from the 9-point fit are presented in Table XXIII in Sec. VII. The new estimates of $g_T^{u,d}$, needed to analyze the contribution of the EDM of the quarks to the neutron EDM, supercede the values presented in Refs. [11, 20].

VI. CONFIRMATION OF THE 2-STATE ANALYSIS

The analysis in the previous sections was predicated on the assumption that the 2-state Ansatz given in Eqs. (9) and (10) resolves the excited-state contamination in the 2- and 3-point functions. In this section, we provide further confirmation of this assumption using additional high-statistics AMA simulations on the a06m310 and a06m220 ensembles with different smearing parameters. These are listed in Table XVIII under the label AMA2.

A comparison of the excited-state contamination and
TABLE XV. Values of the fit parameters defined in Eqs. (11) and (12). The 9-point fit to the isovector charges includes terms with $c_1$, $c_2$, $c_3$ (or $c_3'$ for $g_A^{u-d}$) and $c_4$ (or $c_4'$ for $g_A^{u-d}$). The 9-ptL fit includes the chiral logarithm term $c_3^{\log}$. The 8-pt fit uses the same Ansatz as the 9-pt fit but neglects the $a12m2205$ data point. The last column gives the value of the charge at the physical point.

| ID     | $g_A^{u-d}$ | $g_A^{d-d}$ | $g_A^{u-d}$ | $g_A^{d-d}$ | $g_A^{u-d}$ | $g_A^{d-d}$ | $g_A^{u-d}$ | $g_A^{d-d}$ | $g_A^{u+d}$ | $g_A^{d+d}$ | $g_A^{u+d}$ | $g_A^{d+d}$ | $g_A^{u+d}$ | $g_A^{d+d}$ | $g_A^{u+d}$ |
|--------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 9-pt   | 0.856(27)   | -0.335(15)  | 1.195(33)   | 4.94(30)    | 4.00(22)    | 0.97(12)    | 0.792(42)   | -0.194(14)  | 0.987(51)   | 0.598(36)   |
| 9-ptL  | 0.841(31)   | -0.342(20)  | 1.185(40)   | 5.59(48)    | 4.59(39)    | 1.10(17)    | 0.766(48)   | -0.183(17)  | 0.951(58)   | 0.579(41)   |
| 8-pt   | 0.877(31)   | -0.333(16)  | 1.211(37)   | 5.09(33)    | 4.13(25)    | 0.99(13)    | 0.796(55)   | -0.197(17)  | 0.997(67)   | 0.599(46)   |

TABLE XVII. Estimates of the connected parts of the flavor diagonal charges and $g_T^{u+d}$ with the three different fits described in Table (XV). The estimates for the isovector charges $g_A^{u+d}$ are reproduced from Table (XV) to make comparison easier.

| Ensemble ID | Type | $\sigma$ | $N_{GS}$ | $t_{sep}/a$ | $N_{conf}$ | $N_{HP}$ | $N_{AMA}$ |
|-------------|------|----------|----------|-------------|------------|----------|----------|
| a06m310     | AMA  | 6.5      | 70       | [16, 20, 22, 24] | 1000       | 4000     | 64000    |
| a06m310     | AMA2 | 12       | 250      | [18, 20, 22, 24] | 500        | 2000     | 64000    |
| a06m220     | AMA  | 5.5      | 70       | [16, 20, 22, 24] | 650        | 2600     | 41600    |
| a06m220     | AMA2 | 11       | 230      | [18, 20, 22, 24] | 650        | 2600     | 41600    |

TABLE XVIII. The smearing parameters, the values of $t_{sep}$ and the statistics used in the two AMA simulations on the a06m310 and a06m220 ensembles to test the efficacy of the 2-state fit in controlling excited-state contamination. The second set of AMA measurements with the larger smearing size are labeled AMA2. The number of HP measurements used to correct the bias in the AMA method are listed under $N_{AMA}$.
FIG. 15. The 9-point fit using Eqs. (13) and (14) to the data for the renormalized isovector charges obtained using $Z_{A^0}^{\text{bare},u-d}$, $Z_S g_S^{\text{bare},u-d}$ and $Z_T g_T^{\text{bare},u-d}$. The rest is the same as in Fig. 14.

| ID       | Type | Fit Range | $aM_0$  | $aM_1$  | $A_0^2 \times 10^{11}$ | $A_1^2 \times 10^{11}$ | $A_1^2 / A_0^2$ |
|----------|------|-----------|---------|---------|------------------------|------------------------|-----------------|
| a06m310  | AMA  | 8–30      | 0.3208(23) | 0.56(0) | 0.38(3) | 0.30(10) | 1.66(11) |
| a06m310  | AMA2 | 5–25      | 0.3282(17) | 0.68(5) | 1.32(4)×10$^{-11}$ | 1.5(2)×10$^{-11}$ | 1.16(14) |
| a06m220  | AMA  | 8–30      | 0.3069(18) | 0.63(3) | 11.3(4) | 39.2(5.0) | 3.47(35) |
| a06m220  | AMA2 | 4–30      | 0.3037(13) | 0.64(2) | 2.66(6)×10$^{-9}$ | 3.8(2)×10$^{-9}$ | 1.41(4) |

TABLE XIX. Comparison of the masses $aM_0$ and $aM_1$ and the amplitudes $A_0$ and $A_1$ obtained using the AMA method with different smearing parameters on the a06m310 and a06m220 ensembles. The AMA estimates are the same as in Table III. The smearing parameters and the statistics for the two runs are given in Table XVIII.

| ID       | Type | (0|O$_T$|0) | (0|O$_T$|1) | (1|O$_T$|1) | (0|O$_T$|0) | (0|O$_T$|1) | (1|O$_T$|1) | (0|O$_T$|0) | (0|O$_T$|1) | (1|O$_T$|1) | (0|O$_T$|0) | (0|O$_T$|1) | (1|O$_T$|1) |
|----------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| a06m310  | AMA  | 1.212(14) | −0.060(17) | −1.2(1.4) | 1.18(5) | −0.40(4) | −0.5(1.0) | 0.972(12) | 0.128(10) | 0.50(22) |
| a06m310  | AMA2 | 1.210(13) | −0.042(26) | −2.6(6.2) | 1.17(7) | −0.43(8) | −0.9(25) | 0.987(12) | 0.219(18) | 0.6(4.0) |
| a06m220  | AMA  | 1.234(17) | −0.121(18) | −6.3(3.9) | 1.04(6) | −0.30(4) | −0.7(2.6) | 0.984(10) | 0.103(8) | −0.53(59) |
| a06m220  | AMA2 | 1.222(13) | −0.063(21) | −4.2(3.9) | 0.79(8) | −0.17(7) | 0.25(7) | 0.969(11) | 0.203(16) | 1.6(2.4) |

TABLE XX. Comparison of results with the two different smearing parameters defined in Table XVIII for the three unrenormalized matrix elements $\langle 0|O_T|0 \rangle$, $\langle 1|O_T|0 \rangle$ and $\langle 1|O_T|1 \rangle$ for the isovector axial, scalar and tensor operators using the 2-state Ansatz given in Eqs. (9) and (10). The fit ranges for the 3-point functions are defined under Case 3 in Table V. The AMA estimates are the same as given in Tables VI, VII and VIII.
fits using Eqs. (9) and (10) to the 3-point functions data is shown in Figs. 22 and 23, and the results for the three matrix elements \( \langle 0|O_T|0\rangle \), \( \langle 1|O_T|0\rangle \) and \( \langle 1|O_T|1\rangle \) are given in Table XX. A summary of the notable features is:

- Increasing the smearing size \( \sigma \) reduces the ratio \( A_1/A_0 \) and the relative contribution of the excited-states. Estimates of \( M_0 \) and the isovector charges \( g_A^{u-d} \), \( g_T^{u-d} \) and \( g_V^{u-d} \) (given by \( \langle 0|O_T|0\rangle \)) with the two different smearing sizes agree within 1\( \sigma \). The one exception is \( g_S^{u-d} \) from the \( a06m220 \) ensemble.

- The excited-state contamination in \( g_A^{u-d} \) is significantly reduced with the larger smearing size from 15\% to 5\%. This can be seen by comparing the data at the central values of \( \tau \). The 2-state fit to both sets of data gives consistent estimates of the \( t_{sep} \rightarrow \infty \) value.

- The excited-state effect in \( g_T^{u-d} \) at the central values of \( \tau \) is less than 5\% in all cases as shown in Figs. 10, 22 and 23. Comparing the data with the two smearing sizes, we find that the 2-state fit gives consistent and stable estimates of the \( t_{sep} \rightarrow \infty \) value for both \( a06m310 \) and \( a06m220 \) ensembles.

- The data for \( g_S^{u-d} \) at different \( t_{sep} \) with the larger smearing size overlap and are not well resolved as shown in Figs. 22 and 23. The pattern of variation of the \( a06m220 \) AMA2 data versus \( t_{sep} \) is opposite to that seen in the other three ensembles listed in Table XVIII. The 2-state fit takes this into account with an unreasonably large value of \( \langle 1|O_T|1\rangle \) and with the opposite sign. As a result, the two estimates of \( g_S^{u-d} \) from the \( a06m220 \) ensemble differ by roughly 3\( \sigma \). We consider this inverted pattern of the \( \langle 1|O_T|1\rangle \) contribution in the AMA2 data to be a statistical fluctuation and regard the AMA estimate to be more reliable.

- Estimates of \( \langle 0|O_T|1\rangle \) agree in sign and roughly in magnitude for all the charges.

- Estimates of \( \langle 1|O_T|1\rangle \) for the three charges are poorly determined with either smearing size.

- The differences in \( M_1 \), \( \langle 0|O_T|1\rangle \) and \( \langle 1|O_T|1\rangle \) are large in some cases. These differences reflect the fact that the 2-state fit lumps the contribution of all the excited states into one “effective” excited state, and their contributions vary with the smearing size.
FIG. 17. The 8-point fit to the isovector charges neglecting the $a_{12m220}$ point. The rest is the same as in Fig. 14.

and the fit ranges. Much higher-statistics data with better interpolating operators that enable a three-state fit will be needed to obtain reliable estimates of these first excited-state parameters.

- The errors in the two matrix elements $\langle 0|O_\Gamma|1 \rangle$ and $\langle 1|O_\Gamma|1 \rangle$ given by the 2-state fit are larger in the AMA2 analysis even though the total number of measurements in the two cases are the same. With reduced excited-state contamination, the data at different $t_{sep}$ overlap and the 2-state fit becomes less stable with respect to values of $t_{sep}$ used in the fit. Consequently, higher statistics are needed to provide reliable $t_{sep} \rightarrow \infty$ estimates.

The bottom line is that these two additional simulations validate the results based on 2-state fits to data at multiple values of $t_{sep}$ presented in Sec. V. They also show that the large excited-state contamination in $g_{u-d}^A$ and $g_{u-d}^S$ on the $a = 0.06$ fm lattices with smearing parameter $\sigma \approx 6$ is significantly reduced with $\sigma \approx 11$. On the other hand, estimates at different $t_{sep}$ start to overlap with reduced excited-state contamination, and the 2-state fit becomes less stable. This is most obvious in the $g_{u-d}^S$ data on the $a06m220$ ensemble. In retrospect, a more effective compromise balancing the two effects would have been achieved with an intermediate value for the smearing parameter, $\sigma = 9$ ($\approx 0.55$ fm in physical units), on the $a = 0.06$ fm ensembles.

VII. ASSESSING THE ESTIMATION OF ERRORS

The estimation of errors in our analysis has four main components:

- Statistical and excited-state contamination (SESC): Errors from these two sources are estimated together in the combined 2-state fit.

- Uncertainty in the determination of the renormalization constants $Z_\Gamma$: The $Z$’s are estimated as a function of $q^2$ using the RI-sMOM scheme on the lattice and then converted to $\overline{\text{MS}}$ scheme at 2 GeV using perturbation theory. As discussed in Sec. IV, there is significant spread in the data due to breaking of rotational symmetry on the lattice. Second, the 2-loop series for the matching factor for $g_T^{u-d}$ does not show a convergent behavior. Third, the data for the four charges do not uniformly show a large enough interval, $\eta A_{\text{QCD}} \ll q \ll \xi/\pi/a$, over
which they are independent of \( q^2 \), so we are not able to extract a unique estimate of \( Z_f \). The two methods we use give significantly different estimates. We use this difference, which is larger than the individual statistical uncertainty, to assign the error. These error estimates are added in quadrature to those in the bare charges obtained from the 2-state fit to get the total error in the renormalized charges on each ensemble.

- Discretization errors due to nonzero lattice spacing \( a \), finite-volume effects characterized by \( M_s L \) and uncertainty in the chiral behavior: The errors due to these three systematics are obtained using a simultaneous fit. The Ansatz used for the final results, keeping the lowest-order corrections in each variable, is given in Eqs. 13 and 14.

- Uncertainty due to the number of terms retained in the combined fit Ansatz as discussed in Sec. V.
A recapitulation of the important features observed in the data for the isovector charges is:

- Estimates of the isovector axial charge, $g_S^{u-d}$, converge from below with respect to excited-state contamination on all the ensembles. The data plotted in Fig. 14 show no significant dependence on the pion mass or the lattice volume. The largest variation is the increase with the lattice spacing and the size of the slope is dictated by the smaller estimates on the $a = 0.06$ fm ensembles. Also, as discussed in Sec. V, even though this slope is different in the fits to renormalized charges calculated in the two ways, the extrapolated results are consistent. Overall, the spread in the estimates under changes in the fit Ansatz is small, about 0.03.

- The isovector scalar charge, $g_S^{u-d}$, also converges from below with respect to excited-state contamination. The data show a decrease with the lattice spacing but no significant variation with the pion mass. Our error estimate accounts for (i) the large excited-state contamination on the two finest ensembles, $a06m310$ and $a06m220$; (ii) the uncertainty in the determination of the renormalization constant $Z_S$; and (iii) the larger, by a factor of 3–5, statistical errors compared to those in $g_S^\nu$ and $g_T^\nu$ on the various ensembles as summarized in Table XI. The fits capture the variation of $g_S^{u-d}(a, M_\pi, M_\pi L)$ with respect to both the lattice spacing $a$ and the pion mass $M_\pi$ as shown in Figs. 14 and 17. The largest sensitivity to the fit Ansatz comes from adding a chiral logarithm term, which tends to increase the estimate by about 0.12 as shown in Table XV. However, as shown in Fig. 20, keeping just the leading polynomial correction, $O(M_\pi)$ gives very good fits to the data, and the AIC indicates that adding the chiral logarithm term does not improve the fits significantly. Nevertheless, we will take half the change, 0.06, as an estimate of the systematic error due to the choice of the fit Ansatz.

- Our analysis of the isovector tensor charge, $g_T^{u-d}$, shows that (i) estimates converge from above for each ensemble and the fit using the 2-state Ansatz given in Eqs. (9) and (10) accounts for the excited-
FIG. 22. Comparison of the excited-state contamination in the extraction of unrenormalized isovector charges $g_{\nu-d}^{A,S,T,V}$ from the a06m310 ensemble. The plots on the left are with smearing parameters $\{\sigma = 6.5, N_{GS} = 70\}$ and on the right with $\{\sigma = 12, N_{GS} = 250\}$. Both calculations were done using the AMA method with parameters summarized in Table XVIII.
FIG. 23. Comparison of the excited-state contamination in the extraction of unrenormalized isovector charges \( g_{A}^{u-d} \) from the a06m220 ensemble. The plots on the left are with smearing parameters \( \{ \sigma = 5.5, N_{GS} = 70 \} \) and on the right with \( \{ \sigma = 11, N_{GS} = 230 \} \). Both calculations were done using the AMA method with parameters summarized in Table XVIII.
state contamination within the quoted errors. (ii) The data for the renormalization constant in the RI-sMOM scheme show a window in \( q^2 \) over which the estimates in the \( \overline{\text{MS}} \) scheme at 2 GeV are constant within errors as discussed in Sec. IV and Ref. [11]. On the other hand, the poorly behaved 2-loop series for the matching factor suggests that this systematic uncertainty could be as large as 0.02. We have taken this systematic into account when estimating the error in \( Z_T \) given in Table X. (iii) The estimates from the nine ensembles display little dependence on the lattice spacing, pion mass or the lattice volume, as shown in Fig. 14. (iv) The largest change in estimates, about 0.04, is again due to adding a chiral logarithm term to the fit Ansatz.

Based on the data, fits and trends observed, we propose at an error budget from each of the sources that is summarized in Table XXI. The entries are constructed as follows: For the statistical uncertainty and excited-state contamination, we consider the data shown in Figs. 8, 9, 10, 22 and 23 and the errors in the 3-point function data, the efficacy of the 2-state fit and the difference between the two AMA estimates on the \( a06m310 \) and \( a06m220 \) ensembles. For estimating the uncertainty in the renormalization constants, we use the errors given in Table X, which are consistent with the size of the deviations of \( Z_V g_V^{u-d} \) from unity given in Table XIII. For assessing the error associated with the extrapolation in the lattice spacing, we take half of the total spread in the central values at the three lattice spacings \( a = 0.12, 0.09 \) and 0.06 fm. Similarly, for the dependence on the quark mass, we take half of the spread in the central values at the three masses, \( M_a \approx 135, 220 \) and 310 MeV. The finite-volume correction is observed to be small in all cases and the error budget is assigned to be half the change on going from the 9-point to the 8-point fit estimates shown in Table XV, i.e., the direction is given by the change on removing the smallest \( M_a L \) point \( a12m220S \).

Our combined fits include these systematics and the error estimates given in Tables XV are consistent with the error budget summarized in Table XXI.

An error estimate due to the choice of the fit Ansatz is the least straightforward to assess as discussed next. With nine data points, we can explore only a limited space of lowest order corrections given in Eqs. 11 and 12. Within this subspace, the largest variation with respect to the fit Ansatz is in \( g_S^{u-d} \) and \( g_T^{u-d} \) obtained with and without the chiral logarithm term as shown in Figs. 14 and 16 and quantified in Table XV. As pointed out in Sec. V, in fits with chiral logarithms, the two terms proportional to \( c_3 \) (or \( c_3' \)) and \( c_3^{\log} \) compete and the errors in them are large. The Akaike Information Criterion indicates that including the chiral logarithm term does not improve the fit sufficiently to warrant it. Nevertheless, we take half the spread (0.06 for \( g_S^{u-d} \) and 0.02 for \( g_T^{u-d} \)) between the two 9-point estimates given in Table XV as a conservative estimate of the uncertainty due to the fit Ansatz. Estimates of \( g_A^{u-d} \) are much more stable under changes in the fit Ansatz, with the central value varying between 1.18 and 1.21. Again, we take a conservative value, 0.02, as an estimate of this systematic uncertainty.

In Table XXI, we also indicate the direction in which our analysis changes the estimate as a result of taking into account a given systematic. For example, the slope of the fit to \( g_A^{u-d} \) versus \( a \) shown in Fig. 14 is positive. As a result, the central value after extrapolation to \( a = 0 \) is lower than the data points. We indicate this by attaching a \( \uparrow \) to the estimate shown in Table XXI. For the ratios of renormalization constants, we compare the estimates from method A and B given in Table IX. Taking estimates using method B as the baseline, we assign a \( \downarrow \) if taking the average with method A lowers the final estimate as shown in Table X. The direction of the SESC estimate is taken to be the direction of convergence with \( l_{\text{sep}} \).

Our final estimates for the isovector charges, including a second error to account for the variation in the estimates with the fit Ansatz, are given in Table XXII. Estimates of the flavor-diagonal charges given in Table XXIII and of \( g_T^{u+d} \) given in Table XXII are based on only the connected diagrams. We, therefore, consider it premature to assign an additional systematic uncertainty due to the fit Ansatz.

| Error From | \( g_A^{u-d} \) | \( g_S^{u-d} \) | \( g_T^{u-d} \) | \( g_T^{u+d, \text{con}} \) |
|-----------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| SESC      | 0.02 \( \uparrow \) 0.05 \( \uparrow \) 0.02 \( \downarrow \) | 0.04 \( \uparrow \) 0.04 \( \downarrow \) 0.01 \( \downarrow \) | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) | 0.03 \( \uparrow \) 0.12 \( \uparrow \) 0.04 \( \uparrow \) |
| Z         | 0.01 \( \uparrow \) 0.04 \( \uparrow \) 0.04 \( \downarrow \) | 0.04 \( \downarrow \) 0.04 \( \downarrow \) 0.01 \( \downarrow \) | 0.03 \( \downarrow \) 0.03 \( \downarrow \) 0.02 \( \downarrow \) | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) |
| a         | 0.02 \( \downarrow \) 0.02 \( \downarrow \) 0.02 \( \downarrow \) | 0.04 \( \uparrow \) 0.04 \( \uparrow \) 0.01 \( \downarrow \) | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) | 0.03 \( \uparrow \) 0.12 \( \uparrow \) 0.04 \( \uparrow \) |
| Chiral    | 0.02 \( \uparrow \) 0.02 \( \downarrow \) 0.02 \( \downarrow \) | 0.03 \( \downarrow \) 0.03 \( \downarrow \) 0.02 \( \downarrow \) | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) | 0.03 \( \uparrow \) 0.12 \( \uparrow \) 0.04 \( \uparrow \) |
| Finite volume | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) | 0.01 \( \uparrow \) 0.01 \( \uparrow \) 0.01 \( \uparrow \) | 0.03 \( \uparrow \) 0.12 \( \uparrow \) 0.04 \( \uparrow \) |
| Error quoted | 0.033 | 0.12 | 0.046 |
| Fit Ansatz | 0.02 | 0.06 | 0.02 |

TABLE XXII. Final estimates of the renormalized isovector charges for the proton from the 9-point fit described in Sec. V. The first error includes statistical and all systematic uncertainties except that due to the extrapolation Ansatz, which is given by the second error estimate. As explained in the text, in the connected estimate of \( g_T^{u+d} \) we only give the first error. Estimates for the neutron are obtained by \( u \leftrightarrow d \) interchange.

TABLE XXI. Estimates of the error budget for the three isovector charges due to each of the five systematic effects described in the text. The symbols \( \uparrow \) and \( \downarrow \) indicate the direction in which a given systematic is observed to drive the central value obtained from the 9-point fit. The second last row gives the errors in our best estimate given in Table XV using the 9-point fit. The last row gives the additional systematic uncertainty that accounts for the variations due to the choice of the fit Ansatz.
To summarize, the first error quoted in $g_A^{n-d}$ is dominated by that in $2T$ and, as shown in Table XXI, all five systematic effects are in the same direction. Since the other four systematics are small, we are confident that our error estimate, 0.046, covers these five systematics. Our new result, $g_T^{n-d} = 0.987(51)(20)$, confirms the conclusion reached in Ref. [11] that all the systematics are under control at a few percent level in this calculation.

The extraction of the scalar charge $g_S^{n-d} = 0.97(12)(6)$ is less precise since the statistical errors in $g_S^{n-d}$ on each ensemble are still 10–15%, that is, a factor of 3–5 larger than those in $g_T^{n-d}$. Also, all sources of systematic uncertainty are at the 5% level. The dominant systematic is from including a chiral logarithm in the fit Ansatz—the shift in the estimate is much larger than in $g_S^{n-d}$ or $g_T^{n-d}$. Considering the size and sign of the first five systematic uncertainties, we again conclude that the first error, 0.12, and the additional 0.06 due to the fit Ansatz are conservative.

Our estimate $g_A^{n-d} = 1.195(33)(20)$ is smaller than the experimental result 1.276(3) by about 7%. This difference could be due to a combination of the observed few percent effect in the various systematics. Thus, a higher-statistics study on ensembles at smaller $a$ and closer to the physical $M_T$ is needed to improve the estimate.

### VIII. COMPARISON WITH PREVIOUS WORKS

In this section we compare our results with previous determinations of the isovector charges $g_A^{n-d}$, $g_S^{n-d}$ and $g_T^{n-d}$. In this comparison, it is important to note that we have, for the first time, taken all the systematics into account by uniformly using the 2-state fit with multiple values of $t_{sep}$ to address excited-state contamination and by making a combined fit in the three variables $a$, $M_T^2$ and $M_a L$ using Eqs. 13 and 14. Our error estimates from this combined fit are larger (for example, the fits versus only $M_T^2$, shown in Fig. 14 as grey overlays, have a much narrower error band and give $g_A^{n-d} = 1.25(2)$); however, we claim they are realistic as discussed in Sec. VII. Also, our final results include a second error estimate: the first error includes statistical and all systematic uncertainties except that due to the extrapolation Ansatz, which is given by the second error estimate.

#### A. $g_A^{n-d}$

Calculations of $g_A^{n-d}$ are considered a test of the lattice-QCD method to provide accurate estimates of the properties of the nucleon. A summary of experimental and lattice-QCD determination of $g_A^{n-d}$ is given in Fig. 24. We note that over time the experimental estimate has increased steadily to its present value 1.276(3). On the other hand, most previous lattice-QCD estimates have been in the range 1.1–1.2 [19]. A significant reason for the lattice-QCD estimates being low has been excited-state contamination, since it can make a large negative contribution depending on the nucleon interpolating operator (the smearing parameter $\sigma$ in our study) as shown in Figs. 8, 22 and 23. In this work, we have shown that analyses using a combination of well-tuned smeared sources for generating quark propagators, performing simulations at multiple values of $t_{sep}$, and a simultaneous 2-state fit to the data at a number of values of $t_{sep}$ reduces this contamination to the size of the statistical errors which are about 2%. With $O(50,000)$ measurements on ensembles with $M_a L \gtrsim 4$ and spanning 0.12–0.06 fm in lattice spacing and 135–320 MeV in the pion mass, the uncertainty from the chiral fit and continuum extrapolation is also reduced to about 2% from each of these systematics. Our analysis of the full error budget is presented in Sec. VII.

All but one previous lattice-QCD results underestimate $g_A^{n-d}$ as shown in Fig. 24. The exceptional result is from the RQCD Collaboration [44] that finds a large slope with $M_T^2$ in the renormalization factor independent ratio $g_A/F_\pi$. Extrapolating this ratio to the physical pion mass gave the estimate $g_A = 1.280(44)(46)$ even though the majority of their data for $g_A^{n-d}$ are $\lesssim 1.2$. Our data for $F_\pi$ and $g_A/F_\pi$, given in Table XXIV, show little dependence on the lattice spacing and lattice volume. We, therefore, analyze them in Fig. 25 versus just $M_T^2$ and plot the result of a fit linear in $M_T^2$. The fit shows that our clover-on-HISQ estimate, $g_A/F_\pi = 12.88(15)$, at the physical pion mass remains low by about 7% compared to the experimental value 13.80. This is because our $F_\pi$ data, where $r_1$ is used to set the scale of the HISQ lattices [22], extrapolate to the physical value. On the other hand, the error in the ratio $g_A/F_\pi$ is much smaller than in $g_A$, therefore the deviation is more significant. The difference between the two calculations suggests that further analysis is needed to quantify the various systematics in $g_A^{n-d}$.

To reconcile the roughly 2σ difference between our result $g_A^{n-d} = 1.195(33)(20)$ and the experimental value $g_A^{n-d} = 1.276(3)$ would require all five $O(2%)$ systematics given in Table XXI to eventually move the result in the same direction or one or more of the systematic effects have been grossly underestimated. To gain a better understanding of how the various sources of errors contribute and to reduce the overall uncertainty to $O(2%)$ will require at least $O(200,000)$ measurements on the seven ensembles at different $a$ and $M_a$ used in this study and the analysis of one additional ensemble at $a = 0.06$ fm and $M_a = 135$ MeV. Increasing the statistics by a factor of four will reduce the errors in the data with the largest $t_{sep}$ we have analyzed and thus improve the $t_{sep} \to \infty$ estimates. Adding the point at the physical quark mass and the smallest lattice spacing $a = 0.06$ fm, will further constrain the chiral fit. This level of precision is achievable with the next generation of leadership-class computing resources.
TABLE XXIII. Final estimates of the connected part of the renormalized flavor-diagonal charges of the proton. The estimates for the neutron are obtained by the $u \leftrightarrow d$ interchange.

| ID | $g_A^{u-d}$ | $F_{\pi}^\text{bare}$ (MeV) | $F_{\pi}$ (MeV) | $g_A^{u-d}/F_{\pi}$ (GeV$^{-1}$) |
|----|-------------|-----------------|-----------------|-----------------|
| a12m310* | 1.252(9) | 107.1(1.0) | 102.3(3.4) | 11.62(14) |
| a12m220S | 1.283(39) | 102.4(1.0) | 97.3(3.2) | 12.53(40) |
| a12m220 | 1.273(30) | 104.5(1.0) | 99.2(3.2) | 12.19(31) |

TABLE XXIV. Estimates of the unrenormalized $g_A^{u-d}$ (reproduced from Table XI) and the bare and renormalized $F_{\pi}$ obtained from the HP$^{2}$ measurements. The dominant source of error in the renormalized $F_{\pi}$ is the uncertainty in the $Z_A$ given in Table X. We also give the renormalization factor independent ratio $g_A^{u-d}/F_{\pi}$, calculated as a ratio of the bare quantities, and which is plotted in Fig. 25.

| ID | $g_A^{u-d}$ | $F_{\pi}^\text{bare}$ (MeV) | $F_{\pi}$ (MeV) | $g_A^{u-d}/F_{\pi}$ (GeV$^{-1}$) |
|----|-------------|-----------------|-----------------|-----------------|
| a09m3100 | 1.262(30) | 106.9(1.0) | 101.6(3.3) | 11.80(30) |
| a09m220 | 1.272(30) | 102.8(0.9) | 97.6(3.2) | 12.38(31) |
| a09m130* | 1.255(24) | 97.2(0.8) | 92.4(3.0) | 12.91(26) |
| a06m310* | 1.212(14) | 107.1(0.7) | 104.5(3.3) | 11.25(15) |
| a06m220* | 1.234(17) | 101.3(0.7) | 98.2(3.1) | 12.19(19) |

B. $g_S^{u-d}$

There are few estimates of $g_S^{u-d}$ using lattice QCD. The RQCD Collaboration reported $1.02(18)(30)$ [44], and the LHPC Collaboration obtained $1.08(28)$ [57]. While these estimates are consistent with our result $g_S^{u-d} = 0.97(12)(6)$, it is clear that the errors are still large in all lattice-QCD estimates. Our work suggests that increasing the measurements to $O(200,000)$ on all the ensembles (the same program needed to reduce the overall uncertainty in $g_A^{u-d}$ to 2%) will also reduce the uncertainty in $g_S^{u-d}$ to less than 10%.

Gonzalez-Alonso et al. [58] used the conserved vector current (CVC) relation $g_S/g_V = (M_N - M_P)^{QCD}/(m_d - m_u)^{QCD}$ to obtain $g_S^{u-d}$. In their analysis, the estimates of the two mass differences on the right-hand side were obtained using the global lattice-QCD data. Their result, $g_S^{u-d} = 1.02(8)(7)$, is consistent with our estimate discussed above and shown in Fig. 26. These two lattice-QCD estimates, using CVC versus our direct calculation of the charge, have very different systematic uncertainties, so their consistency is a non-trivial check. We, therefore, consider our result, $g_S^{u-d} = 0.97(12)(6)$, from a direct calculation as having achieved the target accuracy of about 10–15% needed to put bounds on scalar and tensor interactions at the TeV scale when combined with experimental measurements of $b$ and $b_\nu$ parameters in neutron decay experiments with $10^{-3}$ sensitivity [7]. The current and prospective status of these bounds is given in Sec. IX.

We can use CVC in reverse to combine our result $g_S = 0.97(12)(6)$ with the lattice QCD determination of $(m_d - m_u)^{QCD}$ given by the Flavor Lattice Average Group (FLAG) [60] to predict $(M_N - M_P)^{QCD}$. Using the
improves on the value 1.020(76) reported in Ref. [11].\(^4\) It is also consistent with the estimate \(g_T^u\) from the LHPC Collaboration \((N_f = 2 + 1, 16(9)(7)\) MeV), and using the 2+1+1-flavor FLAG estimate \(g_T^u = 1.005(17)(29)\) by the RQCD Collaboration \((N_f = 2, 14)\), and phenomenological estimates (integral over the longitudinal momentum fraction of the experimentally measured quark transversity distributions). Given the consistency of the lattice-QCD estimates and our better understanding of the excited-state contamination and other systematic effects, we consider our error estimate to be conservative and \(g_T^u = 0.987(51)(20)\) a reliable value to use in phenomenology.

### IX. Constraining New Physics Using Precision Beta Decay Measurements

Our improved results for the isovector tensor charges \(g_S^u\) and \(g_T^u\) enable more stringent tests of non-standard scalar and tensor charged-current interactions, parameterized by the dimensionless couplings \(\epsilon_{S,T}\) [7, 69]:

\[
\mathcal{L}_{CC} = -\frac{G_F^{(0)} V_{ud}}{\sqrt{2}} \left[ \epsilon_S \bar{c}(1 - \gamma_5) \nu_e \cdot \bar{u}d \\
+ \epsilon_T \bar{c} \sigma_{\mu\nu}(1 - \gamma_5) \nu_e \cdot \bar{u} \sigma^{\mu\nu}(1 - \gamma_5) d \right].
\]  

\(^4\) The small decrease can be traced back to the better control over excited-state contamination in this study with the AMA method and thus better determination of the \(t_{\text{sep}} \to \infty\) value that converges from above.

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**FIG. 25.** Fits to \(F_\pi\) (left panel) and \(g_A/F_\pi\) (right panel) data given in Table XXIV assuming a linear dependence on \(M^2\) for both. The lattice scale of these HISQ ensembles used to convert \(M^2\) and \(F_\pi\) to physical units was determined using \(r_1\) [22]. Since the extrapolated \(F_\pi\), red star, matches the experimental value at the physical point, the value of the renormalization factor independent ratio \(g_A/F_\pi\) remains about 7% below the experimental result shown as a black star.

**FIG. 26.** A summary plot showing estimates for \(g_S^u\) from lattice QCD and phenomenology. The data are taken from: PNDME'16 (this work); LHPC'12 [57]; PNDME'11 [7]; RQCD'14 [44]. The estimates based on the conserved vector current and phenomenology are updated from: Gonzalez-Alonso [58] and Adler [59]. The rest is the same as in Fig. 24.

2+1-flavor estimates \(m_d = 4.68(14)(7)\) MeV and \(m_u = 2.16(9)(7)\) MeV from FLAG, we get \((M_N - M_P)^\text{QCD} = 2.44(38)\) MeV, and using the 2+1+1-flavor FLAG estimates \(m_d = 5.03(26)\) MeV and \(m_u = 2.36(24)\) MeV gives \((M_N - M_P)^\text{QCD} = 2.59(49)\) MeV. These two estimates update our old “PNDME” value quoted by Gonzalez-Alonso et al. [58] and are now competitive with other lattice QCD estimates given by them.

### C. \(g_T^u\)

In Ref. [11], we presented a detailed discussion of all the errors in the determination of the isovector charge \(g_T^u\) and compared our results with those obtained by other collaborations. Our new estimate, \(g_T^u = 0.987(51)(20)\),
These non-standard couplings, $\epsilon_{S,T}$, can be constrained at low-energy by precision beta-decay measurements (of the pion, neutron, and nuclei) as well as at the Large Hadron Collider (LHC) through the reaction $pp \to e^+e^-X$. The LHC constraint is valid provided the mediator of the new interaction is heavier than a few TeV.

In Fig. 28 (left panel), we update the analysis of constraints on $\epsilon_T$ and $\epsilon_S$ presented in Refs. [7, 69] by using our improved estimate of the tensor charge and the LHC data from the 2012 run at $\sqrt{s} = 8$ TeV, for an integrated luminosity of approximately 20 fb$^{-1}$ [70, 71]. The current bound on $\epsilon_T$ is dominated by the radiative pion decay $\pi \to e^+\gamma$ [72, 73], while the bound on $\epsilon_S$ is dominated by the Fierz interference term in $0^+ \to 0^+$ nuclear beta decays [74].

In the prospective bounds shown in Fig. 28 (right panel), the change in low-energy constraints is due to improvements in experiments: We assume future measurements of the Fierz interference term and the neutrino asymmetry parameter ($b$ and $b_\nu$) in neutron decay will be at the level of $10^{-3}$ [8–10, 75]. A similar constraining power on $\epsilon_T$ can be achieved with a 0.1%-level measurement of the Fierz term in the pure Gamow-Teller $^9\text{He}$ decay [76].

Between the current and prospective constraints, the improvement in the LHC bounds come from both, the increase in center-of-mass energy $\sqrt{s}$ and the integrated luminosity. In both panels, the impact of using our estimates of $g_{ST}$ given in Table XXII over the quark model estimates $0.25 < gS < 1.0$ and $0.6 < gT < 2.3$ [68] is large. Furthermore, the lattice-QCD reduction of uncertainties in $g_{ST}$ implies that the constraining power of beta decays can actually be stronger than of the LHC for this class of non-standard interactions.

The current upper bounds on the effective couplings $\epsilon_{S,T} = (v/\Lambda_{S,T})^2$ correspond to lower bounds for the effective scales $\Lambda_S > 7$ TeV and $\Lambda_T > 13$ TeV. If future low-energy experiments find a nonzero signal, then combined with precision calculations of $g_{ST}$, we will be able to predict the scale of new physics to be probed at the LHC or future colliders. Even without a signal, with improved precision, we will be able to tighten the lower bounds on the scale of new physics in these channels, which will help rule out certain classes of BSM models.

X. CONCLUSIONS

We have presented a high-statistics study of the isovector and flavor-diagonal charges of the nucleon using clover-on-HISQ lattice QCD. By using the AMA error-reduction technique we show that the statistical precision of the data can be improved significantly. Also, keeping one excited state in the analysis of data at multiple values of $t_{sep}$ allows us to isolate and mitigate excited-state contamination. Together, these two improvements allow us to demonstrate that the excited-state contamination in the axial and the tensor channels has been reduced to the 2% level. The high-statistics analysis of nine ensembles covering the range 0.12–0.06 fm in the lattice spacing, $M_\pi = 135–320$ MeV in the pion mass, and $M_\pi L = 3.3–5.5$ in the lattice size allowed us to analyze the systematic errors due to lattice discretization, dependence on the quark mass and finite volume. As a result, this is the first work that is able to include the effect of these three systematic uncertainties by making a simultaneous fit in all the three variables $a$, $M_\pi^2$ and $M_\pi L$. In the case of the isovector charges, we also assign a second error estimate to account for the variation in the results due to the choice of the extrapolation Ansatz as discussed in Sec. VII. Our final estimates are given in Tables XXII and XXIII.

One of the largest sources of uncertainty comes from the calculation of the renormalization constants for the quark bilinear operators. These are calculated nonperturbatively in the RI-sMOM scheme over a range of values of $q^2$. As discussed in Sec. IV, the breaking of the rotational symmetry gives rise to a large spread in the data. After conversion to $\overline{\text{MS}}$ scheme at 2 GeV using perturbation theory, which shows poor convergence for $Z_T$, the data, especially for $g_{ST}^{u-d}$, do not show a large scaling window in which they are independent of $q^2$. Our estimates of errors take into account these uncertainties, and are therefore larger than those obtained by other collaborations.

Our estimate $g_{ST}^{u-d} = 1.195(33)(20)$ is about 2$\sigma$ (about 7%) below the experimental value $g_A/g_V = 1.276(3)$. In Sec. VII we analyze five systematic effects and find that each contributes at the 1–2% level, with roughly equal distribution in sign. Improvement in our understanding of these five systematic factors: residual excited-state
contamination, uncertainty in the determination of the renormalization constants, the Ansatz used for the chiral fit, error in the chiral fit and the continuum extrapolation, requires a still higher-statistics calculation. Based on the various systematic errors discussed in Sec. VII, we claim in Sec. VIII A that the overall uncertainty can be reduced to 2% by increasing the statistics to \(O(200,000)\) measurements on \(O(2000)\) configurations on the seven ensembles shown in Fig. 8 and an additional physical mass HISQ ensemble at \(a = 0.06\) fm. Lastly, to address possible systematic effects due to using the clover-on-HISQ formulation versus a unitary lattice formulation, we have started calculations with similar statistics and methodology using the clover-on-clover formulation [31].

For the tensor charges, we find that the dependence on the lattice volume, lattice spacing and the light-quark mass is small, and a simultaneous fit in these variables, keeping just the lowest-order corrections, gives reliable estimates of the physical value. Our final estimate for the isovector tensor charge, \(g_T^{u-d} = 0.987(51)(20)\), is in good agreement with the previously reported estimates [11] and is more accurate than phenomenological estimates as shown in Fig. 27.

We have also updated our estimates for the connected parts of the flavor-diagonal charges. New estimates of the tensor charges of the proton, needed for the analysis of the contribution of the quark EDM to the neutron EDM [11, 20], are \(g_P^T = 0.792(42)\) and \(g_P^T = -0.194(14)\).

The extraction of the scalar charge of the proton has larger uncertainty. The statistical errors in the lattice data for \(g_S^{u-d}(a, M_\pi, M_\pi L)\) are 3–5 times those in \(g_T^{u-d}(a, M_\pi, M_\pi L)\), and the data show significant dependence on the lattice spacing \(a\) and a weaker dependence on the pion mass \(M_\pi\). Our estimate, \(g_S^{u-d} = 0.97(12)(6)\), is in very good agreement with the estimate \(g_S^{u-d} = 1.02(8)(7)\) obtained using the conserved vector current relation in Ref. [58]. Previous lattice-QCD estimates summarized in Fig. 26 have larger errors but are consistent with these two estimates as discussed in Sec. VIII. Combining our estimate \(g_S^{u-d} = 0.97(12)(6)\) with the 2+1+1-flavor estimate of the difference of light quarks masses \((m_d - m_u)_{QCD} = 2.67(35)\) MeV given by the FLAG [60], we obtain \((M_N - M_P)_{QCD} = 2.59(49)\) MeV.

Finally, our results, \(g_S^{u-d} = 0.97(12)(6)\) and \(g_T^{u-d} = 0.987(51)(20)\), meet the target uncertainty of 15% required to maximize the impact of future measurements of the helicity-flip parts of the neutron decay distribution with \(10^{-3}\) accuracy [7]. The status of current and prospective constraints on novel scalar and tensor interactions, \(\xi_{S,T}\), using our improved estimates of \(g_{S,T}\) are given in Sec. IX. Our goal for the near future is to further understand and reduce all the systematic uncertainties in the estimate of \(g_A^{u-d}\), a benchmark for evaluating the accuracy achievable in lattice-QCD calculations of the matrix elements of quark bilinear operators within

**FIG. 28.** Left panel: current 90% CL constraints on \((\xi_S)\) and \((\xi_T)\) from beta decays \((\pi \to \epsilon \nu \gamma)\) and \(0^+ \to 0^+\) and the LHC \((pp \to \epsilon \nu + X)\) at \(\sqrt{s} = 8\) TeV. Right panel: prospective 90% CL constraints on \((\xi_S)\) and \((\xi_T)\) from beta decays and the LHC \((pp \to \epsilon \nu + X)\) at \(\sqrt{s} = 14\) TeV. The low-energy constraints correspond to 0.1% measurements of \(B, b\) in neutron decay and \(6\) in \(^6\)He decay. In both panels we present the low-energy constraints under two different scenarios for the scalar and tensor charges \(g_{S,T}\): quark model [68] (large dashed contour) and lattice QCD results given in Table XXII (smaller solid contour).
nucleon states.

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