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Flavor diagonal charges of the nucleon and the sigma terms

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Final results from the PNDME calculations of the flavor diagonal charges of the nucleons, $g^{u,d,s}_{A,S,T}$, the pion-nucleon sigma term, $\sigma_{\pi N} = m_{u,d} g_S^{u+d}$, and the strangeness content of the nucleons $\sigma_s = m_s g_S^s$, obtained using eight 2+1+1-flavor HISQ ensembles generated by the MILC collaboration are presented. To remove excited-state contributions, we have carried out both the "standard" and "$N\pi$" analyses and use physics or χPT based reasoning for picking between the two for the final result. To renormalize the charges, we have carried out the calculation of the full mixing matrix for the 2+1-flavor theory using the RI-SMOM scheme on the lattice and then using perturbative results to match to $\overline{MS}$ scheme and run to a common scale of 2 GeV. The chiral-continuum-finite-volume (CCFV) extrapolation is carried out keeping the leading corrections in each. The results for $g^{u,d,s}_{A,S,T}$ are summarized in Table 2 and for the sigma terms in Eq. (4).

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1. Introduction

We present results for the flavor diagonal nucleon charges, $g^{u,d,s}_{A,S,T}$, extracted from the matrix elements of axial, scalar, and tensor quark bilinear operators, $\overline{q}\Gamma q$ with the Dirac matrix $\Gamma = \gamma_\mu\gamma_5, I, \sigma_{\mu\nu}$, respectively, within ground state nucleons. They represent a culmination of the PNDME collaboration's lattice QCD calculations of nucleon charges done using Wilson-clover fermions for valence quarks on eight ensembles generated by the MILC collaboration with 2+1+1-flavors of highly improved staggered quarks (HISQ) [1], and supersede those in our earlier publications [2–4] and updates in conference proceedings [5, 6]. Our previous results for $g^{u,d,s}_{A,T}$ in Refs. [2–4] constitute the FLAG values in the 2024 FLAG report [7] for the 2+1+1-flavor theory. Recent results from the ETM collaboration (also for the 2+1+1-flavor theory using the twisted mass formalism) are consistent with these and our final results except for $g^{u,d}_A$ and $\sigma_{\pi N}$ as discussed later.

The motivation for these calculations and much of the methodology used has already been published for g^q_A in Ref. [2], g^q_T in [3] and for the pion-nucleon sigma term, $\sigma_{\pi N} = m_{u,d} \times g^{u+d}_S$, in [4]. The charges $g^{u,d,s}_A$ give the contributions of the intrinsic spin of the quarks to the nucleon spin; the $g^{u,d,s}_T$ give the contribution of the quark electric dipole moment (EDM) operator to the nucleon EDM; and all three, $g^{u,d,s}_{A,S,T}$, give the coupling of dark matter or Higgs-like interactions with nucleons in the respective channels. In addition, with $g^{u,d,s}_S$ in hand, we calculate the pion-nucleon sigma term, $\sigma_{\pi N} = m_{u,d} g^{u+d}_S$ and the strangeness content of the nucleons $\sigma_s = m_s g^s_S$. These results include a number of improvements over those in our earlier publications [2–4] and conference proceedings [5, 6].

- The calculation has been extended to eight ensembles described in Table 1. The point $a06m220$ is new.
- The disconnected contributions on all ensembles except $a12m220$ are now calculated with operator insertion at all intermediate points t between the nucleon source and the sink points separated by Euclidean time τ.
- The statistics on most of the ensembles have been increased.
- Results for $g^{u,d,s}_S$ are new. In Ref. [4], result for only the renormalization group invariant pion-nucleon sigma term, $\sigma_{\pi N} = m_{u,d} \times g^{u+d}_S$, was presented.
- The calculation of the renormalization of quark bilinears in the 2+1-flavor theory, $Z_{A,S,T}$, has been done nonperturbatively for the clover-on-HISQ formulation using the regularization independent symmetric momentum subtraction (RI-sMOM) scheme [8, 9]. These Zs are then matched to the $\overline{MS}$ scheme and run to 2 GeV using perturbation theory. Our previous calculations [2–4] used $Z_{\rm isoscalar} \approx Z_{\rm isovector}$, i.e., $Z_{\rm u+d} \approx Z_{\rm u\text{-}d}$ for the renormalization constants of the axial and tensor operators. We now confirm that this is a very good approximation having completed the full calculation.
- Resolving and removing the contributions of excited states to nucleon correlation function continues to be a leading systematic. These artifacts have to be removed to get ground state matrix elements. In our recent lattice QCD calculation of the nucleon axial vector form

Ensemble	a (fm)	M_π (MeV)	β	$C_{\rm SW}$	am_{ud}	am_s	$L^3 \times T$	$M_\pi L$
$a15m310$	0.1510(20)	320.6(4.3)	5.8	1.05094	-0.0893	-0.0210	$16^3 \times 48$	3.93
$a12m310$	0.1207(11)	310.2(2.8)	6.0	1.05094	-0.0695	-0.018718	$24^3 \times 64$	4.55
$a12m220$	0.1184(10)	227.9(1.9)	6.0	1.05091	-0.075	-0.02118	$32^3 \times 64$	4.38
$a09m310$	0.0888(8)	313.0(2.8)	6.3	1.04243	-0.05138	-0.016075	$32^3 \times 96$	4.51
$a09m220$	0.0872(7)	225.9(1.8)	6.3	1.04239	-0.0554	-0.01761	$48^3 \times 96$	4.79
$a09m130$	0.0871(6)	138.1(1.0)	6.3	1.04239	-0.058	-0.0174	$64^3 \times 96$	3.90
$a06m310$	0.0582(4)	319.6(2.2)	6.72	1.03493	-0.0398	-0.01841	$48^3 \times 144$	4.52
$a06m220$	0.0578(4)	235.2(1.7)	6.72	1.03493	-0.04222	-0.01801	$64^3 \times 144$	4.41

Table 1: The lattice spacing a, the valence pion mass M_π, gauge coupling β, the Sheikholeslami-Wohlert coefficient C_{SW} defining the clover term in the action, the light quark mass $am_{ud} = 1/2\kappa_{ud} - 4$, the strange quark mass $am_s = 1/2\kappa_s - 4$, the lattice volume $L^3 \times T$, and the lattice size in units of M_π for the eight ensembles analyzed for flavor diagonal charges g_Γ^q.

factor $G_A(Q^2)$ [10–13] and of the pion-nucleon sigma term $\sigma_{\pi N}$ [4], we presented evidence of larger-than-expected excited-state contributions (ESC) from $N\pi$ and $N\pi\pi$ multihadron excited states to the nucleon 3-point correlation functions. Motivated by these works, we continue to study the impact of including $N\pi/N\pi\pi$ states in the analysis of all the flavor diagonal nucleon matrix elements.

For correlation functions with resolvable signal of ESC, fits to get ground state matrix elements (GSME) now include two excited states in the spectral decomposition, and in each case we compare fits with and without including the $N\pi$ excited state. These fits have been made using the full covariance matrix. To reduce ESC, we vary $t_{\rm skip}$, the number of points skipped adjacent to the source and the sink, and the range of source-sink separations (τ values) included in the fits. For final results we take the average of various fits, weighted by the Akaika Information Criteria (AIC) score [14]. For the choice of which strategy ("standard" using first excited-state mass from the 2-point function versus that of the $N\pi$ state) to use for final results, we incorporate input from χPT and physics since the data and the χ^2 of fits, by themselves, do not resolve between the two.

- The renormalized axial, $g_A^{u,d,s}$, and tensor, $g_T^{u,d,s}$, charges are extrapolated to the physical point, $a \to 0$, $M_\pi = 135$ MeV, and $M_\pi L \to \infty$, using the ansatz

$$g(a, M_\pi, M_\pi L) = c_0 + c_a a + c_2 M_\pi^2 + c_3 \frac{M_\pi^2 e^{-M_\pi L}}{\sqrt{M_\pi L}}\,, \tag{1}$$

that includes the leading corrections, pertinent to our lattice setup, in the 3 variables $\{a, M_\pi, M_\pi L\}$. The chiral corrections to $g_S^{u,d}$ and $\sigma_{\pi N}$ are discussed in Sec. 5 [4], and finite-volume corrections are neglected in fits to $\sigma_{\pi N}$ to avoid overparameterization.

2. Resolving excited states: standard method versus including $N\pi$

The 3-point correlation functions used to extract the relevant matrix elements, and from them the charges, have large ESC as illustrated in Fig. 2. These are removed by making fits to their spectral decomposition that we truncate at $n = 2$ excited states, dictated by the quality of the data. In fact, current data are not precise enough to make unconstrained fits with even $n = 1$. We use additional information, as described below, to make $n = 1$ and $n = 2$ fits. The key external inputs needed are the masses of excited states, of which even the mass gap ($\Delta M_1 = M_1 - M_0$) is poorly known for many ensembles.

There are 3 types of fits we consider. (i) Take the ground state amplitude A_0 and masses M_i from fits to the nucleon 2-point correlation functions constructed using the same interpolating operators, (ii) Take the M_i from some other related 3-point functions, or (iii) from the phenomenological values of these excited states. Since the excited states that can contribute significantly can be radial excitations or multihadron states ($N\pi, N\pi\pi, \ldots$) with nucleon quantum numbers, we need to decide which gives the larger ESC. The challenge arises because $M_1 \approx 1250$ MeV for $N\pi$ and ≈ 1500 MeV for the radial excitation. Consequently, even $n = 1$ ES fits give significantly different $\tau \to \infty$ values for these two inputs for M_1. (In all our work, the $N(\vec{p} = 1)\pi(\vec{p} = -1)$ and $N(0)\pi(0)\pi(0)$ are approximately degenerate. We, therefore, use the label "$N\pi$" to imply their joint contribution.)

In general, the coupling of the nucleon interpolating operator is suppressed by $1/L^3$ for each additional particle created (assuming "local" sources which applies to our Wuppertal smeared sources). As a result, the "$N\pi$" state gives a tiny contribution to 2-point functions and has proven challenging to extract its mass from fits. On the other hand, "$N\pi$" contributions to certain matrix elements (thus the corresponding 3-point functions) are sufficiently enhanced to compensate for the $1/L^3$ suppression in the wavefunction. Unfortunately, in these cases, the current data do not, *a priori*, provide guidance as the χ^2 of the fits with the "2-point = standard" versus "$N\pi$" value of M_1 are very similar.

There are two cases in which χPT suggests this enhanced contribution from "$N\pi$" states: (i) the pseudoscalar, G_P, and induced pseudoscalar, $\widetilde{G}_P$, form factors and (ii) the scalar charges $g_S^{u,d}$. The quark line diagrams illustrating why are shown in Fig. 1 (left and middle). One also expects, in χPT, 1-loop contribution to all charges from the diagram in Fig. 1 (right). In the case of the extraction of the axial FF, an enhanced contribution has been confirmed by the analysis of the A_4 correlator and the resulting FF satisfy the (necessary) PCAC relation to within expected discretization effects [10, 12]. Such a data driven confirmation has not yet been achieved for $g_S^{u,d}$!

The final challenge is that $M_{N(1)\pi(-1)}$ becomes smaller than M_{radial} only for $M_\pi \lesssim 200$ MeV. Thus, results are expected to be sensitive to the choice of M_1 only for ensembles with $M_\pi \lesssim$ 200 MeV, which in our case implies that only the $a09m130$ point qualifies.

Our current strategy is to compare results from two 3-state fits: (i) "standard" with M_1 and M_2 taken from the simultaneouly fit to 2-point function within the jackknife/bootstrap procedure, and (ii) "$N\pi$" with $M_1 = M_{N\pi}$, the energy of the non-interacting state with lattice masses and input it using narrow priors, and M_2 the first excited state mass in the 2-point fit. As mentioned above, the charges with possible enhanced ESC are $g_{A,S}^{u,d}$. The data from the $a09m130$ ensemble for g_A^d, g_S^u, g_S^d are shown in Fig. 2. While the "standard" and the "$N\pi$" fits give significantly different extrapolated ($\tau \to \infty$) values, the χ^2 are similar. Clearly, more high statistics data and points with

$M_\pi \lesssim 200$ MeV are needed to resolve between using the "standard" versus "$N\pi$" state analyses.

Our final choice, to take the average of the two fits for $g_A^{u,d}$, "$N\pi$" for $g_S^{u,d}$, and the "standard" for the rest, is based on the arguments given above.

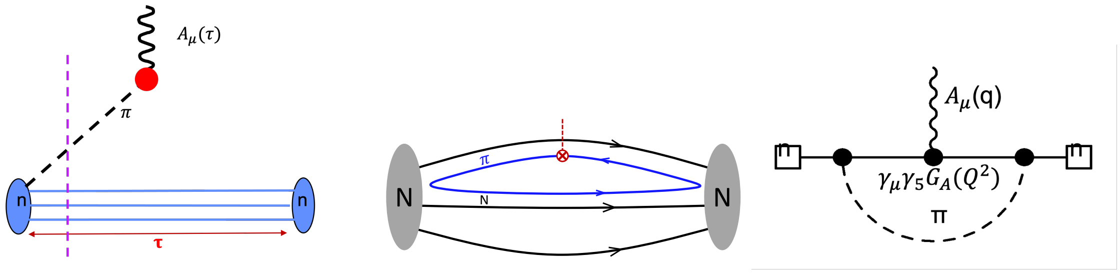

Figure 1: Quark line diagrams illustrating the contribution of $N\pi$ states. (Left) The current A_μ annihilates the pion in the $N\pi$ state produced by the nucleon source. Since the pion is light, the A_μ can couple to it anywhere on the time slice , i.e., giving a compensating enhancement of L^3. See Ref. [13] for a review. (Middle—relevant to $g_S^{u,d}$) the scalar current couples to a light quark loop creating an enhanced $N\pi$ state [4]. (Right) The standard pion loop contribution to all charges that could be $O(5\%)$ be as suggested by χPT.

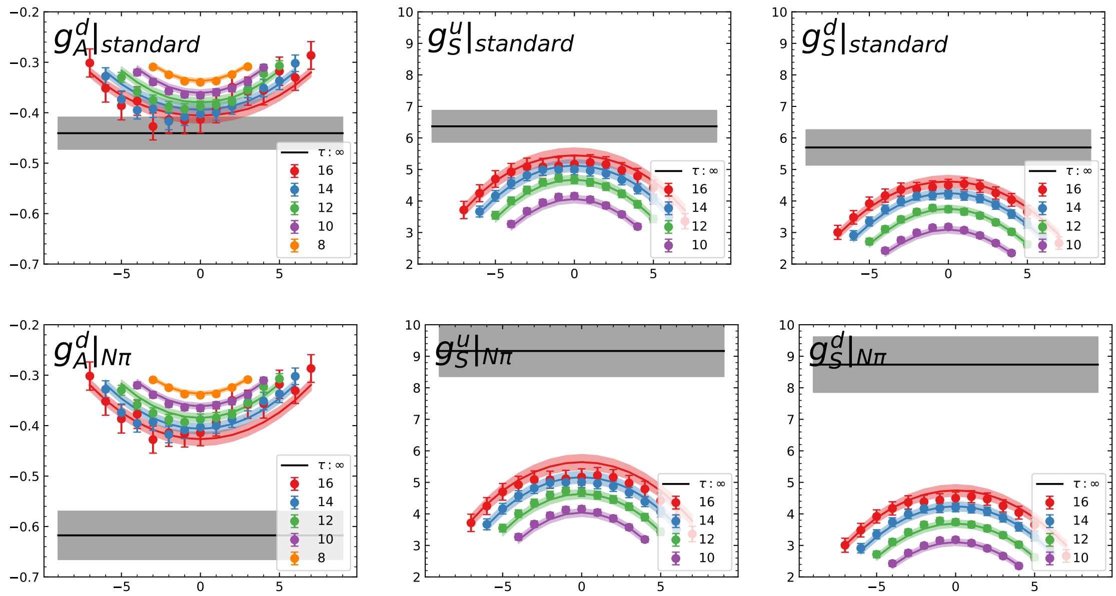

Figure 2: In the absence of ESC, the data for the ratio $C_O^{\rm 3pt}(t,\tau)/C^{\rm 2pt}(t)C^{\rm 2pt}(\tau-t)$ in the limits $(\tau-t)\to\infty$ and $t\to\infty$, should be independent of τ and t, i.e., lie on a horizontal line about $t=\tau/2$ with value that is the desired ground-state value. Current data show large ESC, and the gray band is the estimate of GSME given by a $n=2$ fit to the truncated spectral function. In each column, the data are the same but the top panel shows a fit without the $N\pi$ state and the bottom with. The χ^2 of these fits are similar.

3. Renormalization

The renormalization constants, Z, for the flavor diagonal quark bilinear operators $O^f = \bar\psi^f \Gamma \psi^f$ with Dirac matrix Γ and the flavor index $f=\{u,d,s\}$ are calculated in the $N_f = 2+1$ theory. The lattice calculation, including the mixing, is done in the RI-sMOM scheme [8, 9] on four ensembles, $a15m310$, $a11m310$, $a09m310$, and $a06m310$, i.e., at the four values of the lattice spacing a used in this study. These are used for all values of M_π for that a, i.e., assuming the quark mass dependence can be neglected. Second, the lattice calculation is not fully $O(a)$ improved in either the action or the operators and all the lattice spacing dependent improvement terms in the operators are neglected. Consequently, the results for the renormalized charges are extrapolated to the continuum limit using an ansatz starting with a term linear in a. The calculation is done using momentum source propagators on Landau gauge fixed lattices and includes the mixing of the singlet axial current with the $U(1)_A$ anomaly, for which we use the 2-loop result in Ref. [15].

Two methods, labeled Z_1 and Z_2, are used to calculate the quark field renormalization factor Z_ψ. In Z_1, it is taken from the 2-point function and in Z_2 using the conserved vector charge g_V. These are observed to have different dependence on the quark masses and lattice spacing, however, the results for them and the renormalized charges after extrapolation to the continuum limit using a term linear in a, are consistent. The final results for all charges are taken to be the average of the two estimates.

4. Chiral-continuum-finite-volume extrapolation (CCFV)

For $g_{A,T}^{u,d,s}$, the CCFV fit ansatz is given in Eq. (1). In $g_S^{u,d}$, the leading chiral contribution is from a term $\propto M_\pi$, so we use

$$g_S^{u,d}(a, M_\pi, M_\pi L) = d_0 + d_a a + d_2 M_\pi + d_3 M_\pi^2 + d_4 M_\pi \left(1 - \frac{2}{M_\pi L}\right) e^{-M_\pi L} \,. \qquad (2)$$

Note that the finite-volume term is also modified [4].

In all cases, we find no significant evidence for finite-volume corrections. So we compare results obtained with CCFV versus CC fits. To account for the difference, we have added a systematic uncertainty labeled CC in the results given in Table 2.

5. Pion-nucleon sigma term $\sigma_{N\pi}$

Results for the renormalization group invariant pion-nucleon sigma term were presented in Ref. [4] where it was calculated on each ensemble using the bare quantities $\sigma_{\pi N} = m_l^{\rm bare} g_S^{u+d,\rm bare}$ and the data were extrapolated to the physical point using the N^{2}LO χPT expression [16]:

$$\sigma_{\pi N} = (d_2 + d_2^a a) M_\pi^2 + d_3 M_\pi^3 + d_4 M_\pi^4 + d_{4L} M_\pi^4 \log \frac{M_\pi^2}{M_N^2} \,. \qquad (3)$$

Our χPT analysis and the CC fit in Ref. [4] suggested that all five terms contribute significantly. With data at only three values of $M_\pi \approx 135, 220, 310$ MeV, we can only explore the chiral part of the ansatz with a maximum of three terms. We make a second fit by including one more term, $d_3^\chi M_\pi^3$, but fix the coefficient d_3^χ to its χPT value evaluated with $M_N = 0.939$GeV, $g_A = 1.276$, and $F_\pi = 92.3$MeV [4]. Having addressed the mixing, matching and running pertinent to renormalizing the charges in our Clover-on-HISQ calculation, we now extrapolate g_S^{u+d} and g_S^s using CCFV (and CC) fits and multiply their physical point value by the renormalized quark masses, $(m_u + m_d)/2$

q	g_A^q	g_T^q	$g_S^q\vert_{N\pi}$	$g_S^q\vert_{\text{Standard}}$
u	$0.781(22)(11)_{CC}$	$0.782(26)(11)_{CC}$	$9.36(88)(4)_{CC}$	$6.34(57)(1)_{CC}$
u(PNDME)	$0.777(25)(30)$	$0.784(28)(31)$		
d	$-0.440(29)(9)_{\text{CC}}(24)_{N\pi}$	$-0.195(10)(2)_{CC}$	$8.84(93)(1)_{CC}$	$6.04(63)(1)_{CC}$
d(PNDME)	$-0.438(18)(30)$	$-0.204(11)(10)$		
s	$-0.055(9)(1)_{\text{CC}}$	$-0.0016(12)(1)_{CC}$	$0.66(17)(5)_{CC}$	$0.37(13)(6)_{CC}$
s(PNDME)	$-0.053(8)$	$-0.027(16)$		

Table 2: Final results for the flavor diagonal charges. The subscript CC denotes the systematic uncertainty assigned to account for the difference between the CCFV and CC fit values; and $N\pi$ for that between the the "standard" and $N\pi$ strategies where appropriate. These values are the average of those obtained with the Z_1 and Z_2 renormalization methods. Results for g_A^q and g_T^q supersede those published previously, g_A^q in Ref. [2] and g_T^q in [3], and reproduced here in rows labeled PNDME. We note that the improvements made in this final analysis have not shifted the central values or the errors significantly.

and m_s, respectively, taken from 2024 FLAG report [7] to get the sigma terms. The results are

$$\begin{aligned} \sigma_{\pi N}|_{\text{standard}} &= 42(6)\ \text{MeV} \\ \sigma_{\pi N}|_{N\pi} &= 61(6)\ \text{MeV} \\ \sigma_s|_{\text{standard}} &= 35(13)\ \text{MeV}\,. \end{aligned} \tag{4}$$

Our preferred value is $\sigma_{\pi N}|_{N\pi} = 61(6)$ MeV based on the guidance from χPT that $N\pi$ states make an enhanced contribution to $g_S^{u,d}$ [4].

6. Conclusions

Our final results are summarized in Table 2. Current data do not resolve between the "standard" and "$N\pi$" analyses based on the χ^2 of the ES fits. The charges for which there is a significant difference between the two analyses are g_A^d and $g_S^{u,d,s}$. For g_A^d, the difference is about one combined sigma. An "$N\pi$" analysis is motivated for $g_A^{u,d}$, because of the large contribution of $N\pi$ states to the axial form factors [10, 12]. The $g_S^{u,d,s}$ from the "$N\pi$" analysis are almost 50% larger and lead to a similarly larger value for $\sigma_{\pi N}$ (see Eq. (4)). The motivation for enhanced contribution of $N\pi$ states in $g_S^{u,d,s}$ comes from our χPT analysis in Ref. [4].

The goal is to obtain matrix elements of the various operators within the nucleon ground state using a data driven analysis that also resolves between the "standard" and "$N\pi$" analyses . One approach is to include all the states that make a significant contribution and calculate the full matrix of correlation functions and then carry out a generalized eigenvalue analysis. The other is to increase the statistical precision of the data to reach values of the source-sink separation τ large enough so that ES fits (i.e., their χ^2) discriminate between different choices of excited-state masses, M_i. While the data for all the charges show large ESC, as the statistics are increased, it is already showing the two theoretically required behaviors and achieving which is necessary for robust fits—symmetry of the data about $\tau/2$ and its monotonic convergence with τ. In our ongoing calculations, we are increasing the statistics on two physical mass HISQ ensembles, $a09m135$ and $a06m135$, by 4–6X to extend the signal from $\tau \approx 1.3$ to 1.6 fm. Hopefully, these data will yield a data-driven analysis.

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