The pion–nucleon sigma term from lattice QCD

Rajan Gupta,1,∗†‡ Sungwoo Park,1,∗†‡ Martin Hoferichter,3,‡ Emanuele Mereghetti,4 Boram Yoon,4,§ and Tanmoy Bhattacharya1,∗∗

1Los Alamos National Laboratory, Theoretical Division T-2, Los Alamos, NM 87545, USA
2Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
3Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, University of Bern, Sidlerstrasse 3, 3012 Bern, Switzerland
4Los Alamos National Laboratory, Computer, Computational and Statistical Sciences Division CCS-7, Los Alamos, NM 87545, USA

We present an analysis of the pion–nucleon σ-term, σπN, using six ensembles with 2+1+1-flavor highly improved staggered quark action generated by the MILC collaboration. The most serious systematic effect in lattice calculations of nucleon correlation functions is the contribution of excited states. We estimate these using chiral perturbation theory (χPT), and show that the leading contribution to the isoscalar scalar charge comes from Nπ and Nππ states. Therefore, we carry out two analyses of lattice data to remove excited-state contamination, the standard one and a new one including Nπ and Nππ states. We find that the standard analysis gives σπN = 41.9(4.9) MeV, consistent with previous lattice calculations, while our preferred χPT-motivated analysis gives σπN = 59.6(7.4) MeV, which is consistent with phenomenological values obtained using πN scattering data. Our data on one physical pion mass ensemble was crucial for exposing this difference, therefore, calculations on additional physical mass ensembles are needed to confirm our result and resolve the tension between lattice QCD and phenomenology.

I. INTRODUCTION

This Letter presents results for the pion–nucleon σ-term, σπN ≡ mudgud + d ≡ mud(N(k, s)|iuv + d|N(k, s)) calculated in the isospin symmetric limit with mud = (mu + md)/2 the average of the light quark masses. It is a fundamental parameter of QCD that quantifies the amount of the nucleon mass generated by the u- and d-quarks. The scalar charge gS is determined from the forward matrix element of the scalar density ¯qq between the nucleon state:

\[ g_S^q = \langle N(k = 0, s)|Z_S \bar{q}q|N(k = 0, s)\rangle, \tag{1} \]

where ZS is the renormalization constant and the nucleon spinor has unit normalization. The connection between gS and the rate of variation of the nucleon mass, MN, with the mass of quark with flavor q is given by the Feynman–Hellmann (FH) relation

\[ \frac{\partial M_N}{\partial m_q} = \langle N(k, s)|\bar{q}q|N(k, s)\rangle = g_S^q/Z_S. \tag{2} \]

The charge, gS, determines the coupling of the nucleon to the scalar quark current—an important input quantity in the search for physics beyond the Standard Model (SM), including in direct-detection searches for dark matter [11,8], lepton flavor violation in μ → e conversion in nuclei [9,10], and electric dipole moments [11,14]. In particular, σπN is a rare example of a matrix element that, despite the lack of scalar probes in the SM, can still be extracted from phenomenology—via the Cheng–Dashen low-energy theorem [15,16]—and thus defines an important benchmark quantity for lattice QCD.

The low-energy theorem establishes a connection between σπN and a pion–nucleon (πN) scattering amplitude, albeit evaluated at unphysical kinematics. Since the one-loop corrections are free of chiral logarithms [17,18], the remaining corrections to the low-energy theorem scale as σπN M2π/M2π ≈ 1 MeV, leaving the challenge of controlling the analytic continuation of the isoscalar πN amplitude ΣπN. Stabilizing this extrapolation by means of dispersion relations (and clarifying the relation between σπN and ΣπN), Refs. [19,21] found σπN ≈ 45 MeV based on the partial-wave analyses from Refs. [22,23]. More recent partial-wave analyses [24,25] favor higher values, e.g., σπN = 64(8) MeV [24]. Similarly, χPT analyses depend crucially on the πN input, with σπN prediction varying accordingly [27,28]. Other works that exploit this relation to πN scattering include Refs. [29,30].

The analytic continuation can be further improved in the framework of Roy–Steiner equations [37,45], whose constraints on σπN become most powerful when combined with pionic-atom data on threshold πN scattering [46,50]. Slightly updating the result from Refs. [39,41] to account for the latest data on the pionic hydrogen width [48], one finds σπN = 59.0(3.5) MeV. In particular, this determination includes isospin-breaking corrections [51,54] to ensure that σπN coincides with its definition in lattice QCD calculations [42]. The difference from Refs. [19,21] traces back to the scattering lengths implied by Refs. [22,23], which are incompatible with the modern pionic-atom data. Independent constraints
it is this persistent tension with phenomenology that we expect far lattice QCD calculations \[62–70\] have favored low values versus the pionic-atom result. In contrast, so models \[72\]. In the FH method, the nucleon mass is obtained via a global analysis of low-energy data in the Roy–Steiner reactions \[55–57\] and the charge exchange \[58–61\], and πN state configuration that can give an enhanced contribution.

FIG. 1. The upper connected (left) and disconnected (right) diagrams contribute to the 3-point function that determine the matrix element of flavor-diagonal scalar operators (shown by the symbol ⊗ at time slice \(t\)) within the nucleon state. The black and gray blobs denote nucleon source and sink, separated by Euclidean time \(\tau\). The bottom diagram illustrates that the disconnected diagrams include an \(N\pi\)-intermediate state configuration that can give an enhanced contribution.

from experiment are provided by low-energy \(\pi N\) cross-sections, including more recent data on both the elastic reactions \[55, 57\] and the charge exchange \[58, 61\], and a global analysis of low-energy data in the Roy–Steiner framework leads to \(\sigma_{\pi N} = 58(5)\) MeV \[45\], in perfect agreement with the pionic-atom result. In contrast, so far lattice QCD calculations \[62–70\] have favored low values \(\sigma_{\pi N} \approx 40\) MeV (with the exception of Ref. \[71\]), and it is this persistent tension with phenomenology that we aim to address in this Letter.

There are two ways to calculate \(\sigma_{\pi N}\) using lattice QCD, which are called the FH and the direct methods \[72\]. In the FH method, the nucleon mass is obtained as a function of the bare quark mass \(m_{ud}\) (equivalently \(M_N^2\)) from the nucleon 2-point correlation function, and its numerical derivative multiplied by \(m_{ud}\) gives \(\sigma_{\pi N}\). In the direct method, the matrix element of \(\bar{u}u + \bar{d}d\) is calculated within the ground-state nucleon. Both methods have their challenges. In the FH method, one needs to calculate the derivative about the physical \(m_{ud}\), which is computationally very demanding. Most calculations extrapolate from heavier masses or fit the data for \(M_N\) versus \(M_N^2\) to an ansatz motivated by \(\chi\)PT and evaluate its derivative at \(m_{ud}\). On the other hand, the signal in the matrix element is noisier since it is obtained from a 3-point function with the insertion of the scalar density. In both methods, one has to ensure that all excited-states contamination (ESC) has been removed. Both methods give \(\sigma_{\pi N} \approx 40\) MeV—see Fig. 4 review by the Flavour Lattice Averaging Group (FLAG) in 2019 \[72\], and the two subsequent works \[69, 70\].

Here, we present a new direct-method calculation. Our main message is that \(N\pi\) and \(N\pi\pi\) excited states, which have not been included in previous lattice calculations, can make a significant contribution. We provide motivation for this effect from heavy-baryon \(\chi\)PT \[73, 74\], and show that including the excited states in fits to the spectral decomposition of the 3-point function increases the result by about 50%. Such a change brings the lattice result in agreement with the phenomenological value.

II. LATTICE METHODOLOGY AND EXCITED STATES

The construction of all nucleon 2- and 3-point correlations functions is carried out using Wilson-clover fermions on six 2+1+1-flavor ensembles generated using the highly improved staggered quark (HISQ) action \[75\] by the MILC collaboration \[76\]. In each of these ensembles, the \(u\)- and \(d\)-quark masses are degenerate, and the \(s\)- and \(c\)-quark masses have been tuned to their physical values. Details of the six ensembles at lattice spacings, \(a \approx 0.12, 0.09,\) and 0.06 fm, and \(M_N \approx 315, 230,\) and 138 MeV are given in Table \[1\] and in Table \[II\] and of the analysis in App. \[A\]. To obtain flavor-diagonal charges \(g_S^2\), two kinds of diagrams, called connected and disconnected and illustrated in Fig. 1 are calculated. The details of the methodology for the calculation of the connected contributions (isovector charges) using this clover-on-HISQ formulation are given in Refs. \[77, 78\] and of the disconnected ones in Ref. \[77\].

The main focus of the analysis is on controlling the ESC. To this end, we estimate \(\sigma_{\pi N}\) using two possible sets of excited-state masses, \(M_{i}\) and \(M_{j}\), given in Table \[I\]. These \(M_{i}\) are obtained from simultaneous fits to the zero momentum nucleon 2-point, \(C_{2pt}\), and 3-point, \(C_{3pt}\), functions using their spectral decomposition truncated to four and three states respectively:

\[
\begin{align*}
C_{2pt}(\tau; k) &= \sum_{i=0}^{3} |A_i(k)|^2 e^{-M_i \tau}, \\
C_{3pt}^{S}(\tau; t) &= \sum_{i,j=0}^{2} A_i A_j^{\dagger} \langle i|S|j\rangle e^{-M_i t - M_j (\tau-t)} .
\end{align*}
\]

Here \(A_i\) are the amplitudes for the creation or annihilation of states by the nucleon interpolating operator used on the lattice, \(N = e^{abc} [u^T C_{\gamma_5} (1 + \gamma_4) d^b] u^c\), with color indices \(\{a, b, c\}\) and charge conjugation matrix \(C\). The nucleon source–sink separation is labeled by \(\tau\) and the operator insertion time by \(t\).

The issue of ESC arises because \(N\) couples not only to the ground-state nucleon but to all its excitations including multihadron states with the same quantum numbers. In the current data, the signal in \(C_{3pt}\) extends to \(\tau \approx 1.5\) fm, at which source–sink separation the contribution of excited states is significant as evident from the dependence on \(|\tau, t\rangle\) in the ratio \(R_S(\tau, t) = C_{3pt}(\tau, t)/C_{2pt}(\tau)\) shown in Fig. 2. In the limits \(t \to \infty\) and \((\tau-t) \to \infty\), the ratio \(R_S(\tau, t) \to g_S\). Fits to \(C_{3pt}\) using Eq. \[3\] with the key parameters \(M_i\) left as free parameters have large fluctuations. We, therefore, remove ESC and extract the ground-state matrix element, \(\langle 0|S|0\rangle\), using simultaneous fitting...
TABLE I. The ground- and excited-state masses, $M_0$, $M_1$, and $M_2$, $\chi^2$ of the fit, and the resulting value of the bare isoscalar charge and $\sigma_{\pi N}$ with the two strategies $\{4, 3^*\}$ and $\{4^N\pi, 3^*\}$. The second column gives the bare quark mass $m_{ud}^{bare}$.

| Ensemble ID | $m_{ud}^{bare}$ (MeV) | $M_0$ (GeV) | $M_1$ (GeV) | $M_2$ (GeV) | $\chi^2$ | $g_S$ | $\sigma_{\pi N}$ (MeV) | $M_0$ (GeV) | $M_1$ (GeV) | $M_2$ (GeV) | $\chi^2$ | $g_S$ | $\sigma_{\pi N}$ (MeV) |
|-------------|------------------------|-------------|-------------|-------------|---------|-------|------------------------|-------------|-------------|-------------|---------|-------|------------------------|
| a12m330     | 18.7(5)                | 1.09(1)     | 1.80(12)    | 2.7(1)      | 27/28   | 8.5(0.6) | 160(12)                | 1.09(1)     | 1.71(02)    | 2.0(1)     | 27/28   | 8.5(0.5) | 160(10)                |
| a12m220     | 19.9(5)                | 1.02(1)     | 1.76(08)    | 3.0(3)      | 18/22   | 10.5(0.5) | 104(07)                | 1.01(1)     | 1.50(03)    | 2.6(2)     | 20/22   | 11.8(1.0) | 117(11)                |
| a09m220     | 9.4(1)                 | 1.02(1)     | 1.66(14)    | 2.4(1)      | 35/35   | 10.4(0.8) | 98(07)                 | 1.02(1)     | 1.47(06)    | 2.3(1)     | 35/35   | 11.6(0.9) | 109(09)                |
| a09m130     | 3.5(1)                 | 0.95(1)     | 1.59(09)    | 2.8(2)      | 47/42   | 11.5(0.8) | 40(03)                 | 0.94(1)     | 1.22(01)    | 1.8(1)     | 51/42   | 15.9(2.3) | 55(08)                 |
| a06m330     | 17.2(2)                | 1.11(1)     | 1.80(11)    | 2.9(2)      | 56/60   | 10.4(0.7) | 179(12)                | 1.11(1)     | 1.76(06)    | 2.8(2)     | 56/60   | 10.6(0.6) | 182(10)                |
| a06m220     | 9.1(1)                 | 1.02(1)     | 1.62(14)    | 2.5(2)      | 69/81   | 10.9(1.0) | 98(09)                 | 1.02(1)     | 1.51(07)    | 2.3(1)     | 68/81   | 11.7(0.8) | 106(07)                |

FIG. 2. Results of the $\{4, 3^*\}$ (top row) and $\{4^N\pi, 3^*\}$ (bottom row) fits to the sum of the connected and disconnected data plotted versus $(t - \tau/2)/a$ for ensembles a09m130 and a06m220. Result of the fit is shown by lines of the same color as the data for various $\tau/a$ listed in the label, and the $\tau = \infty$ value is given by the gray band.

fits to $C^{2pt}$ and $C^{3pt}$ with common $M_i$. Statistical precision of the data allowed, without overparameterization, four states in $C^{2pt}$ (labeled $\{4\}$ or $\{4^N\pi\}$), and three states in $C^{3pt}$ (labeled $\{3^*\}$). We also dropped the unresolved $(2S[2])$ term in Eq. 3. Keeping it increases the errors slightly but does not change the values. Using empirical Bayesian priors for $M_i$ and $A_i$ given in Table V we calculate $\sigma_{\pi N}$ for two plausible but significantly different values of $M_1$ and $M_2$ in Table I that give fits with similar $\chi^2$. A similar strategy has been used in the analysis of axial-vector form factors, where also the $N\pi$ state gives a large contribution as discussed in Refs. 79, 80.

Data for $C^{3pt}$, by Eq. 3, should be (i) symmetric about $\tau/2$, and (ii) converge monotonically in $\tau$ for sufficiently large $\tau$, especially when a single excited state dominates. These two conditions are, within errors, satisfied by the data shown in Fig. 2. In the simultaneous fits, $M_1$ and $M_2$ are mainly controlled by the 4-state fits to $C^{3pt}$, however, as discussed in Refs. 78, 80, there is a large region in $M_{1,2} > 0$ in which the augmented $\chi^2$ of fits with different priors for $M_i$ is essentially the same, i.e., many $M_i$ are plausible. This region covers the towers of positive parity $N\pi, N\pi\pi, \ldots$, multihadron states, labeled by increasing relative momentum $k$, that can contribute and whose energies start below those of radial excitations. To obtain guidance on which excited states give large contributions to $C^{3pt}$, we carried out a $\chi PT$ analysis.

We study two well-motivated values of $M_1$ and $M_2$ for the analysis of $C^{3pt}$. The “standard” strategy (called the $\{4, 3^*\}$ fit) imposes wide priors on $M_{i,2}$, mostly to stabilize the fits, while the $\{4^N\pi, 3^*\}$ fits use narrow-width priors for $M_1$ centered about the noninteracting energy of the almost degenerate lowest positive parity multihadron states, $N(1)\pi(-1)$ or $N(0)\pi(0)\pi(0)$. Thus, the label $N\pi$ implies that the contribution of both states is included. Details of extracting the $M_i$ from these four-state fits, $\{4\}$ and $\{4^N\pi\}$ to just $C^{2pt}$, can be found in Ref. 80. For the a09m130 ensemble with $M\approx 138$ MeV, the $\{M_1, M_2\}$ are $\{1.59, 2.8\}$ and $\{1.22, 1.8\}$ GeV for the two cases, as shown in Table I. The fits (see Fig. 2) and the $\chi^2$ with respect to $C^{3pt}$ data are equally good, however, the results for the isoscalar charge $g_S^{2pt}$ differ significantly.

The $\{4, 3^*\}$ fit leads to a result consistent with $\sigma_{\pi N} \approx 40$ MeV, whereas the $\{4^N\pi, 3^*\}$ fit gives $\approx 60$ MeV. The major difference comes from the disconnected quark loop diagram shown in Fig. 1 and is strongly $M_2$ dependent—the effect of the $N\pi$ states is hard to resolve in the $M_\pi \approx 315$ MeV data, debatable in the 230 MeV data, and clear in the $M_\pi = 138$ MeV data.

It is important to point out that the values of $M_1$ and $M_2$ used in both fit strategies are an effective bundling of the many excited states that contribute into two. In fact, as mentioned above, many combinations of $M_1$ and $M_2$ between $\{4, 3^*\}$ and $\{4^N\pi, 3^*\}$ (see Table I) give fits with equally good $\chi^2$ values. Ref. 80 showed that for $\tau \gtrsim 1.0$ fm and for both fit strategies, the dominant ESC in $C^{3pt}$ comes from the first excited state. Thus, operationally, our two results for $\sigma_{\pi N}$ should be regarded as: what happens if the first “effective” excited state has $M_i \approx 1220$ MeV (motivated by $\chi PT$ and corresponding to the lowest theoretically possible states $N\pi$ or $N\pi\pi$) versus 1600 MeV obtained from the standard fit to the 2-point function. To further resolve all the excited states that contribute significantly and their energies in a finite
box requires much higher precision data on additional $M_* \approx 135$ MeV ensembles. In short, while our $\{4^{N\pi}, 3^*\}$ analysis reconciles the lattice and the phenomenological values, it also calls for validation in future calculations.

III. EXCITED STATES IN $\chi$PT

The contributions of low-momentum $N\pi$ and $N\pi\pi$ states to $C^{2pt}$ and $C^{3pt}$ can be studied in $\chi$PT, a low-energy effective field theory (EFT) of QCD that provides a systematic expansion of $\mathcal{R}_S(\tau, t)$ in powers of $Q/\Lambda_\chi$, where $Q$ denotes a low-energy scale of order of the pion mass, $Q \in \{M_\tau, t^{-1}, (\tau - t)^{-1}\}$, while $\Lambda_\chi \approx 1$ GeV is the typical scale of QCD. In contrast to the isovector scalar charge considered in Ref. [84], we find large contributions from the $N(\pi)\pi(-\k)$ and $N(0)\pi(\pi)(-\k)$ states, which can give up to 30% corrections to $\mathcal{R}_S$ and thus affect the extraction of $g_{S\pi\pi}$ and $\sigma_{\pi N}$ in a significant way.

The diagrams contributing to $\mathcal{R}_S$ are shown in Fig. 3, where we assume $\mathcal{N}(x)$ to be a local nucleon source with well defined transformation properties under chiral symmetry. The chiral representation of this class of sources has been derived in Refs. [81] [82] [89]. Details of the calculation at next-to-next-to-leading order $(N^2\text{LO})$ in $\chi$PT and the expansion of $\mathcal{N}$ in terms of heavy nucleon and pion fields are summarized in App. [13]. The crucial observation is that the isoscalar scalar source couples strongly to two pions, so that loop diagrams with the scalar source emitting two pions, which are consequently absorbed by the nucleon, are suppressed by only one chiral order, $Q/\Lambda_\chi$. These diagrams have both $N\pi$ and $N\pi\pi$ cuts, which give rise to ESC to Euclidean Green’s functions. A second important effect is that the next-to-leading-order (NLO) couplings of the nucleon to two pions, parameterized in $\chi$PT by the low-energy constants (LECs) $c_{1,2,3}$, are sizable, reflecting the enhancement by degrees of freedom related to the $\Delta(1232)$. When the pions couple to the isoscalar source, these couplings give rise to large $N^2\text{LO}$ corrections that are dominated by $N\pi\pi$ excited states and have the same sign as the NLO correction. Since, in the isospin-symmetric limit, the isovector scalar source does not couple to two pions, the NLO diagrams and the $N^2\text{LO}$ diagrams proportional to $c_{1,2,3}$ do not contribute to the isovector 3-point function, whose leading ESC arises at $O(Q^2/\Lambda_\chi^2)$. A detailed analysis showing that the functional form of the ESC predicted by $\chi$PT matches the lattice data and fits for sufficiently large time separations $\tau$ is given in App. [B]. In particular, the NLO and $N^2\text{LO}$ ESC can each reduce $\sigma_{\pi N}$ at a level of 10 MeV, thus explaining the $\{4^{N\pi}, 3^*\}$ fits, i.e., a larger value when ESC is taken into account.

IV. ANALYSIS OF LATTICE DATA

Examples of fits with strategies $\{4, 3^*\}$ and $\{4^{N\pi}, 3^*\}$ to remove ESC and obtain $g_{S^\pi\pi}^{u+d, \text{bare}}$ are shown in Fig. 2 and the results summarized in Table 1. The final results are obtained from fits to the sum of the connected and disconnected contributions. These values overlap in all cases with the sum of estimates from separate fits to $g_{S^\pi\pi}^{u+d, \text{conn}}$ and $g_{S^\pi\pi}^{q\bar{q}, \text{dof}}$. From the separate fits, we infer that most of the difference between the two ESC strategies comes from the disconnected diagrams, which we interpret as due to the $N\pi/N\pi\pi$ contributions through quark-level diagrams such as shown in Fig. 1.

Figure 3 shows two chiral fits based on the $N^2$LO $\chi$PT expression extrapolation is carried out using the $N^2$LO $\chi$PT expression [91]:

$$\sigma_{\pi N} = (d_2 + d_2^a) M_\tau^2 + d_3 M_\pi^3 + d_4 M_\pi^4 + d_4 L M_\pi^4 \log \frac{M_\tau^2}{M^2_N}. \tag{4}$$

The $d_i$ in $\chi$PT (henceforth labeled $d_i^a$) are given in Eq. (B11) and evaluated with $M_N = 0.939$ GeV, $g_A = 1.276$, $F_\pi = 92.3$ MeV. Neglected finite-volume corrections can also be estimated in $\chi$PT, see App. [B] and Refs. [78] [90], indicating a correction of less than 1 MeV for the $a09m130$ ensemble.

Figure 3 shows two chiral fits based on the $N^2$LO $\chi$PT expression for $\sigma_{\pi N}$. The $\{2, 2a, 3, 4\}$ fit keeps terms proportional to $\{d_2, d_2^a, d_3, d_4\}$ with all coefficients free. In the $\{2, 2a, 3, 4, 4L\}$ fit we use the $\chi$PT value for $d_3 = d_3^a$, which does not involve any LECs, and include the $d_4$ term. Each panel also shows the six data points obtained with the $\{4, 3^*\}$ and $\{4^{N\pi}, 3^*\}$ strategies and the fits to them. In each fit $d_2^a$ comes out consistent with zero.

The results for $\sigma_{\pi N}$ at the physical point $M_\tau = 135$ MeV from the various fits are essentially given by

FIG. 3. Data for the $\sigma$-term, $\sigma_{\pi N} = m_{ud}^a g_{S^\pi\pi}^{u+d}$, from the two ESC strategies $\{4, 3^*\}$ (gray) and $\{4^{N\pi}, 3^*\}$ (color) are shown as a function of $a$ and $M_\tau^2$. The two left panels show the chiral-continuum (CC) fit $\{2, 2a, 3, 4\}$ and the two right the CC fit $\{2, 2a, 3^*, 4, 4L\}$ described in the text. The result at $M_\tau = 135$ MeV and $\chi^2$/dof of the two fits are given in the legend.
the $a09m130$ point. We have neglected a correction due to flavor mixing inherent in Wilson-clover fermions since it is small as shown in App. [1] Our final result, $\sigma_{\pi N} = 59.6(7.4)$ MeV, is the average of results from the $\{2, 2a, 3, 4\}$ and $\{2a, 3^S, 4, 4L\}$ fits to the $\{4N^\pi, 3^*\}$ data given in Fig. 3 which overlap. In App. [13] we consider more constrained fit variants, which show that the fit coefficients of the $M^2$ and $M^4 \log M^2$ terms are also broadly consistent with their $\chi$PT prediction.

V. CONCLUSIONS

Results for $\sigma_{\pi N}$ were reviewed by FLAG in 2019 [72], and there have been two new calculations since as summarized in App. [13] and shown in Fig. 3. The ETM collaboration [69], using the direct method on one physical mass $2+1+1$-flavor twisted mass clover-improved ensemble, obtained $\sigma_{\pi N} = 41.6(3.8)$ MeV; the BMW collaboration using the FH method and 33 ensembles of $1+1+1+1$-flavor Wilson-clover fermions [70], but all with $M_\pi > 199$ MeV, find $\sigma_{\pi N} = 37.4(5.1)$ MeV. The $\chi$PT analysis of the impact of low-lying excited $N\pi$ states in the FH and direct methods is the same, and as shown in Fig. 3, it mainly affects the behavior for $M_\pi \lesssim 135$ MeV. Our work indicates that previous lattice calculations give the lower value $\sigma_{\pi N} \approx 40$ MeV because in the FH analysis [70] the fit ansatz (Taylor or Padé) parameters are determined using $M_\pi \geq 199$ MeV data, and in the direct method, the $N\pi/N\pi\pi$ states have not been included when extracting the ground-state matrix element [69].

To conclude, a $\chi$PT analysis shows that the low-lying $N\pi$ and $N\pi\pi$ states can make a significant contribution to $g_{\pi NN}^{S+d}$. Including these states in our analysis (the $\{4N^\pi, 3^*\}$ strategy) gives $\sigma_{\pi N} = 59.6(7.4)$ MeV, whereas the standard analysis (the $\{4, 3^*\})$ strategy gives $\sigma_{\pi N} = 41.9(4.9)$ MeV consistent with previous analyses [72]. These chiral fits are shown in Fig. 3. Since the $\{4, 3^*\}$ and $\{4N^\pi, 3^*\}$ strategies to remove ESC are not distinguished by the $\chi^2$ of the fits, we provide a detailed $\chi^2$LO $\chi$PT analysis of ESC, which reveals sizable corrections consistent with the $\{4N^\pi, 3^*\}$ analysis, restoring agreement with phenomenology. Since the effect of the $N\pi$ and $N\pi\pi$ states becomes significant near $M_\pi = 135$ MeV, further work on physical mass ensembles is needed to validate our result and to increase the precision in the extraction of the nucleon isoscalar scalar charge.

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Appendix A: Details of the Lattice Analysis

The parameters of the seven $2+1+1$-flavor ensembles generated using the HISQ action [73] by the MILC collaboration [70] are given in Table [11]. Note that the seventh ensemble, $a09m310$, listed has been used only for the analysis of the nucleon mass in App. [13]. On each of these ensembles, the calculations of the 2- and 3-point functions was carried out using tadpole improved Wilson-clover fermions as described in Ref. [78]. To reduce ESC, smeared sources using the Wuppertal method [92] were used to generate quark propagators.
with parameters given in Ref. [78]. The same smearing was used at the source and sink points.

All correlation functions are constructed using the truncated solver method with bias correction [78, 93, 94]. In this method, high statistics are obtained by using a low-precision (LP) stopping criterion in the inversion of the quark propagators, which was taken to be $r_{LP} \equiv |\text{residue}|_{LP}/|\text{source}| = 10^{-3}$ and $5 \times 10^{-4}$. These estimates are corrected for possible bias using high-precision (HP) measurements with $r_{HP}$ taken to be between $10^{-7}$ and $10^{-8}$ [71, 73]. The number of configurations analyzed, and the number of LP and HP measurements made for the connected and disconnected contributions, are given in Table II. In our data, the bias correction term was found to be a fraction of the $1\sigma$ error in all quantities and for all six ensembles.

For the statistical analysis of the data, we first constructed bias-corrected values for the 2- and 3-point correlation functions, then averaged these over the multiple measurements made on each configuration, and finally binned these. These binned data, 250–320 depending on the ensemble, were analyzed using the single elimination jackknife process. The analysis was repeated to quantify model variation of results by choosing data with different set of source-sink separations $\tau$ and different number of points $\tau_{\text{skip}}$, next to the source and the sink for each $\tau$, skipped in the excited-state fits. The final result was taken to be the average over the model values, weighting each by its Akaike information criteria weight.

The bare quark mass is defined to be $m_{u,d}^{\text{bare}} = 1/2\kappa_l - 1/2\kappa_c$, with the critical value of the hopping parameter, $\kappa_c$, determined using a linear fit to $(aM_\pi)^2$ versus $1/2\kappa$ at each of the three values of $a$. Results for $M_\pi$ are given in Table III and fits to the nucleon mass are discussed in App. C. A subtle point in the renormalization of $\sigma_{\pi N}$ for Wilson-clover fermions is presented in App. D.

The final quoted errors are from the chiral fits shown in Fig. 3 and given in the labels. The error in each data point, $\sigma_{\pi N} = m_{ud}^{\text{bare}} \times g_S^{u+d, \text{bare}}$, combines in quadrature those in $m_{ud}^{\text{bare}}$ and $g_S^{u+d, \text{bare}}$ (see Table II), with the latter given by the appropriate fit used to remove the ESC as illustrated in Fig. 2.

In addition to the simultaneous fits to $C^{2\text{pt}}$ and $C^{3\text{pt}}$ to remove ESC, we have also carried out the full analysis by first calculating the $M_i$ from 4-state fits to $C^{2\text{pt}}$ and using these as input in 3-state fits to $C^{3\text{pt}}$ as described in Ref. [80]. The priors used for the excited state masses $M_i$ and the amplitudes $A_i$ are given in Table V in App. C. The two sets of results for $M_i$ from the two approaches (simultaneous versus individual fits) are consistent and the ground state matrix elements agree within $1\sigma$. This agreement occurs for both strategies, {4, 3}$^*$ and {4N$\pi$, 3}$^*$. The error estimates from the simultaneous fits used to get the final results are slightly larger.

### Appendix B: Chiral Perturbation Theory

The corrections to the nucleon mass and the $\sigma$-term in $\chi$PT have a long history in the literature [17, 18, 74, 95–105]. The LO, NLO, and N$^3$LO diagrams contributing to the isoscalar scalar charge $g_S^{u+d}$ are shown in Fig. 5. In these diagrams, plain and dashed lines denote pions and nucleons in the interaction picture of $\chi$PT, and not the nucleon and pion eigenstates of the full theory.

These diagrams lead to the expansion

$$g_S^{u+d} = g_S^{(0)} + g_S^{(1)}(\frac{M_\pi}{\Lambda_\chi}) + g_S^{(2)}(\frac{M_\pi^2}{\Lambda_\chi^2}) + \ldots$$

where $\Lambda_\chi = 4\pi F_\pi \approx 1$ GeV is the breakdown scale of the chiral expansion. The NLO diagrams $(a_1)$ and $(b_1)$ in Fig. 2 only contribute to the isoscalar channel, implying that the isovector channel has the different expansion

$$g_S^{u-d} = g_S^{(0)} + g_S^{(2)}(\frac{M_\pi^2}{\Lambda_\chi^2}) + \ldots$$

We will show that the same loop diagrams responsible for the NLO and N$^3$LO corrections to $g_S$ also induce a sizable contribution from $N\pi$ and $N\pi\pi$ intermediate states.
To this end, we calculate the ratio $R_N(\tau, t)$ using heavy-baryon $\chi$PT and expand it as

$$R_N(\tau, t) = R_N^{(0)}(\tau, t) + R_N^{(1)}(\tau, t) + R_N^{(2)}(\tau, t),$$  \hspace{1cm} (B3)

including in its definition a factor $m_{ud}$ to make the result $R = m_{ud}R_N$ scale independent and ensure a normalization that facilitates the comparison to $\sigma_{\pi N}$. We assume $N$ to be a local nucleon source, transforming as $(\frac{1}{2}, 0) \otimes (0, \frac{1}{2})$ under the chiral group $SU(2)_L \otimes SU(2)_R$. The heavy-baryon $\chi$PT realization of $N$ was constructed in Ref. [22]

$$N(x) = \left(1 - \frac{\pi^2}{8F^2_\pi} - \frac{\pi \cdot \tau}{2F^2_\pi} \gamma_5\right) N_\nu$, where $N_\nu = (1 + \gamma_4)N_\nu/2$ represents a heavy-nucleon field. At $O(1/M_N)$, Eq. (B4) contains additional LECs, which reduce the predictive power of the calculation.

At LO one simply has $R_N^{(0)} = m_{ud}g_{0N}^2$. The NLO diagrams receive contributions from nucleon, $N\pi$, and $N\pi\pi$ excitations, leading to

$$R_N^{(1)}(\tau, t) = \frac{3g_A^2M_N^2}{8F^2_\pi L^2} \sum_k \frac{k^2}{E^2_\pi} \left[1 - e^{-E_N x t} - e^{-E_N x t B} + \frac{1}{2} e^{-E_N x t} \right] + \frac{1}{4} e^{-2E_N x t} + \frac{1}{4} e^{-2E_N x t B}$$

$$- \frac{3M_N^2}{32F^2_\pi L^3} \sum_k \frac{k^2}{E^2_\pi} \left(e^{-2E_N x t} + e^{-2E_N x t B}\right),$$  \hspace{1cm} (B5)

where $E_\pi = \sqrt{k^2 + M_N^2}$, $E_N = \sqrt{M_N^2 + k^2} - M_N$, $E_{N -} = E_\pi + E_N$, $k = 2\pi n/L$, and $I_B = \tau - t$. $F_\pi = 92.3$ MeV is the pion decay constant, $g_A = 1.276$ the axial charge of the nucleon [107]. The first term in Eq. (B5) is a correction to the ground-state contribution

$$\frac{3g_A^2M_N^2}{8F^2_\pi L^2} \sum_k \frac{k^2}{E^2_\pi} = -\frac{9g_A^2M_N^2}{64\pi F^2_\pi} + \Delta_L\sigma_{\pi N},$$  \hspace{1cm} (B6)

where $\Delta_L\sigma_{\pi N}$ is the finite-volume correction to the $\sigma$-
Finally, diagram \((a_1)\) receiving a contribution from \(N\pi\pi\) intermediate states (nucleon and pion having opposite momenta) and from an \(N\pi\pi\) state (the nucleon at rest and the two pions carrying momenta \(\pm k\)). The \(N\pi\) and \(N\pi\pi\) states with zero pion momentum vanish due to the prefactor \(k^2\). The amplitude of the \(N\pi\) contribution is suppressed by \((M_N L)^3\) compared to \(g_{S}^{(0)}\), but enhanced by the large coupling of a scalar source to the pion, making it suppressed by only a single chiral order. The last line of Eq. (15) originates from diagram \((b_1)\). In this case the dominant excited state is \(N\pi\pi\), with the two pions at zero momentum. Diagram \((g_2)\) arises from the last term in the square bracket in Eq. (14). Though formally NLO, this diagram vanishes up to \(O(1/M_N)\) corrections, and thus the topology \((g_2)\) only contributes to NLO. Similarly, the diagram with the pion emitted by \(\tilde{\nu}\) and absorbed by \(\tilde{N}\) vanishes at NLO.

At NLO there are several contributions. They come from loop corrections to the LO (diagrams \((a_2)\), \((b_2)\), and \((c_2)\)) and diagrams with subleading interactions in the chiral Lagrangian and the scalar source coupling to the pions (diagrams \((d_2)\), \((e_2)\), and \((f_2)\)). Here, diagrams \((a_2)\) and \((b_2)\) are exactly canceled by the NLO corrections to the 2-point function. This is in contrast to the isovector case, in which they are responsible for the leading ESC:

\[
R_{\text{isovector}}^{(2)}(\tau, t) = -m_{ud} g_S^{(0)} \frac{g_A^2}{2F_\pi^2} \frac{1}{L^3} \sum_k \frac{k^2}{E_\pi^3} \left[ 1 - e^{-E_\pi t} - e^{-E_\pi t_B} + e^{-E_\pi \tau} \right]. 
\] (B7)

This result agrees with the corrections to the isovector scalar charge computed in Ref. [33], once we expand in the limit \(M_\pi \gg |k|\).

Diagram \((c_2)\) only contributes to the ground state, and diagrams \((d_2)\) and \((e_2)\) are recoil corrections. A first effect of these diagrams is to shift the energy excitation of the \(N\pi\) state from \(E_\pi\) to \(E_\pi + \tilde{E}_N\). The remaining recoil corrections are

\[
R_{\text{recoil}}^{(2)} = -\frac{9g_A^2 M_N^2}{32M_N F_\pi^2 L^3} \sum_k \frac{(k^2)^2}{E_\pi^5} \left[ 1 - \frac{2}{3} e^{-E_\pi t} \right. \\
- \frac{2}{3} e^{-E_\pi t_B} + \frac{2}{3} e^{-E_\pi \tau} - \frac{1}{6} e^{-2E_\pi t} - \frac{1}{6} e^{-2E_\pi t_B} \\
+ \frac{3g_A^2 M_N^2}{32M_N F_\pi^2 L^3} \sum_k \frac{1}{E_\pi} \left[ 1 - \frac{2}{3} e^{-E_\pi t} - \frac{1}{2} e^{-2E_\pi t_B} \right] \\
+ \frac{2k^2}{E_\pi^2} \left( 1 - e^{-E_\pi t} - e^{-E_\pi t_B} + e^{-E_\pi \tau} \right) \right]. 
\] (B8)

Finally, diagram \((d_2)\) receives contributions from the LECs \(c_{1,2,3}\), which contribute to \(\pi N\) scattering at NLO in \(\chi\)PT. Including diagram \((c_2)\), they give

\[
R_{c_1}^{(2)} = -\frac{3M_N^2}{4F_\pi^2} \frac{1}{L^3} \sum_k \frac{1}{E_\pi} \left[ (c_2 + 2c_3) E_\pi^2 \right. \\
+ (2c_1 - c_3) M_N^2 \left( 1 - \frac{1}{2} e^{-2E_\pi t} - \frac{1}{2} e^{-2E_\pi t_B} \right) \\
+ \frac{3M_N^2}{F_\pi^2} \frac{1}{L^3} \sum_k \frac{1}{E_\pi} \left[ E_\pi c_1 \right]. 
\] (B9)

The energy gap in this case is \(\approx 2M_\pi\), since \(k = 0\) is allowed. The LECs \(c_{1,2,3}\) have been determined most reliably by an analysis of \(\pi N\) scattering using Roy–Steiner equations, matched to \(\chi\)PT in the subthreshold region [40, 41]. We will use the N3LO values

\[
c_1 = -1.11(3) \text{ GeV}^{-1}, \quad c_2 = 3.13(3) \text{ GeV}^{-1}, \\
c_3 = -5.61(6) \text{ GeV}^{-1}, 
\] (B10)

which correspond to NLO in the scalar form factor. We neglect the N2LO diagrams with pions emitted by the nucleon source, represented by \((g_2)\), \((h_2)\), and \((i_2)\) in Fig. 5, given that for a local source the NLO contribution is already small. Of these diagrams, \((g_2)\) produces N2LO recoil corrections, \((h_2)\) contains unknown LECs that appear in the expansion of the source, and \((i_2)\) cancels in the ratio between the 2- and 3-point function. While we have assumed local nucleon sources, the relative importance of the diagrams in Fig. 5 depends on the details of the lattice realization of \(\tilde{N}\). However, for the Gaussian smearing applied in this work with \(r_s \sim 0.6\) fm, corrections in addition to diagram \((b_1)\) scale as \((r_s M_N)^2 \sim 0.2\) and can therefore be neglected, see also Refs. [31, 109].

In the infinite-volume limit, the ground-state pieces of Eqs. (B5), (B8), and (B9) reproduce the N2LO expression for the \(\sigma\)-term (in the form given in Ref. [41])

\[
\sigma_{\pi N} = m_{ud} \frac{\partial M_N}{\partial m_{ud}} = m_{ud} g_S^{d+d} \\
= -4c_1 M_\pi^2 - \frac{9g_A^2 M_N^3}{64\pi F_\pi^2} - \frac{3M_N^4}{64\pi^2 F_\pi^2} \log \frac{M_N^2}{M_N^2} + 1 \\
+ (\frac{g_A^2}{M_N} - 8c_1 + c_2 + 4c_3) \\
+ 2M_\pi^2 \left( e_1 + \frac{3}{128\pi^2 F_\pi^2} (c_2 - \frac{2g_A^2}{M_N^2} + c_1 (l_{1/2} - 1)) \right), 
\] (B11)

except for the LO contribution proportional to \(c_1 M_N^2\), its quark-mass-renormalization proportional to \(l_{3/2} - 1\), and the N2LO LEC \(c_1\), all of which only contribute to the ground state. All other terms in Eq. (B11) can be obtained by replacing the finite-volume sum \(1/L^3 \sum_k\) with infinite-volume integrals in Eqs. (B5), (B8), and (B9).

To assess the importance of the \(N\pi\) and \(N\pi\pi\) contributions we define

\[
\delta \sigma_{\pi N}(\tau, t) = R(\tau, t) - \lim_{t, \tau \to \infty} R(\tau, t). 
\] (B12)
FIG. 6. (Left) Excited-state corrections from different truncations to the isoscalar scalar charge \( g_S \) in \( \chi PT \). (Right) Estimates for \( R_S(\tau, t) \) from the \( N^2LO \) analysis for the a09m130 ensemble, which should be compared to the data in Fig. 2 (and the shape with that of the separate contributions shown in Fig. 7). We assume \( g_S = 18 \) is the asymptotic value in both cases.

The contributions to \( \delta \sigma_{\pi N} \) from the NLO diagrams (including the formally \( N^2LO \) correction from \( \hat{E}_N \)) and from the \( N^2LO \) diagrams are evaluated in Table III using the parameters of the a09m130 lattice ensemble, for two choices of source–sink separation, \( \tau = 16a \) and \( \tau = 12a \). We list separately the corrections from diagram \((a_1)\) and \((b_1)\) in Fig. 5 as the first is dominated by \( N\pi \) excited states, the second by \( N\pi\pi \). Similarly, the \( N^2LO \) corrections from the diagrams proportional to the LECs \( c_{1,2,3} \) receive contributions from \( N\pi\pi \) states, while the recoil corrections in Eq. (B8) are dominated by \( N\pi \). From Table III we see that \( R^{(1)} \) and \( R^{(2)} \) are of similar size and the most important contributions come from diagram \((a_1)\) and from Eq. (B9). The nucleon source and recoil contributions are substantially smaller.

We also note that the ESC is amplified by the presence of several states close in energy. We can see this in the left panel of Fig. 6, where the red and orange curves denote the NLO and \( N^2LO \) corrections, including states up to \( |n_{\text{max}}| = 1 \), while the green and blue curves include states up to \( |n_{\text{max}}| = 3 \). In the continuum, the effect of the entire tower of excited states can be resummed, with the result shown in the last line of Table III and by the purple line in Fig. 6. The comparison to the different \( |n_{\text{max}}| \) values indicates the degree of convergence, which is ultimately determined by \( t \) and \( \tau \) via the exponential suppression of the continuum integrals. Indeed, we see that for \( \tau = 16a \) the corrections at \( t = 8a \) beyond \( |n_{\text{max}}| = 3 \) are around 10%, but twice as large for \( \tau = 12a, t = 6a \).

Away from \( t \sim \tau/2 \), the integrals become increasingly dominated by large-momentum modes, leading to the eventual breakdown of the chiral expansion. For this reason, the expansion becomes less reliable for small and large \( t \), which explains why the functional form predicted by \( \chi PT \), see the right panel of Fig. 6, suggests a faster decrease towards the edges than observed in the lattice data, see Figs. 2 and 7. (Note that in fits to remove the excited-state effects in the lattice data, we neglect \( t_{\text{skip}} \) points next to the source and the sink for each \( \tau \).) In the
FIG. 8. Chiral fits to the data for the $\sigma$-term, $\sigma_{\pi N} = m_\pi g_\pi^{\pi N}^d$, from the two ESC strategies $\{4,3^*\}$ (gray) and $\{4N^*, 3^*\}$ (color) shown as a function of $M^2$. The four chiral fits are $\{2^\chi, 3^\chi, 4\}$, $\{2^\chi, 3^\chi, 4, 4L\}$, $\{2^\chi, 3^\chi, 4, 4L^*\}$, and $\{2^\chi, 3^\chi, 4, 4L^*\}$. The result at $M_\pi = 135$ MeV and the $[\chi^2/dof]$ of the chiral fits for the two ESC strategies are given in the legend.

| chiral fit          | $d_2$ (GeV$^{-1}$) | $d_3$ (GeV$^{-2}$) | $d_4$ (GeV$^{-3}$) | $\chi^2/dof$ | $\sigma_{\pi N}$ (MeV) | $d_2$ (GeV$^{-1}$) | $d_3$ (GeV$^{-2}$) | $d_4$ (GeV$^{-3}$) | $\chi^2/dof$ | $\sigma_{\pi N}$ (MeV) |
|---------------------|-------------------|-------------------|-------------------|-------------|------------------------|-------------------|-------------------|-------------------|-------------|------------------------|
| Chiral fit $\{2\chi, 3\chi, 4\}$ | 2.56(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) | 2.56(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) |
| Chiral fit $\{2\chi, 3\chi, 4, 4L\}$ | 3.44(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) | 3.44(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) |

| {4N$^*$, 3$^*$} | $d_2$ (GeV$^{-1}$) | $d_3$ (GeV$^{-2}$) | $d_4$ (GeV$^{-3}$) | $\chi^2/dof$ | $\sigma_{\pi N}$ (MeV) | $d_2$ (GeV$^{-1}$) | $d_3$ (GeV$^{-2}$) | $d_4$ (GeV$^{-3}$) | $\chi^2/dof$ | $\sigma_{\pi N}$ (MeV) |
|-----------------|-------------------|-------------------|-------------------|-------------|------------------------|-------------------|-------------------|-------------------|-------------|------------------------|
| Chiral fit $\{2\chi, 3\chi, 4\}$ | 2.57(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) | 2.57(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) |
| Chiral fit $\{2\chi, 3\chi, 4, 4L\}$ | 3.44(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) | 3.44(15) | 2.18(1.4) | 11.35 | -- | 3.30(3.3) |

TABLE IV. Chiral fit coefficients with the ansatz $d_2M^2_\pi + d_3M^3_\pi + d_4M^4_\pi + d_{4L}M^4_{\pi N}\log(M_\pi/M_N)^2$. Here the $\chi^2/\text{dof}$ values for $d_i$ are calculated using Eq. (B11) and with $M_N = 0.939$ GeV, $g_A = 1.276$, $F_\pi = 92.3$ MeV. $d_{4L}$ includes the chiral logarithm in $\tilde{c}_3 = -\log M^2_\pi + \text{finite}$. The lower table gives the coefficients for the fits including an $aM^2_\pi$ term, as discussed in Sec. IV.

center, however, the EFT expansion should be reliable, in particular for the $\tau = 16a$ variant, which leads to the conclusion that NLO and N$^2$LO contributions can each lead to a reduction of $\sigma_{\pi N}$ at the level of 10 MeV. Note that Fig. 7 shows the behavior versus $t$ and $\tau$ for the individual contributions, i.e., insertions on the $u$, $d$, and the disconnected loop $l$.

While in Table III and Fig. 6 we focused on the ensemble with the lightest pion mass, we find agreement between the $\chi$PT expectations and the fits in Fig. 2 also for the remaining ensembles. For example, with the parameters of the $a09m220$ ensemble, $\chi$PT predicts the difference between the lattice data and the extrapolated value of $g_S$ to be 3 at $\tau = 2 = 8a$, in good agreement with the left panel in the second row of Fig. 2. Similarly, for the $a09m220$ and $a09m210$ ensembles we obtain that $g_S$ is shifted by 2.8 and 1.6, at $\tau = 2 = 12a$.

Finally, using Eq. (B11), we have carried out the following chiral fits to the lattice data: $\{2, 3\}$, $\{2^\chi, 3^\chi, 4\}$, $\{2, 3^\chi, 4, 4L\}$, $\{2^\chi, 3^\chi, 4, 4L\}$, and $\{2^\chi, 3^\chi, 4, 4L^*\}$, in addition to the fits $\{2, 3\}$, $\{2^\chi, 3^\chi, 4\}$, $\{2^\chi, 3^\chi, 4, 4L\}$ already shown in Fig. 2. Four of these additional fits are shown in Fig. 8 with resulting fit parameters given in Table IV. (We neglect possible discretization errors in these fits as they are not resolved in our best fits shown in Fig. 2.) We see that for the $\{4N^*, 3^*\}$ strategy all fit variants lead to parameters that agree with the $\chi$PT prediction, including evidence for the nonanalytic $M^2_\pi$ term from the $\{2, 3\}$ and $\{2, 3^\chi, 4\}$ fits, with changes in $\sigma_{\pi N}$ consistent with the uncertainty assigned to the least constrained fits ($\{2, 3\}$ and $\{2^\chi, 3^\chi, 4, 4L\}$), whose average we quote as our central result. Even in the most-constrained case ($\{2^\chi, 3^\chi, 4, 4L^*\}$) a good fit of the data is obtained, in marked contrast to the $\{4, 3^*\}$ strategy, in which case the $\chi^2/\text{dof}$ becomes unacceptable when imposing the maximum amount of chiral constraints.

The expressions in Eqs. (B5), (B6), and (B9) can also be used to assess the importance of finite-volume corrections to $g_S$. Focusing on the ground-state contributions, we can write $\Delta L \sigma_{\pi N}$ in Eq. (B10) as

$$\Delta_L \sigma_{\pi N} = -\frac{3g_\pi^2M^2_\pi}{64\pi F^2} \sum_{n \neq 0} e^{-M_\pi L/n} \left( 1 - \frac{2}{M_\pi L/n} \right).$$

Similarly, for the $c_i$ contributions (B9) we obtain

$$\Delta_L^{(2)} \sigma_{\pi N} = \frac{3M^4}{8\pi^2 F^2} \sum_{n \neq 0} \left( 2c_1 - c_3 \right) K_0 \left( M_\pi L/n \right) + (c_2 + 4c_3 - 4c_1) K_1 \left( M_\pi L/n \right),$$

in terms of the Bessel functions $K_0$ and $K_1$. Using the parameters of the $a09m130$ lattice ensemble, we get

$$\Delta_L \sigma_{\pi N} = -0.77 \text{ MeV}, \quad \Delta_L^{(2)} \sigma_{\pi N} = -0.43 \text{ MeV}.$$
implying that the finite-volume corrections are controlled at the level of about 1 MeV.

We end this appendix by pointing out a subtlety. We have used the lowest-order (linear) relation between $M_N^2$ and $1/2\kappa$ to get $m_{ud}^{\text{bare}}$ as we have ensembles at only two values of $M_N$ at each $\kappa$. Higher-order corrections give the LEC $l_3$ term in Eq. (B11). Removing it changes the $\chi$PT prediction of the $d_{4L}^{\chi}$ term in Table XVIII from 11.35 to 9.70, however, the results of the $\{2,3,4\}$ and $\{2^*,3^*,4,4L^\chi\}$ fits do not change significantly.

### Appendix C: Chiral fits to the Nucleon Mass

In both types of analyses, simultaneous fits to $C^{2pt}$ and $C^{3pt}$ and individual fits to them, we have used the same empirical Bayesian priors for the amplitudes and masses of the three excited states determined using the procedure described in Ref. [78]. The central values of these priors and their widths for $\{4,3^*\}$ and $\{4^N\pi,3^*\}$ fits are given in Table XV. The resulting $M_0$, $M_1$, and $M_2$ that enter in $\{3^*\}$ fits to $C^{3pt}$ are given in Table IV and are essentially the same from the two types of analyses. The result for the nucleon mass on the seventh ensemble, a09m310, used only for the analysis of $M_N$ in this section, is 1.09(1) GeV from both analyses.

In this section, we study the chiral behavior of the nucleon mass $M_N \equiv M_0$ using the $N^2$LO $\chi$PT result, which has a form similar to Eq. (4):

$$M_N = e_0 + e_2 M_\pi^2 + e_3 M_\pi^3$$

$$+ e_4 M_\pi^4 + e_{4L} M_\pi^2 \log \frac{M_N^2}{M_Z^2},$$

(C1)

with the $\chi$PT expressions for the $c_i$ given, e.g., in Ref. [11]. Even ignoring discretization and finite-volume corrections and fitting the lattice data using Eq. (C1) we face two challenges. First, as evident from the data for $M_0$ in Table IV there is no significant difference between the $\{4,3^*\}$ and $\{4^N\pi,3^*\}$ results. Therefore, we cannot comment on the impact of $N\pi$ states in the analysis of $M_N$. Second, as shown in Fig. 9 at least three parameters ($c_0$ and two more) are needed to fit the data. With data at essentially only three values of $M_\pi$, even these fits are overparameterized. In short, data at many more values of the lattice parameters, especially in $M_N^2$, are needed to quantify the lattice artifacts and check the prediction of $\chi$PT. The most constrained fit, $\{2,3,4\}$ and $\{2^*,3^*,4,4L^\chi\}$ fits do not change significantly.

### Appendix D: Renormalization

In this appendix we discuss the renormalization of the quark mass and scalar charge for fermion schemes that break chiral symmetry such as Wilson-clover fermions. We will do this using the notation and results given in Ref. [110] for an $N_f$ flavor theory with two light degenerate flavors, $m_u = m_d = m_1$, and $N_f - 2$ heavier flavors denoted generically by $m_s$. Here $m_i$ and $\hat{m}_i$ denote the bare and renormalized quark masses for flavor $i$ and we will neglect all $O(a)$ terms as they do not effect the continuum limit. These discretization errors start at $O(a)$ in our calculation.

We start with Eq. (26) in Ref. [110]:

$$m_j = Z_m \left[ m_j + (r_m - 1) \sum_{i=1}^{N_f} m_i \right],$$

(D1)

where $m_j$ are defined as $(1/2\kappa_i) - (1/2\kappa^0_f)$ with $\kappa_i$ the Wilson hopping parameter and $\kappa^0_f$ its critical value defined to be the point at which all pseudoscalar masses vanish, i.e., the $SU(N_f)$ symmetric limit. Using $Z_m$ to denote the flavor nonsinglet and $Z_m r_m$ the isosinglet renormalization constants, one has the relation [110]

$$\sum_s m_s = \frac{N_f}{Z_m [2 + (N_f - 2) r_m]} \sum_s \hat{m}_s$$

$$+ \frac{2(N_f - 2)(1 - r_m)}{2 + (N_f - 2) r_m} m_i,$$

(D2)

and

$$\hat{m}_i = \frac{N_f Z_m r_m}{2 + (N_f - 2) r_m} m_i + \frac{r_m - 1}{2 + (N_f - 2) r_m} \sum_s m_s,$$

(D3)
from which we obtain,

$$m_l(\hat{m}_l = 0) = \frac{1}{N_f Z_m r_m} \sum_s \hat{m}_s.$$  \hspace{1cm} \text{(D4)}

So, we have

$$\hat{m}_l = \frac{N_f Z_m r_m}{2 + (N_f - 2) r_m} \left[ m_l - m_l(\hat{m}_l = 0) \right]_{\text{fixed } \sum_s \hat{m}_s}. \hspace{1cm} \text{(D5)}$$

Similarly, for the scalar density $S_l$ with flavor $i$, and its expectation value $\langle S_l \rangle$ in any fixed state we have from Eqs. (22–23) in \[110\]

$$\langle S_l \rangle = Z_S \left[ \frac{(N_f - 2) + 2 r_s}{N_f} \langle S_l \rangle + \frac{r_s - 1}{N_f} \sum_s S_s \right], \hspace{1cm} \text{(D6)}$$

with $Z_S$ and $Z_{SfS}$ the nonsinglet and the singlet renormalization constants. Using $Z_S Z_m = 1$ and $r_s r_m = 1$ \[110\], we get the desired result

$$\hat{m}_l \langle S_l \rangle = \left[ m_l - m_l(\hat{m}_l = 0) \right]_{\text{fixed } \sum_s \hat{m}_s} \times \left( \langle S_l \rangle + \frac{1 - r_m}{2 + (N_f - 2) r_m} \sum_s S_s \right), \hspace{1cm} \text{(D7)}$$

showing that mixing between flavors in Wilson-like formulations gives rise to a correction to $\sigma_{\pi N}$, i.e., the second term on the second line. To explain this, we need to clarify an important point about the notation. In this work we have defined $\kappa_e$ as the point at which $M^2_e$ vanishes with all the $m_s$ kept at their physical values. The difference in the definition of the chiral point, $\kappa^0_c$ versus $\kappa_c$, leads to a difference in the definition of the bare quark masses. The connection is that the bare quark mass used in this work is the same as $m_l - m_l(\hat{m}_l = 0)_{\text{fixed } \sum_s \hat{m}_s}$ in Eq. \[D7\].

We have not calculated $\langle \sum_s S_s \rangle$ that is needed to evaluate the correction to the isoscalar scalar charge, however, it is relatively small since $|1 - r_m| \lesssim 2\%$ for the six ensembles and $\langle \sum_s S_s \rangle < \langle S_l \rangle$. At the precision at which we are working in this paper, and since the focus is on showing that there is a difference in the result depending on the excited state analyses, i.e., between $\{4, 3^*\}$ and $\{4^N, 3^*\}$, this correction is neglected. Also, note that $r_m = 1$ for lattice QCD formulations that preserve chiral symmetry, in which case there is no correction.

**Appendix E: Update of FLAG 2019 Results for $\sigma_{\pi N}$**

Figure 4 gives an update on the summary of results for $\sigma_{\pi N}$ presented in the FLAG review 2019 \[22\] using the same notation. We focus on a comparison of results from lattice QCD and those from $\pi N$ scattering data. For the lattice data, we retain only the 2+1 and 2+1+1 (and 1+1+1+1) flavor results obtained since 2015. (See Refs. \[62, 63, 66, 67, 111, 117\] for other determinations included in the FLAG review.) Moreover, Fig. 4 does not include results from calculations that analyze more than one lattice data set within the FH approach \[118, 130\], or results that use a mixture of lattice QCD and phenomenological analyses \[131\]. Most of the recent lattice results are clustered around $\sigma_{\pi N} \approx 40$ MeV, while the phenomenological estimates are at $\sigma_{\pi N} \approx 60$ MeV, as is our result with $N\pi/N\pi\pi$ included when removing ESC.

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[1] H. Hellman, *Einführung in die Quantenchemie* (Franz Deuticke, Leipzig und Wein, 1937).

[2] R. P. Feynman, *Phys. Rev.* **56**, 340 (1939).
[3] J. Gasser and A. Zepeda, Nucl. Phys. B **174**, 445 (1980).
[4] A. Bottino, F. Donato, N. Fornengo, and S. Scopel, Astropart. Phys. **13**, 215 (2000) arXiv:hep-ph/9909228.
[5] A. Bottino, F. Donato, N. Fornengo, and S. Scopel, Astropart. Phys. **18**, 205 (2002) arXiv:hep-ph/0112299.
[6] J. R. Ellis, K. A. Olive, and C. Savage, Phys. Rev. D **77**, 065026 (2008) arXiv:0801.3656 [hep-ph].
[7] A. Crivellin, M. Hoferichter, and M. Procura, Phys. Rev. D **89**, 054021 (2014) arXiv:1312.4951 [hep-ph].
[8] M. Hoferichter, P. Klos, J. Menéndez, and A. Schwenk, Phys. Rev. Lett. **119**, 181803 (2017) arXiv:1708.02245 [hep-ph].
[9] V. Cirigliano, R. Kitano, Y. Okada, and P. Tuzon, Phys. Rev. D **80**, 013002 (2009) arXiv:0904.0957 [hep-ph].
[10] A. Crivellin, M. Hoferichter, and M. Procura, Phys. Rev. D **89**, 093024 (2014) arXiv:1404.7134 [hep-ph].
[11] J. Engel, M. J. Ramsey-Musolf, and U. van Kolck, Prog. Part. Nucl. Phys. **71**, 21 (2013) arXiv:1303.2371 [nucl-th].
[12] J. de Vries and Ulf-G. Meißner, Int. J. Mod. Phys. E **25**, 1641008 (2016) arXiv:1509.07331 [hep-ph].
[13] J. de Vries, E. Merighetti, C.-Y. Sung, and A. Walker-Loud, Phys. Lett. B **760**, 254 (2017) arXiv:1612.01567 [hep-lat].
[14] N. Awad, K. K. Sahoo, N. Yoshinaga, T. Sato, K. Asai, and B. P. Das, Eur. Phys. J. A **53**, 54 (2017) arXiv:1703.01570 [hep-ph].
[15] T. P. Cheng and R. F. Dashen, Phys. Rev. Lett. **28**, 594 (1971).
[16] L. S. Brown, W. J. Pardee, and R. D. Peccei, Phys. Rev. D **4**, 2801 (1971).
[17] V. Bernard, N. Kaiser, and Ulf-G. Meißner, Phys. Lett. B **389**, 144 (1996) arXiv:hep-ph/9607245.
[18] T. Becher and H. Leutwyler, JHEP **06**, 017 (2001) arXiv:hep-ph/0103263.
[19] J. Gasser, H. Leutwyler, M. P. Locher, and M. E. Sainio, Phys. Lett. B **213**, 85 (1988).
[20] J. Gasser, H. Leutwyler, and M. E. Sainio, Phys. Lett. B **253**, 252 (1991).
[21] J. Gasser, H. Leutwyler, and M. E. Sainio, Phys. Lett. B **253**, 260 (1991).
[22] R. Koch and E. Pietarinen, Nucl. Phys. A **336**, 331 (1980).
[23] G. Höhler, *Methods and Results of Phenomenological Analyses*, edited by H. Schopper, Landolt-Boernstein - Group I Elementary Particles, Nuclei and Atoms, Vol. 9b2 (Springer-Verlag Berlin, Heidelberg, 1983).
[24] R. A. Arndt, W. J. Briscoe, I. I. Strakovsky, and R. L. Workman, Phys. Rev. C **74**, 045205 (2006) arXiv:nucl-th/0605082.
[25] R. L. Workman, R. A. Arndt, W. J. Briscoe, M. W. Paris, and I. I. Strakovsky, Phys. Rev. C **86**, 035202 (2012) arXiv:1204.2277 [hep-ph].
[26] M. M. Pavan, T. I. Strakovsky, R. L. Workman, and R. A. Arndt, PiN Newslett. **16**, 110 (2002) arXiv:hep-ph/0110066.
[27] N. Fettes and Ulf-G. Meißner, Nucl. Phys. A **676**, 311 (2000) arXiv:hep-ph/0002162.
[28] J. M. Alarcón, J. Martin Camalich, and J. A. Oller, Phys. Rev. D **85**, 051503(R) (2012) arXiv:1110.3797 [hep-ph].
[29] R. Koch, Z. Phys. C **15**, 161 (1982).
[30] T. E. O. Ericson, Phys. Lett. B **195**, 116 (1987).
