Lattice Computation of the Nucleon Scalar Quark Contents at the Physical Point

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We present a QCD calculation of the u, d, and s scalar quark contents of nucleons based on 47 lattice ensembles with $N_f = 2 + 1$ dynamical sea quarks, 5 lattice spacings down to 0.054 fm, lattice sizes up to 6 fm, and pion masses down to 120 MeV. Using the Feynman-Hellmann theorem, we obtain $f_{ud}^N = 0.0405(40)(35)$ and $f_s^N = 0.113(45)(40)$, which translates into $\sigma_{\pi N} = 38(3)(3)$ MeV, $\sigma_{sN} = 105(41)(37)$ MeV, and $y_N = 0.20(8)(8)$ for the sigma terms and the related ratio, where the first errors are statistical and the second errors are systematic. Using isospin relations, we also compute the individual up and down quark contents of the proton and neutron (results in the main text).

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Introduction.—The scalar quark contents of nucleons, N, are important properties of these particles that are conveniently parametrized by the dimensionless ratios,

$$f_{ud}^N = m_{ud}\frac{\langle N|\bar{u}u + \bar{d}d|N\rangle}{2M_N^2} \equiv \frac{\sigma_{\pi N}}{M_N},$$
$$f_q^N = m_q\frac{\langle N|\bar{q}q|N\rangle}{2M_N^2} \equiv \frac{\sigma_{qN}}{M_N}, \quad (1)$$

where N can be either a proton, p, or a neutron, n, at rest, the quark field $q = u$, d, or s and $m_{ud} = (m_u + m_d)/2$ is the average u-d quark mass. We use the relativistic normalization $\langle N(\vec{p}\,')|N(\vec{p})\rangle = 2E_{\vec{p}}(2\pi)^3\delta^{(3)}(\vec{p}\,' - \vec{p})$. With unit normalization, the r.h.s. of Eq (1) would be multiplied by a factor $2M_N$. Note that in the isospin limit, $m_u = m_d$, $f_{ud}^n = f_{ud}^p$ and $f_s^n = f_s^p$ and we will generically call these quantities f_{ud}^N and f_s^N, respectively. Although they cannot directly be accessed in experiment, they are scheme and scale-independent quantities that allow us to translate quark-level couplings into effective, scalar couplings with a nucleon. They are related to a wide variety of observables such as pion and kaon-nucleon scattering amplitudes, quark-mass ratios or quark-mass contributions to nucleon masses. Their knowledge is also very important for dark matter (DM) searches, as they allow us to convert DM-quark couplings into spin-independent, DM-nucleon cross sections.

Early determinations of $\sigma_{\pi N}$ [1–3] were obtained using π-N scattering data. They rely on a difficult extrapolation of the amplitude to the unphysical Cheng-Dashen point, where small $SU(2)$ chiral perturbation theory (χPT) corrections [4–9] can be applied to obtain $\sigma_{\pi N}$. The two results [2,3] differ by nearly two standard deviations and a factor of about 1.4, for reasons discussed in Refs. [8–10]. σ_{sN} is then obtained from $\sigma_{\pi N}$ using results for m_s/m_{ud} and $SU(3)$ χPT [11–13]. Propagating the two determinations of $\sigma_{\pi N}$ leads to a factor of 3 difference in σ_{sN} at the 1.5σ level, which gets squared in DM-nucleon cross sections. This situation has prompted new phenomenological and model studies (some using published lattice results) [8,10,14–19] as well as a number of lattice calculations [20–31] (see Fig. 2). Recent critical reviews of $\sigma_{\pi N}$ can be found in Refs. [9,32].

Here we report on an *ab initio*, lattice QCD calculation, via the Feynman-Hellmann (FH) theorem, of the nucleon scalar quark contents, f_{ud}^N and f_s^N, in the isospin limit. We also compute the four quantities, $f_{u/d}^{p/n}$, to leading order in an expansion in $\delta m = m_d - m_u$, assuming $m_{ud} \sim \delta m$, which is well satisfied in nature. All of our results are accurate up to very small, subleading isospin-breaking corrections. For $f_{u/d}^{p/n}$ this represents a marked improvement over the standard approach [33], which is only accurate up to much larger $SU(3)$-flavor breaking corrections.

Numerical setup.—The data set at the basis of this study consists of 47 ensembles with tree-level-improved Symanzik gauge action and $N_f = 2 + 1$ flavors of clover-improved Wilson quarks, the latter featuring 2 levels

of HEX smearing [34]. The ensembles are made up of approximately 13 000 configurations altogether and, on average, around 40 measurements for each correlator are performed on each configuration. The ensembles are obtained with 5 lattice spacings a (ranging from 0.054 fm to 0.116 fm), lattice sizes up to 6 fm and pion masses, M_π, down to 120 MeV. This setup allows for a consistent control of systematic uncertainties when reaching the physical point (Φ), i.e., when interpolating to physical $m_{ud}^{(\Phi)}$ and $m_s^{(\Phi)}$ and extrapolating to $a \to 0$ and $V \to \infty$.

Methodology.—We use the FH theorem to compute the quark contents via the derivative of the nucleon mass with respect to the quark masses

$$f_{ud}^N = \frac{m_{ud}}{M_N}\frac{\partial M_N}{\partial m_{ud}}\bigg|_\Phi, \qquad f_s^N = \frac{m_s}{M_N}\frac{\partial M_N}{\partial m_s}\bigg|_\Phi, \tag{2}$$

thus avoiding a computation of the 3-point functions required for a direct calculation of the matrix elements.

To determine the individual u and d contents of the proton and neutron, we start from the simple algebraic identity (again, $\delta m = m_d - m_u$)

$$f_{u/d}^p = \left(\frac{1}{2} \mp \frac{\delta m}{4m_{ud}}\right) f_{ud}^p + \left(\frac{1}{4} \mp \frac{m_{ud}}{2\delta m}\right)\frac{\delta m}{2M_p^2}\langle p|\bar{d}d - \bar{u}u|p\rangle. \tag{3}$$

Note that the QCD Hamiltonian can be decomposed as

$$H = H_{\rm iso} + H_{\delta m}, \qquad H_{\delta m} = \frac{\delta m}{2}\int d^3x(\bar{d}d - \bar{u}u), \tag{4}$$

where $H_{\rm iso}$ denotes the full isospin symmetric component, including the m_{ud} term. To leading order in δm, the shift δM_N to the mass of $N = p$ or n, due to the perturbation $H_{\delta m}$, is

$$\delta M_N = \frac{\langle N|H_{\delta m}|N\rangle}{\langle N|N\rangle} = \frac{\delta m}{4M_N}\langle N|\bar{d}d - \bar{u}u|N\rangle. \tag{5}$$

Moreover, in the isospin limit $M_n = M_p$ and $\langle n|\bar{d}d - \bar{u}u|n\rangle = \langle p|\bar{u}u - \bar{d}d|p\rangle$, so that, up to higher-order isospin-breaking corrections, the n-p mass difference is

$$\Delta_{\rm QCD}M_N = 2\delta M_p = \frac{\delta m}{2M_p}\langle p|\bar{u}u - \bar{d}d|p\rangle. \tag{6}$$

Using this relation, introducing the quark-mass ratio $r = m_u/m_d$, and remembering that, in the isospin limit, $f_{ud}^p = f_{ud}^N$, we obtain

$$f_u^{p/n} = \left(\frac{r}{1+r}\right)f_{ud}^N \pm \frac{1}{2}\left(\frac{r}{1-r}\right)\frac{\Delta_{\rm QCD}M_N}{M_N},$$
$$f_d^{p/n} = \left(\frac{1}{1+r}\right)f_{ud}^N \mp \frac{1}{2}\left(\frac{1}{1-r}\right)\frac{\Delta_{\rm QCD}M_N}{M_N}, \tag{7}$$

where the upper sign is for p and the lower one for n and where $M_N = M_n = M_p$ is the nucleon mass in the isospin limit. These equations hold up to very small $O(\delta m^2, m_{ud}\delta m)$ corrections. Analogous expressions were obtained independently in Ref. [35], using $SU(2)$ χPT.

Extracting hadron and quark masses.—Quark and hadron masses are extracted as detailed in Ref. [34], with the quark masses determined using the "ratio-difference method." In addition, to reliably eliminate excited state effects in hadron correlators we have used a procedure similar to that suggested in Ref. [36]. For each of our four hadronic channels, we fit the corresponding correlator $C(t)$ to a single-state ansatz. We use the same minimal start time for our fit interval, $t_{\rm min}$, and the same maximum plateau length, Δt, for all ensembles: $t_{\rm min}$ and Δt are fixed in physical and lattice units, respectively. They are determined by requiring that the distribution of fit qualities over our 47 ensembles be compatible with a uniform distribution to better than 30%, as given by a Kolmogorov-Smirnov (KS) test. An identical procedure is followed to determine the axial Ward identity (AWI) masses.

Computing physical observables.—On each of our 47 ensembles, we extract M_π, M_K, M_N, and M_Ω as well as the light and strange quark masses, m_{ud} and m_s, as explained in the last paragraph. We define $M_{K^\chi}^2 = M_K^2 - M_\pi^2/2$ and work in a massless scheme so the lattice spacings a depend only on the coupling β. These lattice spacings, together with all other quantities, are determined from a global combined fit of the form

$$M_X^{n_X} = [1 + g_X^a(a)][1 + g_X^{\rm FV}(M_\pi, L)](M_X^{(\Phi)})^{n_X} \times (1 + c_X^{a,ud}(a)\tilde{m}_{ud} + c_X^{a,s}(a)\tilde{m}_s + \text{h.o.t.}), \tag{8}$$

for $M_X = (aM_X)/a(\beta)$, with $X = N, \Omega, \pi, K_\chi$, $n_X = 2$ for $X = \pi$ and 1 otherwise and where (aM_X) is the hadron mass in lattice units, as determined on a single ensemble. The quark mass terms, renormalized in the renormalization group invariant (RGI) scheme, are defined as

$$\tilde{m}_q = m_q^{\rm RGI} - m_q^{(\Phi)}, \qquad m_q^{\rm RGI} = \frac{(am_q)}{aZ_S[1 + g_q^a(a)]}, \tag{9}$$

with renormalization constants Z_S from [34]. By h.o.t. we denote higher-order terms in the mass Taylor expansions, and $g_X^a(a)$ parametrizes the continuum extrapolation of $M_X^{(\Phi)}$, while $g_X^{\rm FV}(M_\pi, L)$ parametrizes its finite-volume corrections, according to Refs. [37,38]. The $c_X^{a,q}(a)$, $q = ud, s$, are equal to $c_X^q[1 + g_X^{a,q}(a)]$, where the $g_X^{a,q}(a)$ parametrize the continuum extrapolation of the slope parameters c_X^q. We define the physical point via M_π, M_{K^χ} and M_Ω. Thus, for those quantities, $M_X^{(\Phi)}$ are fixed to 134.8 MeV, 484.9 MeV [39], and 1672.45 MeV [40],

respectively. Moreover, the corresponding discretization terms, $g_X^a(a)$, vanish by definition, leaving only $g_N^a(a)$.

Statistical and systematic uncertainties.—To estimate systematic errors, we follow the extended frequentist method developed in Refs. [36,41]. To account for remnant, excited-state contributions in correlator and AWI mass fits, in addition to the time range $(t_{\min}, \Delta t)$, obtained through the KS test, we consider a more conservative range with $t_{\min}$ increased by 0.1 fm, while keeping Δt fixed. Truncation errors in the m_{ud} Taylor expansion are estimated by pruning the data with two cuts in pion mass, at 320 MeV and 480 MeV. In addition, we consider higher-order terms proportional to $\tilde{m}_{ud}^2$ (or also a χPT-inspired $[(m_{ud}^{\mathrm{RGI}})^{3/2} - (m_{ud}^{(\Phi)})^{3/2}]$ for M_N), $\tilde{m}_{ud}^3$, $\tilde{m}_{ud}\tilde{m}_s$, and $\tilde{m}_{ud}^2\tilde{m}_s$ in Eq. (8). Systematic effects from terms of even higher order, which our results are not accurate enough to resolve, are estimated by replacing the Taylor expansions that include higher-order terms with their inverse, in the spirit of Padé approximants. Regarding cutoff effects, our action formally has leading corrections of $O(\alpha_s a)$, which are often numerically suppressed by HEX smearing, leaving a dominant $O(a^2)$ term [42]. We estimate the uncertainty associated with the continuum extrapolation of the leading $M_N^{(\Phi)}$ term in Eq. (8) by allowing $g_N^a(a)$ to be proportional to either $\alpha_s a$ or a^2. Moreover, so as not to overfit the lattice results, we neglect corrections whose coefficients are larger than 100% except for the ones proportional to $\tilde{m}_{ud}^2$ (or $[(m_{ud}^{\mathrm{RGI}})^{3/2} - (m_{ud}^{(\Phi)})^{3/2}]$) in M_N.

This procedure leads to 192 different analyses, each one providing a result for the observables of interest. Our final results are obtained by weighing these 192 values with Akaike's information criterion (AIC), the AIC-weighed mean and standard deviation corresponding to the central value and systematic error of the given observable, respectively [36]. The statistical error is then the bootstrap error of the AIC-weighed mean. The results were crosschecked by replacing the AIC weight with either a uniform weight or a weight proportional to the quality of each fit. In both cases we obtained consistent values for all of our observables.

The results thus obtained account for uncertainties associated with the continuum extrapolation of the leading $M_N^{(\Phi)}$ term in Eq. (8), but not of the subleading f_{ud}^N or even smaller contribution, f_s^N. Indeed, the discretization terms, $g_N^{a,q}(a)$, were set to zero in the above analyses. To account for those uncertainties, we allow the terms $g_N^{a,q}(a)$ to be proportional to $\alpha_s a$ or a^2. To stabilize the corresponding fits, we fix $M_N^{(\Phi)}$ to its experimental value. Even then, we find that within their statistical errors, our results only support discretization corrections in $c_N^{a,ud}(a)$. Including these, and performing the same variation of 192 analyses as in the procedure described above, we find that the central value of f_{ud}^N increases by 0.0024 and f_s^N decreases by 0.038 compared to our standard analysis. At first sight one may be surprised by the fact that adding discretization terms to f_{ud}^N has a larger effect on f_s^N. However, these terms are small corrections to the ud-mass dependence of M_N in the range of masses considered, but they are of similar size to the s-mass dependence of M_N and interfere with it. We expect the continuum extrapolation error on f_s^N to be much smaller than the variation observed here and therefore consider this variation to be a conservative estimate of continuum extrapolation uncertainties. We take this variation to be our estimate of the uncertainty associated with the continuum extrapolation of the quark contents, add it in quadrature to the systematic error obtained in our standard analysis, and propagate it throughout.

Results and discussion.—The fit qualities in this study are acceptable, with an average $\chi^2/\mathrm{d.o.f.} = 1.4$. Since we do not use the nucleon for scale setting, its physical value constitutes a valuable crosscheck of our procedure. Of course, here we only use the results of our standard analysis, in which this mass is a free parameter. We obtain $M_N = 929(16)(7)$ MeV, which is in excellent agreement with the isospin averaged physical value 938.9 MeV, as obtained by averaging p and n masses from [40]. Typical examples of the dependence of M_N on m_{ud}^{RGI} and m_s^{RGI} are shown in Fig. 1.

The final results for the isospin-symmetric, scalar quark contents are

$$f_{ud}^N = 0.0405(40)(35), \qquad f_s^N = 0.113(45)(40). \tag{10}$$

Here the systematic error includes the continuum extrapolation uncertainty discussed in the preceding section. As a further crosscheck, we have performed an additional, full analysis where we replace, for each lattice spacing, the renormalized quark masses in Eq. (8) by the ratio of the lattice quark masses to their values at the physical mass point. In this analysis, the need for renormalization factors is obviated, because they cancel in the ratios. However, eight additional parameters are required: at each of our five lattice spacings, two parameters are needed to specify the values of the ud and s quark masses corresponding to the physical mass point, while only the two parameters $m_q^{(\Phi)}$, $q = ud, s$, of Eq. (8) are needed for our standard analysis. Nevertheless, the results obtained with this alternative approach are in excellent agreement with the results from our main strategy.

It is straightforward to translate the results of Eq. (10) into σ terms. We obtain $\sigma_{\pi N} = 38(3)(3)$ MeV and $\sigma_{sN} = 105(41)(37)$ MeV. Another quantity of interest in that context is the so-called strangeness content of the nucleon, $y_N = 2\langle N|\bar{s}s|N\rangle/\langle N|\bar{u}u + \bar{d}d|N\rangle$, that we obtain with m_s/m_{ud} determined self-consistently in our calculation. Our result is $y_N = 0.20(8)(8)$.

Now, using Eq. (7), together with the result for f_{ud}^N, the strong isospin splitting of the nucleon mass, $\Delta_{\mathrm{QCD}} M_N = 2.52(17)(24)$ MeV from Ref. [36], and the quark-mass ratio $r = 0.46(2)(2)$ from Ref. [39], we find

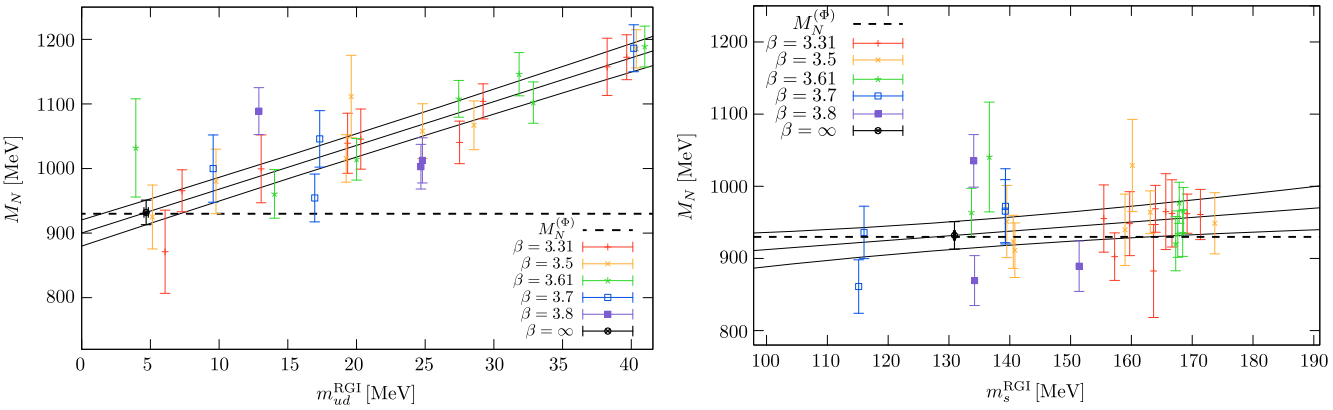

FIG. 1. Typical dependence of M_N on $m_{ud}^{\rm RGI}$ (left panel) and $m_s^{\rm RGI}$ (right panel). The black open circle represents our result for $M_N^{(\Phi)}$ in this particular fit, while the horizontal line corresponds to its experimental value. Dependencies of M_N on variables not shown in these plots have been eliminated using the function obtained in the fit.

$$f_u^p = 0.0139(13)(12), \qquad f_d^p = 0.0253(28)(24),$$
$$f_u^n = 0.0116(13)(11), \qquad f_d^n = 0.0302(28)(25). \qquad (11)$$

Another interesting quantity is $z_N \equiv \langle p|\bar{u}u|p\rangle/\langle p|\bar{d}d|p\rangle = \langle n|\bar{d}d|n\rangle/\langle n|\bar{u}u|n\rangle$, where the last equality holds in the isospin limit. We find it to be $z_N = 1.20(3)(3)$. This is significantly smaller than the value of 2 that one would obtain if the scalar densities $\bar{u}u$ and $\bar{d}d$ were replaced by the number density operators, $\bar{u}\gamma^0 u$ and $\bar{d}\gamma^0 d$.

We compare our results for f_{ud}^N and f_s^N to phenomenological and lattice findings in Fig. 2. Our result for f_{ud}^N points to a rather low value, for instance compared to the recent, precise, phenomenological determination of Ref. [8]. Regarding f_s^N, our value is typically larger than most other lattice results. Note that our error bars are not smaller than those of all previous lattice based calculations. However, unlike previous calculations, ours are performed directly at that physical mass point and do not require uncertain extrapolations to physical m_{ud}, nor do they make use of $SU(3)\,\chi$PT (e.g., in replacing m_s by $M_{K^\chi}^2$ in the definition of f_s^N or in constraining the m_s-dependence of M_N with the m_{ud} and m_s dependence of the baryon octet), whose systematic errors are difficult to estimate. Given this full model independence, our total 13% error on f_{ud}^N is quite satisfactory. Unfortunately, the overall uncertainty on f_s^N is still large, at 53%. The reason for this lies in the small m_s dependence of M_N, as shown in Fig. 1, which is a major drawback of the present approach based on the FH theorem. To try to improve on the precision, the whole analysis has also been carried out by fixing $M_N^{(\Phi)}$ to its experimental value. However, the impact on the central values and error bars is small and therefore we do not retain this approach for our main analysis. To our

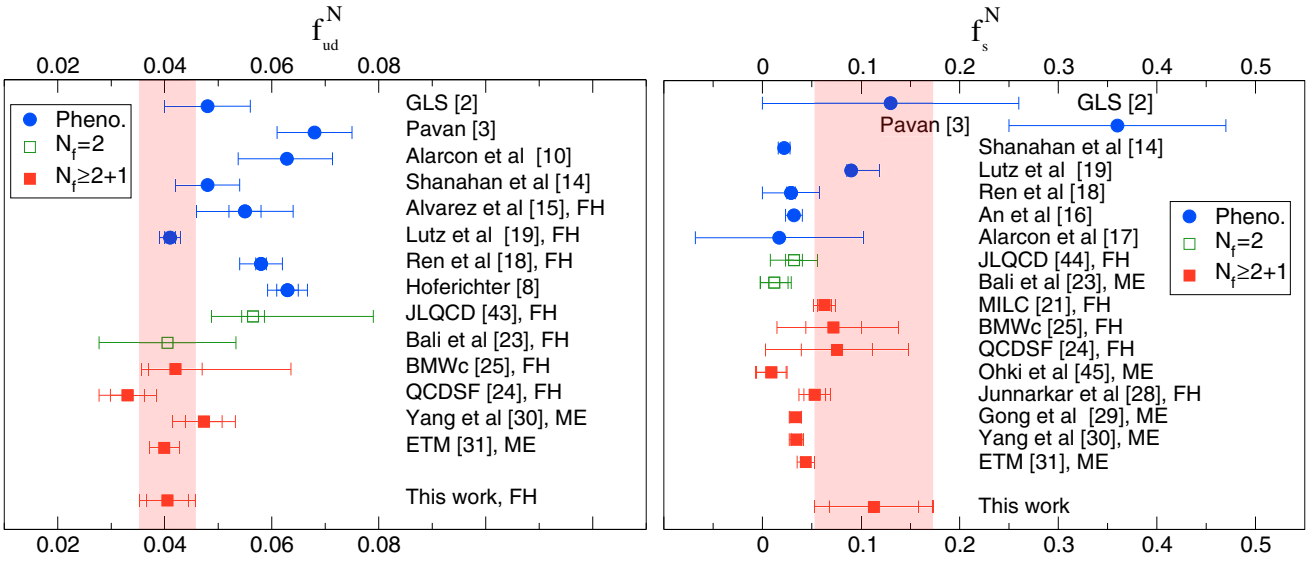

FIG. 2. Comparison of our results for f_{ud}^N (left panel) and for f_s^N (right panel) with values from the literature. Numbers are from Refs. [2,3,10,14,15,19,18,8,43,23,25,24,30,31,29,16,17,21,44,45,28]. For lattice based determinations "FH" denotes studies that use the Feynman-Hellmann theorem while "ME" denotes direct computations of the matrix element.

understanding, in the FH approach the uncertainty on f_s^N can be narrowed only by reducing the statistical error on the data and by increasing the lever arm on m_s.

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