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Chiral Extrapolation of Lattice Moments of Proton Quark Distributions

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We present the resolution of a long-standing discrepancy between the moments of parton distributions calculated from lattice QCD and their experimental values. We propose a simple extrapolation formula for the moments of the nonsinglet quark distribution $u - d$, as a function of quark mass, which embodies the general constraints imposed by the chiral symmetry of QCD. The inclusion of the leading nonanalytic behavior leads to an excellent description of both the lattice data and the experimental values of the moments.

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Although historically, deep-inelastic scattering from the nucleon provided an important test of perturbative QCD, precision measurements of parton distribution functions (PDFs) in these experiments now provide crucial, fundamental information about the nonperturbative structure of the nucleon. Recent discoveries that have had a profound impact on our understanding include the proton spin crisis [1], the Gottfried sum rule violation [2], and to a certain extent the nuclear EMC effect [3]. Future experiments aimed at testing whether $\Delta\bar{u}$ and $\Delta\bar{d}$ are equal or whether $s(x)$ differs from $\bar{s}(x)$ should also serve to deepen our understanding of the nonperturbative origin of parton distributions.

A decade or more of rigorous, nonperturbative calculations of the moments of PDFs in the nucleon within lattice QCD has so far led to a major impasse. The values of the first three nontrivial moments typically lie some 50% above the corresponding experimental data. Since PDF moments are benchmark calculations of hadron structure in lattice QCD, an unresolved discrepancy of this order of magnitude in such fundamental quantities would seriously undermine the credibility of any *ab initio* calculation of hadronic properties, and therefore represents a crucial challenge in hadronic physics. In this Letter we explain for the first time the physics required to resolve this problem. We show that inclusion of the nonanalytic chiral behavior of the moments of $u - d$ as a function of quark mass removes the discrepancy.

At first sight, when one thinks of structure functions in terms of light-cone correlation functions of currents measured at high energy and momentum transfer, it may appear remarkable that spontaneous chiral symmetry breaking and the associated pion cloud could play an essential quantitative role. Indeed, the 50% effects may seem all the more puzzling when chiral corrections to lattice hadron mass calculations are known to be far smaller. However, as discussed below, moments of structure functions correspond to matrix elements of local operators in the hadron ground state. Furthermore, by the familiar variational principle in

quantum mechanics, a first-order error in the wave function yields a first-order error in matrix elements of general operators while producing only a second-order error in the energy, so much larger errors in operators than masses should be expected.

Lattice calculations of parton distributions in Euclidean space-time are based on the operator product expansion—one calculates the matrix elements of certain local operators. The results are directly related to the moments of the measured PDFs:

$$\langle x^n \rangle_q = \int_0^1 dx x^n [q(x, Q^2) + (-1)^{n+1} \bar{q}(x, Q^2)], \quad (1)$$

where the distribution $q(x, Q^2)$ is a function of the Bjorken variable x and the momentum scale Q^2 . The operator product expansion relates the moments $\langle x^n \rangle_q$ to forward nucleon matrix elements of local twist-2 operators, which for nonsinglet distributions are given by $\mathcal{O}_{\{\mu_1, \dots, \mu_n\}} = \bar{\psi} \gamma_{\{\mu_1} \overleftrightarrow{D}_{\mu_2} \dots \overleftrightarrow{D}_{\mu_n\}} \psi$, where ψ is the quark field, D_μ the covariant derivative, and $\{\dots\}$ represents symmetrization of the Lorentz indices. As a result of operator mixing on the lattice, all lattice calculations have so far been restricted to $n \leq 3$. Nevertheless, many features of the PDFs can be reconstructed from just the lowest few moments [4].

Early calculations of structure functions within lattice QCD were performed by Martinelli and Sachrajda [5]. The data used in the present analysis, shown in Fig. 1 for the $n = 1, 2$, and 3 moments of the $u - d$ difference at next-to-leading order (NLO) in the $\overline{\text{MS}}$ (modified minimal subtraction) scheme, are taken from the more recent and extensive calculations by the QCDSF [6–8] and MIT [9] groups. The data include results from quenched simulations at $\beta = 6.0$ for several values of κ , which for a world average lattice spacing of $a = 0.1$ fm correspond to quark masses ranging from 30 to 190 MeV. In addition, we include unquenched data from the MIT group, which has also performed the first full QCD calculations at

$\beta = 5.6$ (corresponding to the same a as for the quenched data with $\beta = 6.0$) using the SESAM configurations [10]. The unquenched results are consistent with the quenched data, indicating that internal quark loops do not appear to play an important role at the quark masses considered. Rather than show the moments versus the scale and renormalization scheme dependent quark mass, we plot the data as a function of the pion mass squared, $m_\pi^2 \propto m_q$. For the $n = 1$ moment we retain only the data corresponding to the statistically most accurately determined operator $\mathcal{O}_{44} - 1/3 \sum_{i=1}^3 \mathcal{O}_{ii}$ [6–9]. To avoid finite volume effects [11], we exclude points at the lowest quark masses from the data sets of Refs. [7] and [9]. The moments correspond to a momentum scale of $Q^2 = 1/a^2 \approx 4 \text{ GeV}^2$.

Note that matrix elements of the operators $\mathcal{O}_{\{\mu_1 \dots \mu_{n+1}\}}$ include both connected and disconnected diagrams, corresponding to operator insertions in quark lines which are connected or disconnected (except through gluon lines) with the nucleon source. Since the evaluation of disconnected diagrams is considerably more difficult numerically, only exploratory studies of these have been completed [12] and the present work will treat only connected diagrams. However, because the disconnected contributions are flavor independent (for equal u and d quark masses), they cancel exactly in the *difference* of u and d moments. Therefore it is appropriate to compare connected contributions to lattice $u - d$ moments with moments of phenomenological PDFs [13].

To compare the lattice results with the experimentally measured moments, one must extrapolate the data from the lowest quark mass used ($\sim 50 \text{ MeV}$) to the physical value ($\sim 5\text{--}6 \text{ MeV}$). Naively one extrapolates to the physical quark mass assuming that the moments depend linearly on the quark mass. However, as shown in Fig. 1 (long-dashed lines), a linear extrapolation of the world lattice data for the $u - d$ moments overestimates the experimental values by some 50% in all cases. This suggests that important physics is still being omitted from the lattice calculations and their extrapolations. It is crucial, if one is to have confidence in lattice calculations of hadronic observables, that the origin of this discrepancy is identified.

Indeed, one knows on very general grounds that a linear extrapolation in $m_q \sim m_\pi^2$ must fail because it omits the crucial nonanalytic structure associated with chiral symmetry breaking. Even at the lowest quark mass accessed on the lattice, the pion mass is over 300 MeV . Earlier studies of chiral extrapolations of lattice data for hadron masses [14], magnetic moments [15], and charge radii [16] have shown that for quark masses above $50\text{--}60 \text{ MeV}$, hadron properties behave very much as one would expect in a constituent quark model, with relatively slow, smooth behavior as a function of the quark mass. However, for $m_q \lesssim 50 \text{ MeV}$ one typically finds the rapid, nonlinear variation expected from the nonanalytic behavior of Goldstone boson loops [17]. The transition occurs when the pion Compton wavelength becomes

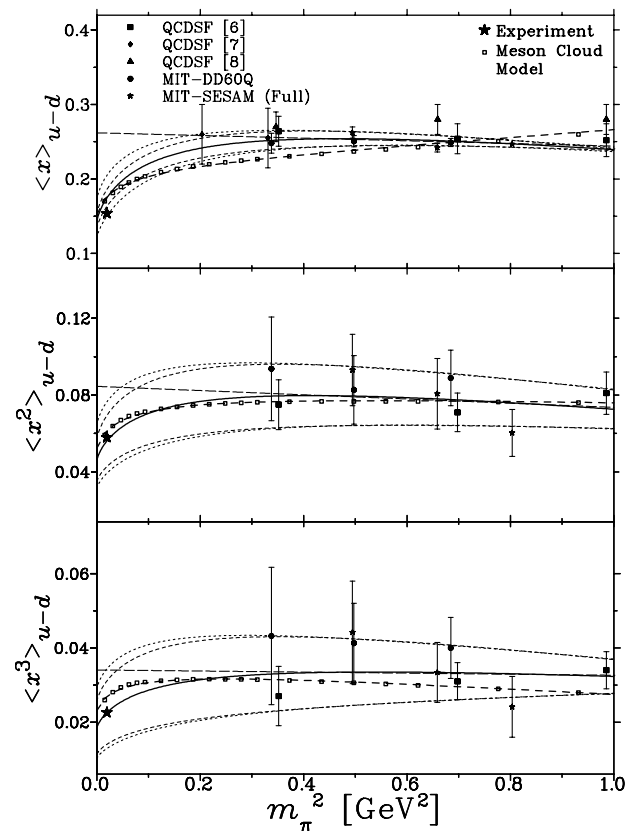


FIG. 1. Moments of the $u - d$ quark distribution. The straight (long-dashed) lines are linear fits to the data, while the curves have the correct LNA behavior in the chiral limit. For each moment, the best fit to the lattice data using Eq. (3) is shown by the solid curve (with $\mu = 550 \text{ MeV}$), while the inner envelope about this represents the statistical errors in the data. The best fit parameters are the following: $a_1 = 0.1427$, $b_1 = -0.0624 \text{ GeV}^{-2}$, $a_2 = 0.0459$, $b_2 = -0.0245 \text{ GeV}^{-2}$, $a_3 = 0.0184$, $b_3 = -0.00666 \text{ GeV}^{-2}$, which give a χ^2 per degree of freedom of 0.98, 0.60, and 0.60 for $n = 1, 2$, and 3 , respectively. The effect of the uncertainty in the parameter μ is illustrated by the outer lower (upper) short-dashed curves, which correspond to $\mu = 450$ (650) MeV . The small squares are the meson cloud model results [24], and the dashed curve through them best fits using Eq. (3). The star represents the phenomenological values taken from NLO fits [13] in the $\overline{\text{MS}}$ scheme.

larger than the pion source, essentially the size of the extended nucleon.

Following the earlier work on chiral extrapolations of physical observables, we expand the moments $\langle x^n \rangle_q$ at small m_π as a series in m_π^2 . Generally the expansion coefficients are (model-dependent) free parameters. On the other hand, the pion cloud of the nucleon gives rise to unique terms whose nonanalyticity in the quark mass arises from the infrared behavior of the chiral loops. Hence they are generally model independent. In fact, the leading nonanalytic (LNA) term for the u and d distributions arising from a one-pion loop behaves as [18]

$$\langle x^n \rangle_q^{\text{LNA}} \sim m_\pi^2 \log m_\pi. \quad (2)$$

Experience with the chiral behavior of masses and magnetic moments shows that the LNA terms alone are not sufficient to describe lattice data for $m_\pi \gtrsim 200$ MeV [14,15], so that extrapolation of lattice data to $m_\pi \sim 0$, through the chiral transition region, requires a formula which is consistent with both the heavy quark and chiral limits of QCD.

In order to fit the lattice data at larger m_π , while preserving the correct chiral behavior of moments as $m_\pi \rightarrow 0$, the moments of $u - d$ are fitted with the form

$$\langle x^n \rangle_{u-d} = a_n + b_n m_\pi^2 + a_n c_{\text{LNA}} m_\pi^2 \ln\left(\frac{m_\pi^2}{m_\pi^2 + \mu^2}\right), \quad (3)$$

where the parameters a_n and b_n are *a priori* undetermined, and the mass μ essentially determines the scale above which Goldstone boson loops no longer yield rapid variation, typically at scales ~ 500 MeV. (In fact, the mass μ corresponds to the upper limit of the momentum integration if one applies a sharp cutoff in the pion loop integral [19].) The coefficient $c_{\text{LNA}} = -(3g_A^2 + 1)/(4\pi f_\pi)^2$ has been calculated in chiral perturbation theory [20]. In the limit $m_\pi \rightarrow 0$ the form in Eq. (3) is therefore the most general expression for moments of the PDFs at $\mathcal{O}(m_\pi^2)$ which is consistent with chiral symmetry. At larger m_π values, where chiral loops are suppressed, the argument of the logarithm in Eq. (3) ensures that the effects of this term are switched off.

Having motivated the functional form of the extrapolation formula, we next apply Eq. (3) to the lattice data from Refs. [6–9]. In principle, Eq. (3) is only strictly applicable to full (unquenched) QCD, and quenched chiral perturbation theory should be used to extrapolate quenched data at small quark masses where the effects of pion and spurious η loops will dominate the m_π dependence. However, at the large quark masses where lattice calculations are currently performed, chiral effects are strongly suppressed and, as shown in Fig. 1, quenched and unquenched results are statistically indistinguishable and have therefore been combined to improve overall statistics.

While the current lattice data are at values of m_π too high to display any deviation from constituent quark behavior, it is not *a priori* obvious why a lowest order form should be able to fit data at $m_\pi \sim 1$ GeV. Hence, it is useful to note that studies based on chiral quark models suggest that Eq. (3) can indeed provide a very good parametrization of the m_π dependence of PDF moments. We illustrate this by taking a simple meson cloud model of the nucleon, based on the MIT bag with pion cloud corrections introduced perturbatively in an expansion in the infinite momentum frame [21] about “bare” nucleon states — analogously to the cloudy bag model (CBM) [22]. Earlier studies of the N and Δ masses [14] and the nucleon magnetic moments [15] established that the CBM gives a good description of the lattice data over a wide range of quark mass. The details of structure function calculations

in the meson cloud model are well known and can be found in the literature [23,24] (see also [25]). Since the model is not our main focus here, we simply show the results for the $n = 1, 2$, and 3 moments (for a bag radius of 0.8 fm and a πNN dipole vertex form factor mass of 1.3 GeV [23,24]). These are denoted in Fig. 1 by the small squares, and the χ^2 fits to these using the form (3) are represented by the dashed curves through them. Clearly, Eq. (3) provides an excellent fit to model data, which are also in qualitative agreement with the calculated lattice moments. These results give us confidence that a fit to the lattice data based on Eq. (3) should be reasonable.

The results of the best χ^2 fit to the lattice data for each moment are given by the central solid lines in Fig. 1. The inner envelopes around these curves represent fits to the extrema of the error bars. For the central curves, the value of the mass parameter μ that is most consistent with all experimental moments is $\mu = 550$ MeV. This value of μ is comparable to the scale at which the behavior found in other observables, such as magnetic moments and masses, switches from smooth and constituent quarklike (slowly varying with respect to the current quark mass) to rapidly varying and dominated by Goldstone boson loops. The similarity of these scales for the various observables simply reflects the common scale at which the Compton wavelength of the pion becomes comparable to the size of the hadron (without its pion cloud). We also note that this is similar to the scale predicted by the χ^2 fits to the meson cloud model in Fig. 1.

At present, all of the lattice data are in a region where the moments show little variation with m_π^2 . This, together with the relatively large errors, means that one cannot distinguish between a linear extrapolation and one that includes the correct chiral behavior, as Fig. 1 illustrates. Consequently, it is not possible to determine μ from the current lattice data. In fact, with the current errors it is possible to consistently fit both the lattice data and the experimental values with μ ranging from ~ 400 to 700 MeV. The dependence on μ is illustrated in Fig. 1 by the difference between the inner and outer envelopes on the fits. The former are the best fits to the lower (upper) limits of the error bars, while the latter use $\mu = 450$ (650) MeV instead of the central value of $\mu = 550$ MeV. Data at smaller quark masses are therefore crucial to constrain this parameter and guide an accurate extrapolation.

These results have significant implications for lattice calculations. Unlike heavy quark systems, where it may be acceptable to work in a reasonably small volume, calculations of the nucleon require an accurate representation of the pion cloud. Hence the volume must be sufficiently large that the pion Compton wavelength of a reasonably light pion fits well within the volume. Even though one need not calculate at the physical pion mass, the pion must be light enough that the parameters of a systematic chiral extrapolation are well determined statistically. Specifically, from Fig. 1 it is clear that 5% measurements

down to $m_\pi^2 = 0.05 \text{ GeV}^2$ [requiring a spatial volume of order $(4.3 \text{ fm})^3$] would provide data for an accurate chiral extrapolation. This will require Terascale calculations [26], first in the quenched approximation with chiral fermions and eventually in full QCD, which is necessary to produce the full pion cloud and the correct chiral behavior embodied in the leading nonanalytic structure. While this is demanding, with the hybrid Monte Carlo algorithm of Ref. [27] requiring 8 Teraflops-years for full QCD, since the total computational cost of this algorithm varies as $m_\pi^{-7.25}$, we note that this is still a factor of 26 less than that necessary for a brute force evaluation at the physical quark mass. Indeed, the discovery reported here brings reliable calculations of hadronic properties within the capability of the next generation of computers that will be available in the next 2–3 years.

In summary, we have investigated the quark mass dependence of moments of quark distribution functions, with emphasis on both the physics in the chiral limit and the scale at which the pion Compton wavelength corresponds to the intrinsic size of the nucleon. We proposed a low order formula for the m_π dependence of moments, which embodies the leading nonanalytic behavior expected from the chiral properties of QCD, and used it to extrapolate the available lattice data to the physical region. The applicability of a low order expansion for the lattice data is also supported by phenomenological chiral quark model studies. Compared with linear extrapolations, which drastically overestimate the experimental values, we find that within the current errors there is no evidence of a discrepancy between the lattice data and experiment once the correct dependence on quark mass near the chiral limit is incorporated. This observation resolves an important long-standing problem with *ab initio* calculations of hadron structure in QCD which has persisted for more than a decade. It not only removes a serious threat to the credibility of current lattice calculations, but also provides the foundation for quantitative calculation of hadron observables with the next generation of Terascale computers.

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