ADP-01-07/T442
JLAB-THY-01-09
CTP-3092

Chiral Extrapolation of Lattice Moments of Proton Quark Distributions

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Abstract

The behavior of the first three nontrivial moments of the nonsinglet quark distribution $u - d$ in the proton is studied as a function of quark mass in order to guide the extrapolation of lattice QCD calculations to the physical region. We propose a simple extrapolation formula, embodying the general constraints of the chiral symmetry of QCD, which provides an excellent fit to the lattice data and the experimental values for each moment.

The measurement of parton distributions has had a deep impact on our understanding of the nonperturbative structure of hadrons. Crucial discoveries have included the proton spin crisis [1], the SU(2) flavor symmetry violation of the proton sea [2], and to a certain extent the nuclear EMC effect [3]. The possibility that $\Delta\bar{u}$ may not be equal to $\Delta\bar{d}$ or that s may differ from $\bar{s}$ will also be tested in future experiments, which will lead to still deeper understanding of the nonperturbative origin of parton distributions.

There are numerous studies of such nonperturbative phenomena within QCD-motivated quark models, and even some important model independent results [4]. However, ultimately one must calculate these phenomena directly from QCD itself, and lattice field theory is the only quantitative tool currently available. Naive extrapolation of existing lattice data to physical quark masses shows a systematic discrepancy of more than 30% between the low moments of quark distributions and experiment. In this Letter we present results of a new analysis of lattice QCD data on the first three nontrivial moments of the nonsinglet parton distribution $u-d$ based on a consistent chiral extrapolation of the moments to the physical region, which for the first time resolves the discrepancy.

Since lattice QCD is formulated in Euclidean space, it is not possible to calculate parton distribution functions (PDFs), defined as light-cone correlation functions, directly on the lattice. Using the operator product expansion, however, one can calculate the *moments* of the PDFs, defined as:

$$\langle x^n \rangle_q = \int_0^1 dx\ x^n\ \left(q(x,Q^2) + (-1)^{n+1} \bar{q}(x,Q^2) \right)\ , \tag{1}$$

where the distribution $q(x,Q^2)$ is a function of the Bjorken scaling 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 $\mathcal{O}_{\{\mu_1 \cdots \mu_{n+1}\}} = \overline{\psi}\ \gamma_{\{\mu_1}\ \overleftrightarrow{D}_{\mu_2}\ \ldots\ \overleftrightarrow{D}_{\mu_{n+1}\}}\ \psi$, where ψ is the quark field, D_μ the covariant derivative and $\{\ldots\}$ represents symmetrization of the Lorentz indices.

The discretization of space-time on the lattice means that lattice versions of the operators $\mathcal{O}_{\{\mu_1 \cdots \mu_{n+1}\}}$ transform according to the hypercubic subgroup, H(4), of the rotational group O(4). Operators irreducible with respect to O(4) decompose, however, into several irreducible representations of H(4), and for $n > 3$ the required lattice operators mix with lower spin operators. As a result 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 [5].

Early calculations of structure functions within lattice QCD were performed by Martinelli and Sachrajda [6]. The data used in this analysis, shown in Fig. 1 for the $n = 1$, 2 and 3 moments of the $u-d$ difference in the $\overline{\rm MS}$ scheme, are taken from the more recent analyses by the QCDSF [7–9] and MIT [10] groups[1]. 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

[1]A jackknife error analysis of the MIT data for the $u-d$ difference was performed to take into account correlations between errors on the individual u and d moments. This may, however, unduly underweight the QCDSF data.

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 [11]. Quite interestingly, these 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 better determined operator $\mathcal{O}_{44} - 1/3 \sum_{i=1}^{3} \mathcal{O}_{ii}$ [7–10]. To avoid finite volume effects [12], we exclude points at the lowest quark masses from the data sets of Refs. [8] and [10]. The moments correspond to a momentum scale of $Q^2 = 1/a^2 \approx 4$ GeV^2.

Note that matrix elements of the operators $\mathcal{O}_{\{\mu_1 \cdots \mu_{n+1}\}}$ 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 evaluation of disconnected diagrams is considerably more difficult numerically, only exploratory studies of these have been completed [13] 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 in the *difference* of u and d moments. Therefore it is valid to compare connected contributions to lattice $u - d$ moments with moments of phenomenological PDFs [14].

To compare the lattice results with the experimentally measured moments, one must extrapolate the data from the lowest quark mass used (~ 50 MeV) to the physical value ($\sim$ 5–6 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 more than 30% in all cases. This suggests that important physics is still being omitted from the lattice calculations and their extrapolations.

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 [15], magnetic moments [16] and charge radii [17] have shown that for quark masses above 50–60 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 $m_q \lesssim 50$ MeV one typically finds the rapid, non-linear variation expected from the nonanalytic behavior of Goldstone boson loops [18]. The transition occurs when the pion Compton wavelength becomes 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 infra-red 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 [4]:

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

Contributions from a Δ isobar in the intermediate state also enter at this order [4], but because of the N–Δ mass difference these are generally less important. Next-to-leading nonanalytic terms in the moment expansion are of order m_π^3 or higher. Contributions from the coupling to the pion give rise to LNA terms for the n-th moment which are higher order in m_π^2, namely $\sim m_\pi^{n+3} \log m_\pi$ for odd n and $\sim m_\pi^{n+2} \log m_\pi$ for even n [4]. The coupling to a nucleon which is not dressed by a pion cloud (a 'bare' nucleon) does not give rise to nonanalytic terms. This contribution is, however, important at large m_π, where the effects of pion loops are suppressed, and the moments depend linearly on the quark mass. 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 [15,16], 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 $m_\pi \to 0$, the moments of $u - d$ are fitted with the form:

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

where the coefficient $c_{\rm LNA} = -4g_A^2/(4\pi f_\pi)^2$, and g_A and f_π are understood to be evaluated in the chiral limit. 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 cut-off in the pion loop integral.) In contrast to other quantities, such as masses, magnetic moments or charge radii, the overall coefficient of the LNA term in Eq.(3) contains the model-dependent factor, a_n. This arises from the convolution-like diagram [4,19], in which the moments of the 'bare' nucleon distribution, to which the current couples, are multiplied by moments of the pion distribution in the nucleon. Note however, that the form of the extrapolation formula in Eq.(3), and in particular the presence of the LNA term $m_\pi^2 \ln m_\pi$, *does not* itself rely on the convolution approximation. Multi-meson loops and other non-convolution contributions implicit in a full lattice calculation cannot produce the LNA behavior in Eq.(2) and will in general give rise to higher order corrections [20] — the *only* source of the LNA structure is the coupling to a nucleon dressed by a one pion loop. Therefore in the limit $m_\pi \to 0$ the form in Eq.(3) is 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. [7–10]. One potential concern that could be raised at this point is whether Eq.(3), which is derived from full (unquenched) QCD, can be used to extrapolate quenched QCD data. While this issue will be relevant at small quark masses, where the effects of pion loops will dominate the m_π dependence, at the presently large quark masses where lattice calculations are performed the effects of pion loops are suppressed. In consequence, one does not expect large differences between quenched and full QCD. The unquenched lattice data shown in Fig. 1 indeed confirm this.

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. On the other hand, studies based on chiral quark models suggest that Eq.(3) can indeed provide a very good parameterization of the m_π dependence of PDF moments. We illustrate this by taking a simple and phenomenologically successful model of the nucleon based on the MIT bag with pion cloud corrections introduced perturbatively in an expansion about 'bare' nucleon states — essentially the cloudy bag model (CBM) [21]. The feature of the model germane to the chiral extrapolation of lattice data is that it is consistent with the chiral properties of QCD, and in particular that it reproduces the LNA behavior of chiral perturbation theory [17,18]. Earlier studies of the N and Δ masses [15] and the nucleon magnetic moments [16] also showed that the CBM gave a good description of the lattice data over a wide range of quark mass.

The details of structure function calculations in the CBM are well known and can be found in the literature [22,23] (see also [20]). 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 [19,23]). 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 the CBM 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 (for parameters a_n and b_n) 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. The value of μ required here is similar to the scale at which the behavior found in other observables, such as magnetic moments and masses, switches from smooth and constituent quark-like (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 CBM in Fig. 1.

At present all of the lattice data are in a region where the moments vary smoothly with m_π^2 — essentially linearly. 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 MeV 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 perform an accurate extrapolation.

In summary, we have investigated the quark mass dependence of moments of quark distribution functions, paying particular attention to the behavior of moments in the chiral limit. 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 generally 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.

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 $m_\pi^2 = 0.05$ GeV^2 (requiring a spatial volume of order $(4.3\ \mathrm{fm})^3$) would provide data for an accurate chiral extrapolation. This will require Terascale calculations [24], 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.

ACKNOWLEDGMENTS

We would like to thank C. Boros, D. Dolgov, R. Edwards, R. Horsley, C. Michaels and D. Richards for helpful discussions and communications. This work was supported by the Australian Research Council, the U.S. Department of Energy contract DE-AC05-84ER40150, under which the Southeastern Universities Research Association (SURA) operates the Thomas Jefferson National Accelerator Facility (Jefferson Lab), and cooperative research agreement DE-FC02-94ER40818.

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FIGURES

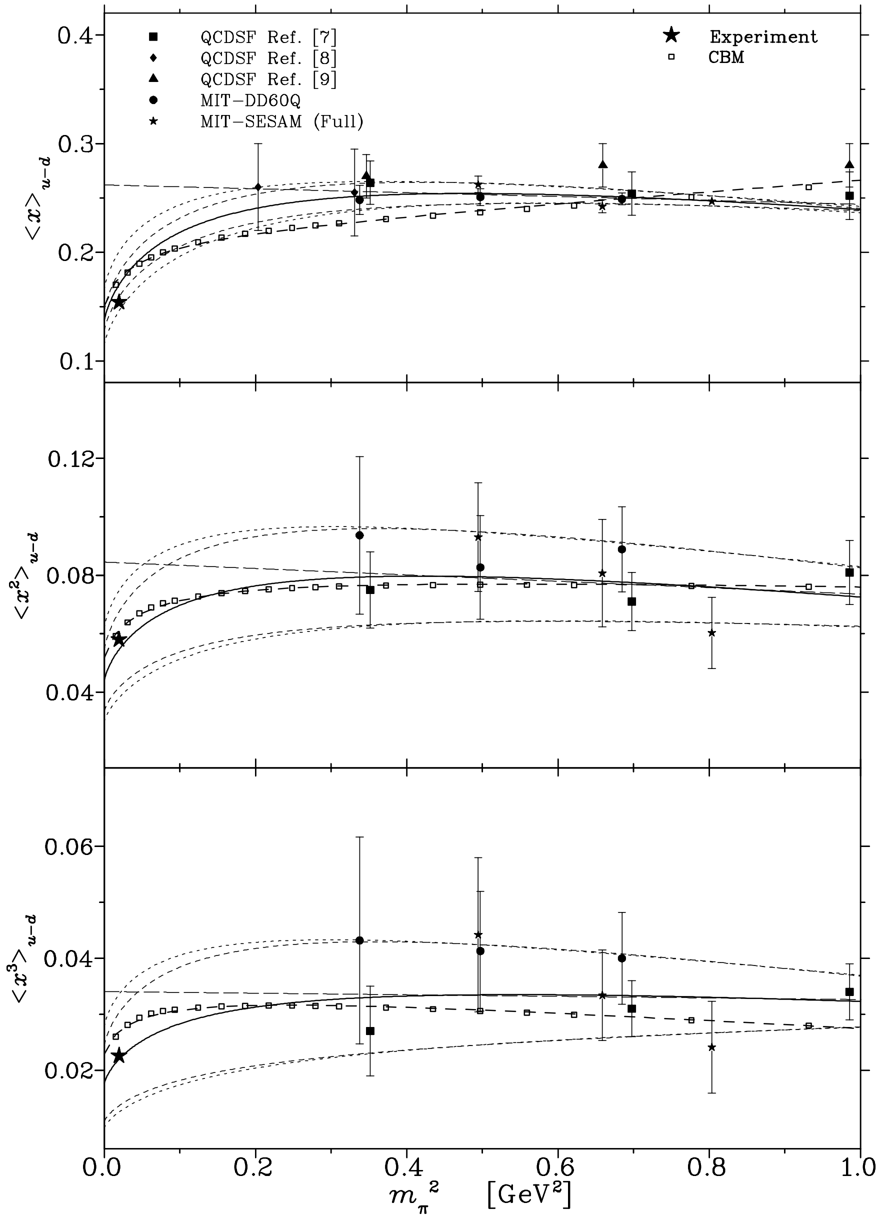

FIG. 1. Moments of the $u-d$ quark distribution. The straight (long-dashed) lines are linear fits to the data, while the curves have the correct LNA behavior in the chiral limit. For each moment, the best fit to the lattice data using Eq.(3) is shown by the solid curve (with $\mu = 550$ MeV), while the inner envelope about this represents the statistical errors in the data. The best fit parameters are: $a_1 = 0.1364$, $b_1 = -0.0648\,\mathrm{GeV}^{-2}$, $a_2 = 0.0438$, $b_2 = -0.0252\,\mathrm{GeV}^{-2}$, $a_3 = 0.0176$, $b_3 = -0.00693\,\mathrm{GeV}^{-2}$, which give a χ^2 per degree of freedom of 0.9, 0.5 and 0.5 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 CBM results, and the dashed curve through them best fits using Eq.(3). The star represents the phenomenological values taken from NLO fits [14] in the $\overline{\mathrm{MS}}$ scheme.