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Charge Symmetry Breaking in Parton Distribution Functions from Lattice QCD

R. Horsley,[1] Y. Nakamura,[2,3] D. Pleiter,[4] P.E.L. Rakow,[5] G. Schierholz,[6]
H. Stüben,[7] A.W. Thomas,[8] F. Winter,[1,2] R.D. Young,[8] and J.M. Zanotti[1]
(CSSM and QCDSF/UKQCD Collaborations)

[1] *School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, UK*
[2] *Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany*
[3] *Center for Computational Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan*
[4] *Deutsches Elektronen-Synchrotron DESY, 15738 Zeuthen, Germany*
[5] *Theoretical Physics Division, Department of Mathematical Sciences, University of Liverpool, Liverpool L69 3BX, UK*
[6] *Deutsches Elektronen-Synchrotron DESY, 22603 Hamburg, Germany*
[7] *Konrad-Zuse-Zentrum für Informationstechnik Berlin, 14195 Berlin, Germany*
[8] *CSSM, School of Physics and Chemistry, University of Adelaide, Adelaide SA 5005, Australia*

By determining the quark momentum fractions of the octet baryons from $N_f = 2 + 1$ lattice simulations, we are able to predict the degree of charge symmetry violation in the parton distribution functions of the nucleon. This is of importance, not only as a probe of our understanding of the non-perturbative structure of the proton but also because such a violation constrains the accuracy of global fits to parton distribution functions and hence the accuracy with which, for example, cross sections at the LHC can be predicted. A violation of charge symmetry may also be critical in cases where symmetries are used to guide the search for physics beyond the Standard Model.

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Charge symmetry is related to the invariance of the QCD Hamiltonian under rotations about the 2-axis in isospace, turning u quarks to d and protons to neutrons. Extensive studies in nuclear systems have shown that it is an excellent symmetry [1], typically accurate to a fraction of a percent (e.g. $m_n - m_p \sim 0.1\%$). At the quark level it is, of course, very badly broken but this is hidden by dynamical chiral symmetry breaking. There has been extensive theoretical work on the effect of the $u - d$ mass difference on parton distribution functions (PDFs), where charge symmetry (CS) implies [2, 3]:

$$u^p(x, Q^2) = d^n(x, Q^2), \quad d^p(x, Q^2) = u^n(x, Q^2) \; . \quad (1)$$

Within the MIT bag model, Sather [4] and Rodionov *et al.* [5] found that charge symmetry violation (CSV) in the singly represented valence sector, $\delta d(x) \equiv d^p(x) - u^n(x)$, could be as large as 5% in the intermediate to large range of Bjorken x. Furthermore, these authors also found that $\delta u(x) \equiv u^p(x) - d^n(x)$ was similar in magnitude but of opposite sign.

Only recently has a global analysis of PDFs allowed for CSV, with Martin *et al.* [6] finding a best fit that is remarkably close to the predictions of Ref. [5] for both the magnitude and shape of $\delta d(x)$ and $\delta u(x)$. Unfortunately, the errors on their result are currently too large to be of phenomenological use but at the larger end CSV could lead to considerable uncertainties in the predictions for some processes of interest at the LHC. The need for urgency in obtaining better constraints on CSV in PDFs has recently become apparent in connection with the search for physics beyond the Standard Model using neutrino deep-inelastic scattering. Indeed, the level of CSV predicted in Refs. [4, 5] would reduce the 3σ discrepancy with the Standard Model reported by the NuTeV collaboration [7] by at least one standard deviation [8, 9]. It was argued by Londergan and Thomas that for the second moments, which are relevant to the NuTeV measurement, namely $\langle x\delta d^-(x)\rangle$ and $\langle x\delta u^-(x)\rangle$ (where the superscript minus indicates a C-odd or valence distribution function), the results had very little model dependence [10]. Further, future planned new-physics searches will benefit from improved constraints on CSV, such as the parity-violating deep inelastic scattering program at Jefferson Lab [11].

In this Letter we report the first lattice QCD determination of the CSV arising from the $u - d$ mass difference. Our results are deduced by studying the second moments of the parton distribution functions as we vary the light (degenerate u, d) and strange quark masses in a $N_f = 2 + 1$ lattice simulation. The sign and magnitude of the effect which we find are consistent both with the estimates based on the MIT bag model [10] and with the best fit global determination of Ref. [6]. However, the uncertainties in this work are considerably smaller than those derived from the global analysis.

Because of valence quark normalisation, the first moments of $\delta u^-(x)$ and $\delta d^-(x)$ must vanish. Hence the second moment (which we label δq^-) is the first place where CSV can be visible in the valence quark distributions,

$$\delta u^- = \int_0^1 dx\, x(u^{p-}(x) - d^{n-}(x)) = \langle x\rangle^p_{u^-} - \langle x\rangle^n_{d^-} \; , \quad (2)$$

$$\delta d^- = \int_0^1 dx\, x(d^{p-}(x) - u^{n-}(x)) = \langle x\rangle^p_{d^-} - \langle x\rangle^n_{u^-} \; . \quad (3)$$

κ_l	κ_s	m_π [MeV]	m_K [MeV]	$\langle x\rangle_u^\Sigma/\langle x\rangle_u^p$	$\langle x\rangle_s^\Sigma/\langle x\rangle_d^p$	$\langle x\rangle_s^\Xi/\langle x\rangle_u^p$	$\langle x\rangle_u^\Xi/\langle x\rangle_d^p$
0.12083	0.12104	460(17)	401(15)	1.0263(51)	0.960(12)	0.993(23)	1.044(28)
0.12090	0.12090	423(15)	423(15)	1.0	1.0	1.0	1.0
0.12095	0.12080	395(14)	438(16)	0.9888(44)	1.0344(70)	1.010(25)	0.985(24)
0.12100	0.12070	360(13)	451(16)	0.9670(83)	1.059(14)	1.019(26)	0.953(29)
0.12104	0.12062	334(12)	463(17)	0.9631(94)	1.082(18)	1.037(29)	0.940(30)

TABLE I. Pion and kaon masses on $24^3 \times 48$ lattices with lattice spacing, $a = 0.083(3)$fm [12], where the error on the lattice spacing has been included in the errors for m_π and m_K. The last four columns contain our results for ratios of the hyperon quark momentum fractions.

As detailed below, these CSV momentum fractions are related to the hyperon moments by

$$\delta u^- \sim \langle x\rangle_{u^-}^\Sigma - \langle x\rangle_{s^-}^\Xi \tag{4}$$

$$\delta d^- \sim \langle x\rangle_{s^-}^\Sigma - \langle x\rangle_{u^-}^\Xi \ , \tag{5}$$

in the limit where the strange and light quarks have almost equal mass.

In the numerical calculation of these moments, our gauge field configurations have been generated with $N_f = 2+1$ flavours of dynamical fermions, using the Symanzik improved gluon action and nonperturbatively $\mathcal{O}(a)$ improved Wilson fermions [13]. The quark masses are chosen by first finding the $\mathrm{SU}(3)_{\mathrm{flavour}}$-symmetric point where flavour singlet quantities take on their physical values and then varying the individual quark masses while keeping the singlet quark mass $\overline{m}_q = (m_u+m_d+m_s)/3 = (2m_l + m_s)/3$ constant [12]. Simulations are performed on lattice volumes of $24^3 \times 48$ with lattice spacing, $a = 0.083(3)$fm. A summary of our dynamical configurations is given in Table I. More details regarding the tuning of our simulation parameters can be found in Ref. [12].

On the lattice, we compute moments of the quark distribution functions, $q(x)$

$$\langle x^{n-1}\rangle_q^B = \int_0^1 dx\, x^{n-1}(q^B(x) + (-1)^n \bar{q}^B(x)) \ , \tag{6}$$

where x is the fraction of the momentum of baryon B carried by the quarks, by calculating the matrix elements of local twist-2 operators

$$\langle B(\vec{p})|\left[\mathcal{O}_q^{\{\mu_1\cdots\mu_n\}} - \mathrm{Tr}\right]|B(\vec{p})\rangle = 2\langle x^{n-1}\rangle_q^B [p^{\mu_1}\cdots p^{\mu_n} - \mathrm{Tr}] \ , \tag{7}$$

where $\mathcal{O}_q^{\mu_1\cdots\mu_n} = i^{n-1}\bar{q}\gamma^{\mu_1}\overleftrightarrow{D}^{\mu_2}\cdots\overleftrightarrow{D}^{\mu_n} q$.

In this paper we consider only the quark-line connected contributions to the second ($n = 2$) moment, $\langle x\rangle_q$, which means we only include the part of $\bar{q}^B$ coming from quark-line connected backward moving quarks, the so-called Z-graphs. While the contributions from disconnected insertions are expected to be small, in the following analysis we will focus on differences of baryons and so these contributions will cancel in the $\mathrm{SU}(3)_{\mathrm{flavour}}$ limit and should be negligible for small expansions around this limit, as considered here.

We use the standard local operator $\mathcal{O}_q^{\langle x\rangle} = \mathcal{O}_q^{44} - 1/3(\mathcal{O}_q^{11} + \mathcal{O}_q^{22} + \mathcal{O}_q^{33})$. The matrix element in Eq. (7) is obtained on the lattice by considering the ratio:

$$R(t,\tau,\vec{p}) = \frac{C_{3\mathrm{pt}}(t,\tau,\vec{p})}{C_{2\mathrm{pt}}(t,\vec{p})} = -\frac{E_{\vec{p}}^2 + \frac{1}{3}\vec{p}^{\,2}}{E_{\vec{p}}}\langle x\rangle \ , \tag{8}$$

where $C_{2\mathrm{pt}}$ and $C_{3\mathrm{pt}}$ are lattice two and three-point functions, respectively, with total momentum, $\vec{p}$, (in our simulation we consider only $\vec{p} = 0$). The operator $\mathcal{O}_q^{\langle x\rangle}$ is inserted into the three-point function, $C_{3\mathrm{pt}}(t,\tau,\vec{p})$ at time, τ, between the baryon source located at time, $t = 0$, and sink at time, t.

The operators used for determining the quark momentum fractions need to be renormalised, preferably using a nonperturbative method such as RI′-MOM [14–16]. Here, however, we will only present results for ratios of quark momentum fractions so that the renormalisation constants cancel and hence our results are scale and scheme independent. In Fig. 1 we present results for the ratio of the $u(s)$-quark momentum fraction of the $\Sigma(\Xi)$ baryon to the momentum fraction of the u in the proton. They are also given in Table I, as a function of m_π^2, normalised with the centre-of-mass of the pseudoscalar meson octet, $X_\pi = \sqrt{(2m_K^2 + m_\pi^2)/3} = 411$ MeV. Here we see the strong effect of the decrease (increase) in the light (strange) quark momentum fractions as we approach the physical point. In particular, we see that the heavier strange quark in the Ξ^0 carries a larger momentum fraction than the up quark in the proton. We also notice that the up quark in the Σ^+ has a smaller momentum fraction than the up quark in the proton. This is a purely environmental effect since the only difference between these two measurements is the mass of the spectator quark (s in Σ^+, d in p). This implies that the momentum fraction of the strange quark in the Σ should be larger than that of the down quark in the proton, which is exactly what we see in Fig. 2.

To infer the level of CSV relevant to the nucleon, we only need to consider a small expansion about the $\mathrm{SU}(3)_{\mathrm{flavour}}$ symmetric point, for which linear flavour expansions prove to work extremely well [12]. For instance, we can write

$$\delta u = m_\delta \left(-\frac{\partial\langle x\rangle_u^p}{\partial m_u} + \frac{\partial\langle x\rangle_u^p}{\partial m_d}\right) + \mathcal{O}(m_\delta^2) \, , \tag{9}$$

where $m_\delta \equiv (m_d - m_u)$ and we have already made use of charge symmetry by equating $\partial\langle x\rangle_d^n/\partial m_d = \partial\langle x\rangle_u^p/\partial m_u$

FIG. 1. Ratio of doubly represented quark momentum fractions, $\langle x\rangle_u^\Sigma/\langle x\rangle_u^p$ and $\langle x\rangle_s^\Xi/\langle x\rangle_u^p$ as a function of m_π^2/X_π^2, where we have determined X_π from the masses in Tab. I.

FIG. 2. Ratio of singly represented quark momentum fractions, $\langle x\rangle_s^\Sigma/\langle x\rangle_d^p$ and $\langle x\rangle_u^\Xi/\langle x\rangle_d^p$ as a function of m_π^2/X_π^2, where we have determined X_π from the masses in Tab. I.

and $\partial\langle x\rangle_d^n/\partial m_u = \partial\langle x\rangle_u^p/\partial m_d$. A similar expression holds for δd.

Near the $\mathrm{SU}(3)_{\mathrm{flavour}}$ symmetric point, we note that the up quark in the proton is equivalent to an up quark in a Σ^+ or a strange quark in a Ξ^0, which we describe collectively as the "doubly-represented" quark [17].

The local derivatives required for δu can be obtained by varying the masses of the up and down quarks independently. Within the present calculation, we note that the difference $\langle x\rangle_s^\Xi - \langle x\rangle_u^p$ measures precisely the variation of the doubly-represented quark matrix element with respect to the doubly-represented quark mass (while holding the singly-represented quark mass fixed). Similar variations allow us to evaluate the other required derivatives, where we write

$$\frac{\partial\langle x\rangle_u^p}{\partial m_u} \simeq \frac{\langle x\rangle_s^{\Xi^0} - \langle x\rangle_u^p}{m_s - m_l}\,,\ \frac{\partial\langle x\rangle_u^p}{\partial m_d} \simeq \frac{\langle x\rangle_u^{\Sigma^+} - \langle x\rangle_u^p}{m_s - m_l}\,, \quad (10)$$

$$\frac{\partial\langle x\rangle_d^p}{\partial m_u} \simeq \frac{\langle x\rangle_u^{\Xi^0} - \langle x\rangle_d^p}{m_s - m_l}\,,\ \frac{\partial\langle x\rangle_d^p}{\partial m_d} \simeq \frac{\langle x\rangle_s^{\Sigma^+} - \langle x\rangle_d^p}{m_s - m_l}\,. \quad (11)$$

With these expressions and Eq. (9), we obtain the relevant combinations for our determination of CSV in the nucleon

$$\delta u = m_\delta \frac{\langle x\rangle_u^{\Sigma^+} - \langle x\rangle_s^{\Xi^0}}{m_s - m_l}\,,\ \delta d = m_\delta \frac{\langle x\rangle_s^{\Sigma^+} - \langle x\rangle_u^{\Xi^0}}{m_s - m_l}\,. \quad (12)$$

By invoking the Gell-Mann–Oakes–Renner relation and normalising to the total nucleon isovector quark momentum fraction, we write

$$\frac{\delta u}{\langle x\rangle_{u-d}^p} = \frac{m_\delta}{\overline{m}_q} \frac{(\langle x\rangle_u^{\Sigma^+} - \langle x\rangle_s^{\Xi^0})/\langle x\rangle_{u-d}^p}{(m_K^2 - m_\pi^2)/X_\pi^2}\,, \quad (13)$$

$$\frac{\delta d}{\langle x\rangle_{u-d}^p} = \frac{m_\delta}{\overline{m}_q} \frac{(\langle x\rangle_s^{\Sigma^+} - \langle x\rangle_u^{\Xi^0})/\langle x\rangle_{u-d}^p}{(m_K^2 - m_\pi^2)/X_\pi^2}\,. \quad (14)$$

Written in this way, the fractional CSV terms are just the slopes of the curves shown in Fig. 3 (evaluated at the symmetry point) multiplied by the ratio $m_\delta/\overline{m}_q$. By fitting the slopes, we obtain

$$\frac{\delta u}{\langle x\rangle_{u-d}^p} = \frac{m_\delta}{\overline{m}_q}(-0.221 \pm 0.054) \quad (15)$$

$$\frac{\delta d}{\langle x\rangle_{u-d}^p} = \frac{m_\delta}{\overline{m}_q}(0.195 \pm 0.025) \quad (16)$$

Chiral perturbation theory yields the quark mass ratio $m_\delta/\overline{m}_q = 0.066(7)$ [18] and the isovector momentum fraction is experimentally determined to be $\langle x\rangle_{u-d}^p \simeq 0.158$ at $4\,\mathrm{GeV}^2$. Substituting these values into Eqs. (15) and (16) yields the first lattice QCD estimates of the CSV momentum fractions

$$\delta u = -0.0023(6), \quad \delta d = 0.0020(3). \quad (17)$$

The first observation we make is that these results are roughly equal in magnitude and have opposite sign. These values are slightly larger than, but within errors in agreement with, the phenomenological predictions of [5, 8], where within the MIT bag model (at a scale $Q^2 \simeq 4\,\mathrm{GeV}^2$) they found $\delta u^- = -0.0014$ and $\delta d^- = 0.0015$. They are also consistent with the best-fit values of the phenomenological analysis of MRST [6], $\delta u^- = -\delta d^- = -0.002^{+0.009}_{-0.006}$ (90% CL).

While our work provides the first nonperturbative QCD result to give a clear indication of the sign and magnitude of the CSV in these moments, we point out that it is based on lattice simulations using a single volume and lattice spacing. To achieve a precise quantitative determination will require a detailed study of the finite-volume

FIG. 3. The difference between the doubly and singly represented quarks in the Σ and Ξ as a function of the strange/light quark mass difference. We deduce δu and δd, respectively, from the slopes of these curves (c.f. Eqs. (15) and (16)).

and discretisation effects which we plan to address by extending these calculations to larger volumes and a second lattice spacing. Additionally, it is well known that lattice results for the second moment of the iso-vector nucleon PDFs, $\langle x \rangle_{u-d}$, do not agree well with experiment (see e.g. [19]). Based on chiral perturbation theory it is expected that finite size effects and chiral corrections are potentially large [20–23], but this has so far not been confirmed by lattice calculations. This discrepancy may also be due to a mismatch of lattice nucleon matrix elements and perturbative Wilson coefficients. However, what concerns us here are ratios of moments of PDFs, in which such effects cancel out. For example, we find $\langle x \rangle^p_u / \langle x \rangle^p_d \approx 2.3$ in good agreement with $\langle x \rangle^p_{u^-} / \langle x \rangle^p_{d^-} = 2.40(6)$ found in [24]. We are also encouraged that lattice results for the ratio $\langle x \rangle_{(u-d)} / \langle x \rangle_{(\Delta u - \Delta d)}$ agree well with experiment [25]. Lastly, we have estimated the CSV associated only with the $u - d$ mass difference. It is important to also find a method to investigate the CSV induced by electromagnetic effects which is expected [6, 26] to be of a similar size. The determination of this effect is, however, a separate calculation which will have no impact on our result.

In summary, we have performed the first lattice determinations of the quark momentum fractions of the hyperons, Σ and Ξ in $N_f = 2 + 1$ lattice QCD. By examining the $\mathrm{SU}(3)_{\mathrm{flavour}}$-breaking effects in these momentum fractions, we are able to extract the first QCD determination of the size and sign of charge-symmetry violations in the parton distribution functions in the nucleon, δu and δd. Although our lattice calculations are restricted to the second ($n = 2$) moment of the C-even quark distributions, our results for $\delta u = -0.0023(6)$, $\delta d = 0.0020(3)$ are in excellent agreement with earlier phenomenological calculations [5, 8].

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