## Exploring the Nucleon Structure from First Principles of QCD

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Abstract. Quantum Chromodynamics (QCD) is generally assumed to be the fundamental theory underlying nuclear physics. In recent years there is progress towards investigating the nucleon structure from first principles of QCD. Although this structure is best revealed in Deep Inelastic Scattering, a consistent analysis has to be performed in a fully non-perturbative scheme. The only known method for this purpose are lattice simulations. We first sketch the ideas of Monte Carlo simulations in lattice gauge theory. Then we comment in particular on the issues of chiral symmetry and operator mixing. Finally we present our results for the Bjorken variable of a single quark, and for the second Nachtmann moment of the nucleon structure functions.

## 1. Introduction

For 37 years we have a strong candidate for a fundamental theory underlying nuclear physics. There is a well-founded paradigm that the whole of nuclear physics can in principle be explained by QCD. Nevertheless this theory has hardly been represented at this workshop, because most talks referred to complex phenomena, which can in practice still not be computed based on QCD. Effective approaches — like the shell-model — are popular for this purpose. They are often successful for specific questions, but they all have their limitations.

In this contribution we do address QCD, and we report in particular on progress in the understanding of the nucleon structure function from first principles. This is obviously a non-perturbative task, and the only method to tackle it systematically are lattice simulations.

The formulation of QCD looks amazingly simple: it deals with quarks with a local SU(3) symmetry ("colour symmetry"), which gives rise to strong interaction mediated by 8 gauge bosons ("gluons"); one for each generator of the gauge group SU(3). Since the latter is non-Abelian, the gluons also interact among each other, which makes the dynamics of the system complicated. In the low energy regime, which dominates our daily experience, the gauge coupling is strong, and the interactions are extremely involved. This can be seen for instance from the

fact that the fundamental masses of the lightest (valence) quark flavours — which we assume to be generated by the Higgs mechanism — only contribute about 2~% to the nucleon mass; all the rest is contained in some dense "foam" of gluons and sea-quarks.

So far perturbation theory could be carried out for some quantities up to  $\alpha_s^4$ , with  $\alpha_s = g_s^2/4\pi$ ,  $g_s$  being to strong gauge coupling. This is applicable to a number of high energy processes, dominated by the exchange of few gluons. A suitable method for that purpose is dimensional regularisation, which is, however, strictly limited to perturbation theory.

On the other hand, the lattice regularisation enables a fully non-perturbative treatment, *i.e.* we can really address finite values of  $\alpha_s$ . Here we refer to the functional integral formulation of quantum field theory, which is (in principle) based on an integration over all possible configurations of the fields involved. The partition function, and all n-point functions that can be derived from it, are then given by an integration over all these configurations with a phase factor  $\exp(iS)$ , where S is the action of the configuration. The convergence of such integrals can be improved drastically by moving to Euclidean space-time, *i.e.* by invoking an "imaginary time" (Wick rotation). This changes the factor mentioned above to  $\exp(-S_E)$ , where  $S_E$  is the Euclidean action. This transition is justified in view of the expectation values of n-point functions if four conditions — known as the "Osterwalder-Schrader axioms" — hold. For many theories, including QCD at zero vacuum angle  $\theta$  and zero baryon density,  $S_E$  is real positive for all configurations, hence the factor  $\exp(-S_E)$  can be interpreted as a probability distribution for the possible field configurations.

Lattice studies consider discrete points in a finite volume of Euclidean space-time. The matter fields — in this case the quark fields  $\bar{\Psi}$ ,  $\bar{\Psi}$  — are located on these lattice sites, while the gauge field variables  $U_{\mu} \in SU(3)$  live on the links connecting nearest neighbour sites. Thus the functional integral is completely well-defined. Most theories of interest are bilinear in the fermion fields. Then the action takes the structure  $S_{\rm E}[\bar{\Psi},\Psi,U]=\bar{\Psi}M[U]\Psi+S_{\rm gauge}[U]$ , where the indices of  $\bar{\Psi}$ ,  $\Psi$  run over all lattice sites, and on each site over all internal degrees of freedom. The fermion matrix M contains the gauge couplings between neighbouring sites (due to the discrete covariant derivative in the Dirac operator).  $S_{\rm gauge}$  is the pure gauge part of the action. In accordance with the Spin-Statistics Theorem, the components of the spinor fields  $\bar{\Psi}$ ,  $\Psi$  are given by Grassmann variables, *i.e.* they anti-commute, and the corresponding integration yields

$$Z = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi\mathcal{D}U \exp(-S_{\mathrm{E}}[\bar{\Psi},\Psi,U]) = \int \mathcal{D}U \det M[U] e^{-S_{\mathrm{gauge}}[U]}. \tag{1}$$

The functional measure  $\mathcal{D}U$  now represents the integral over the (compact, gauge invariant) Haar measure for each link variable. Thus we preserve exact gauge invariance on the regularised level. For system sizes of interest, it is still far beyond our ability to compute this integral explicitly. Hence the method of choice is to generate a large set of gauge configurations with the given probability distribution; moreover the configurations should be well de-correlated, *i.e.* statistically independent from each other. There are powerful algorithms for this purpose, see Refs. [1] for reviews. Once such a set of configurations is generated, it can be used to measure observables of interest. This approximate functional integral yields results for expectation values with statistical errors (due to the finite sample of configurations) and systematic errors (finite lattice spacing, finite volume etc.). These errors can be estimated and reduced with additional computational effort. The important point, however, is that the result is fully non-perturbative. This allows us nowadays for instance to calculate the light hadron spectrum from first principles of QCD up to a precision of a few percent. The results agree with phenomenology within these errors.

Our daily experience is dominated by nuclear physics at low energy. Regarding QCD this implies a dominance by the light quark flavours, in particular the flavours u and d. Their masses

are very small compared to  $\Lambda_{\rm QCD}$  — the intrinsic scale of QCD, which provides a scale for the hadron masses. Hence these quarks have an approximate chiral symmetry, which is of prominent importance in low energy QCD. To briefly review this property, we first note that fermion fields can be decomposed into "left- and right-handed" components by means of the chiral projectors,

$$\Psi_{L,R} = \frac{1}{2} (1 \pm \gamma_5) \Psi , \quad \bar{\Psi}_{L,R} = \bar{\Psi} \frac{1}{2} (1 \mp \gamma_5) .$$
 (2)

In the chiral limit (zero quark masses) these two components decouple. It is allowed to add quark masses to the Lagrangian, since QCD is a vector theory — the left- and right-handed components couple in the same way to the gauge field — (unlike the electroweak sector of the Standard Model). From a perturbative perspective, the approximate chiral symmetry still protects the masses of light quarks from large renormalisation. Based on this property, it is occasionally claimed that there is no hierarchy problem for fermion masses. However, it is the non-perturbative level that ultimately matters for physics, and there it is highly non-trivial to implement (approximate) chiral symmetry in a regularised system. A quite obvious ansatz is the Wilson lattice fermion, which starts from the naïve discretisation of the derivative in the Dirac operator, and subtracts a discrete Laplacian to send the fermion doublers to the cutoff scale. However, this extra term breaks chiral symmetry explicitly. As a consequence, under gauge interaction the fermion masses are renormalised such that they naturally end up at the cutoff scale as well. The (observed) property  $m_{u,d} \ll \Lambda_{\rm QCD}$  can then only be attained by a tedious fine-tuning of negative bare quark masses, i.e. the hierarchy problem is back.

Only at the very end of the last century was there a breakthrough in the formulation of chiral lattice fermions, which overcomes this problem, at least in vector theories. A key observation was that a lattice modified version of chiral symmetry of the form [2]

$$\bar{\Psi} \to \bar{\Psi} \Big( 1 + \varepsilon \Big[ 1 - \frac{a}{2} D \Big] \gamma_5 \Big) , \quad \Psi \to \Big( 1 + \varepsilon \gamma_5 \Big[ 1 - \frac{a}{2} D \Big] \Big) \Psi$$
 (to  $O(\varepsilon)$ ), (3)

is sufficient to rule out additive mass renormalisation. Here a is the lattice spacing, and in the continuum limit this turns into the standard chiral transformation (infinitesimal form). Even on the lattice the fermionic Lagrangian  $\bar{\Psi}D\Psi$  is invariant, if the lattice Dirac operator D fulfils the Ginsparg-Wilson relation (GWR)

$$\{D, \gamma_5\} \equiv D\gamma_5 + \gamma_5 D = aD\gamma_5 D . \tag{4}$$

On the other hand, the functional measure  $\mathcal{D}\bar{\Psi}\mathcal{D}\Psi$  is not invariant, and this is just what it takes to reproduce the axial anomaly correctly [2].

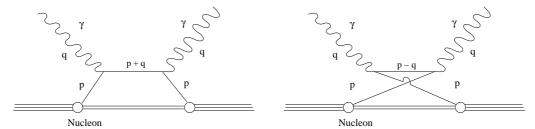
Solutions to the GWR can be constructed based on block spinor renormalisation group transformations ("perfect lattice fermion") [3, 4], or by pulling apart the chiral modes in an extra "dimension" ("Domain Wall Fermion") [5]. By integrating out that "dimension", one obtains — for  $\gamma_5$ -Hermitian operators,  $D^{\dagger} = \gamma_5 D \gamma_5$  — the "overlap Dirac operator"  $D_{\text{ov}}$  [6],

$$aD_{\text{ov}} = 1 + A_{\text{ov}} , \quad A_{\text{ov}} = A/\sqrt{A^{\dagger}A} , \quad A = aD - 1 .$$
 (5)

It is easy to verify that it satisfies the GWR, which can now be written as  $D_{\text{ov}} + D_{\text{ov}}^{\dagger} = aD_{\text{ov}}^{\dagger}D_{\text{ov}}$ . For the kernel D we can insert for instance the Wilson operator [6], but properties like scaling, locality and approximate rotation symmetry can be improved by using a better kernel [7].

In addition to the exact, lattice modified chiral symmetry, the GWR also prevents uncontrolled operator mixing on the regularised level [4]. This powerful property is very helpful, for instance for the numerical study of a fully non-perturbative Operator Product Expansion (OPE).

We now summarise our lattice OPE project [8, 9, 10] as an example for the application of chiral quarks in lattice QCD. This takes us beyond the hadron spectrum; we investigate the internal structure of the nucleon (see Ref. [11] for a recent review). Phenomenologically this structure is revealed in Deep Inelastic Scattering of a lepton on a nucleon target. This scattering is dominated by a one-photon exchange involving a single quark, as sketched below.



Although this is a high energy process, there are problems with a perturbative treatment due to ambiguous UV and IR divergences. A fully satisfactory study based on QCD has to be consistently non-perturbative, *i.e.* it is a challenge for the lattice. The involvement of a single quark implies that chirality is conserved, hence the use of Ginsparg-Wilson quarks is appropriate. In our simulations we applied 2 flavours of degenerate overlap valence quarks with masses of 29 MeV and 73 MeV, which correspond to pion masses of 280 MeV and 440 MeV, respectively. The goal is the evaluation of the product of electromagnetic currents  $J_{\mu}$  — of the photon exchange, with large transfer momentum q — between quark states of low momentum p. This product is decomposed by the OPE as follows,

$$W_{\mu\nu} \simeq \langle \Psi(p)|J_{\mu}(q)J_{\nu}(-q)|\Psi(p)\rangle = \sum_{m,i,n} C_{\mu\nu,i,\mu_{1}...\mu_{n}}^{(m)}(q)\langle \Psi(p)|\mathcal{O}_{i,\mu_{1}...\mu_{n}}^{(m)}|\Psi(p)\rangle . \tag{6}$$

 $C^{(m)}$  are Wilson coefficients, which are independent of the target and therefore of p, and  $\mathcal{O}^{(m)}$  are *local* operators, which are relevant to describe the nucleon structure. They involve the quark momentum components  $p_{\mu_j}$ . We further use the Clifford index  $i = 1 \dots 16$ , and the index m to distinguish operators with the same symmetries.

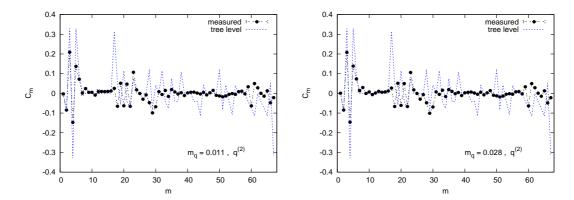
A truncation of the OPE on the right-hand-side of eq. (6) requires the scale separation

$$p^2 \ll q^2 \ . \tag{7}$$

We probed three photon momenta,  $|q^{(1)}| = 2.2 \text{ GeV}$ ,  $|q^{(2)}| = 3.3 \text{ GeV}$ ,  $|q^{(3)}| = 4.4 \text{ GeV}$ . Based on the above scale separation, we truncated the quark bilinears at  $O(|p|^3)$ . Thus we still include 1360 operators, but for photon momenta  $q \propto (1,1,1,1)$  they occur in only 67 equivalence classes. The strategy is now to measure the elements of  $W_{\mu\nu}$  and  $\langle \mathcal{O}^{(m)} \rangle$  for a multitude of low quark momenta p, and solve eq. (6) for the Wilson coefficients. They are over-determined in this way, but by means of a Singular Value Decomposition we arrived at reliable values [8]. In Fig. 1 we compare the results obtained numerically at photon momentum  $q^{(2)}$  to the Wilson coefficients at tree level in the chiral limit. We see that they follow the same pattern, though gauge interaction reduces the absolute values significantly. In particular the coefficients  $C_1$  and  $C_7 \dots C_{16}$  vanish in the chiral limit, because they are attached to operators with an even power of  $\gamma$ -matrices. We obtain small absolute values for them also in the interacting case at finite quark mass, which confirms that chiral symmetry on the lattice works, and it suppresses operator mixing.

As a first application, we evaluate the Bjorken variable x for one unpolarised quark. The expectation value  $\langle x \rangle$  measures the nucleon momentum fraction carried by the quark involved in the Deep Inelastic Scattering. To be explicit, we consider the tensor [9]

$$T_{\mu\nu} = \frac{1}{4} \text{Tr}[S^{-1}(p)W_{\mu\nu}(p,q)] = \delta_{\mu\nu}W_1 + p_{\mu}p_{\nu}W_2 + (p_{\mu}q_{\nu} + p_{\nu}q_{\mu})W_4 + q_{\mu}q_{\nu}W_5 , \qquad (8)$$



**Figure 1.** The Wilson coefficients for quark masses  $m_q = 0.011$  and  $m_q = 0.028$  in lattice units, corresponding to 29 MeV and 73 MeV. In both cases the photon momentum amounts to 3.3 GeV. The results for the 67 independent coefficients are compared to their values on tree level. We see a similar pattern, with reduced absolute values under interaction. The coefficients which vanish in the chiral limit,  $C_1$  and  $C_7 \dots C_{16}$ , are still small at finite quark mass, which confirms the validity of our method.

where S is the quark propagator. The Dirac-index structure is not visible here due to the trace (terms with  $W_3$  and  $W_6$  would occur for polarised targets).

In particular  $T_{\mu\mu}$  is directly related to the Bjorken variable in the high energy Bjorken limit. In this limit, the Minkowski space momenta obey  $(p \cdot q)^2 \gg p^2 q^2$ . Among the 22 operators in the expansion of  $T_{\mu\mu}$  we focus on those with spin 2, where the Bjorken limit leads to [9]

$$\langle x \rangle = \frac{q^2 \left[ T_{\mu\mu} \right]_{\text{spin } 2}}{2 \sum_{\mu > \nu} p_{\mu} p_{\nu}} \,. \tag{9}$$

Fig. 2 (on the left) shows the numerator against the denominator of the right-hand-side in eq. (9). A broad range of points measured at  $m_q = 73$  MeV is consistent with a linear behaviour, which allows us to read off  $\langle x \rangle$  from the slope (the errors are statistical only),

$$\langle x \rangle|_{q^{(1)}} = 0.44(9) , \quad \langle x \rangle|_{q^{(2)}} = 0.73(5) , \quad \langle x \rangle|_{q^{(3)}} = 0.60(5) .$$
 (10)

Finally we proceed to the nucleon structure function [10]. On a lattice of spacing a, a generic moment can be expanded as

$$\mathcal{M}(q^2) = c_2(q^2a^2)A_2(a^2) + \frac{c_4(q^2a^2)}{q^2}A_4(a^2) + \dots$$
(11)

where  $A_n$  are reduced nucleon matrix elements (the Lorentz structure is factored out),  $c_n$  are the corresponding Wilson coefficients, and n is the twist. Both factors are bare quantities. If one tries to replace a by some scale  $\mu$  of a soft renormalisation scheme, one runs into ambiguities, which do not occur on the lattice with its hard momentum cutoff  $\pi/a$ .

In our study, we evaluated the (spin averaged) nucleon matrix elements for all 67 types of operators, and extracted moments of the structure function by Nachtmann integration of the hadronic tensor [12]. This allows us in particular to project out operators of spin 2. For instance, the traceless form of  $W_{\mu\nu}$  leads to

$$\mathcal{M}(q^2) = \frac{3q^2}{(4\pi)^2} \int d\Omega_q \ n_\mu \Big( W_{\mu\nu} - \frac{1}{4} \delta_{\mu\nu} W_{\lambda\lambda} \Big) n_\nu \ \to \ \int_0^1 dx \ \Big( F_2(x, q^2) + \frac{1}{6} F_L(x, q^2) \Big) \ . \tag{12}$$

Here n is a constant 4-vector with  $n^2 = 1$ , and the last expression in eq. (12) refers again to the Bjorken limit. By means of a further projection [10] we can separate the structure functions  $F_2$ 

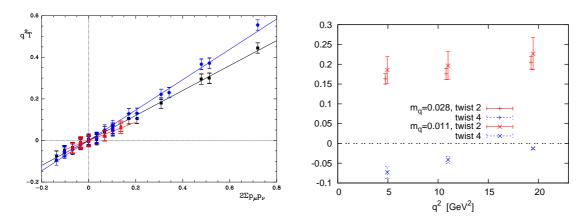


Figure 2. On the left: The term  $q^2T_{\mu\mu}$  for spin 2, versus  $2\sum_{\mu>\nu}p_{\mu}p_{\nu}$  (numerator and denominator in eq. (9)). The squares, circles and triangles refer to photon momentum  $q^{(1)}$ ,  $q^{(2)}$ ,  $q^{(3)}$ , respectively. In all three cases the data points are compatible with a linear behaviour. Thus the slope allows for the determination of the Bjorken variables  $\langle x \rangle$  given eq. (10). On the right: The nucleon moment  $\mathcal{M}_2$  against the photon momentum squared. We distinguish the contributions of twist 2 and twist 4. In all cases the result for our two quark masses agree within statistical errors. For large  $q^2$  the twist 4 contribution seems to vanish, whereas the twist 2 contribution stabilises at a finite value in the range  $\approx 0.5...0.8$ .

and  $F_L$ . Based on the numerical measurement of the matrix elements, we can carry out the first integral in eq. (12). Thus we arrive at explicit and non-perturbative results for  $\mathcal{M}$ .

Our results for the second moment  $\mathcal{M}_2$  are shown in Fig. 2 (on the right). They agree within the errors for both quark masses, at all three photon momenta, which suggests that they may be valid up to the physical pion mass. As we increase the photon momentum (*i.e.* the transfer momentum in the hard scattering), the twist 4 contribution tends to vanish, while the twist 2 term stabilises at a moderate value. As usual the numerical errors increase for lighter quarks.

These results demonstrate that the explicit determination of the nucleon structure functions—as observed in Deep Inelastic Scattering—directly from QCD is feasible, in the framework of a non-perturbative regularisation free of ambiguities. Moreover we obtained explicit results for the Bjorken variable of the quark involved in this scattering. Our results provide insight into the nucleon structure. For a detailed discussion we refer to Ref. [10].

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## References

- $[1] \ \ \text{Kennedy AD 2006 hep-lat/0607038. L\"{u}scher M 2010 arXiv:1002.4232 [hep-lat]}.$
- [2] Lüscher M 1998 Phys. Lett. B **428** 342.
- [3] Ginsparg PH and Wilson KG 1982 Phys. Rev. D 25 2649.Bietenholz W and Wiese U-J 1996 Nucl. Phys. B 464 319.
- [4] Hasenfratz P 1998 Nucl. Phys. B **525** 401.
- [5] Kaplan D 1992 Phys. Lett. B 288 342.
- [6] Neuberger H 1998 Phys. Lett. B 417 141, 1998 Phys. Lett. B 427 353.
- [7] Bietenholz W 1999 Eur. Phys. J. C 6 537.
- [8] Bietenholz W, Cundy N, Göckeler M, Horsley R, Perlt H, Pleiter D, Rakow PEL, Schierholz G, Schiller A, Streuer T and Zanotti JM 2009 PoS(LAT2009)138 [arXiv:0910.2437 [hep-lat]].
- [9] Bietenholz W, Cundy N, Göckeler M, Horsley R, Perlt H, Pleiter D, Rakow PEL, Schierholz G, Schiller A, Streuer T and Zanotti JM 2009 PoS(LAT2009)139 [arXiv:0911.4892 [hep-lat]].
- [10] QCDSF Collaboration, in preparation.
- [11] Hägler Ph 2009 arXiv:0912.5483 [hep-lat].
- [12] Nachtmann O 1973 Nucl. Phys. B 63 237.