First moments of the nucleon transverse quark spin densities using lattice QCD

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We present a calculation of the Mellin moments of the transverse quark spin densities in the nucleon using lattice QCD. The densities are extracted from the unpolarized and transversity generalized form factors extrapolated to the continuum limit using three $N_f = 2 + 1 + 1$ twisted mass fermion gauge ensembles simulated with physical quark masses and spanning three lattice spacings. The first moment of transversely polarized quarks in an unpolarized nucleon shows an interesting distortion, which can be traced back to the sharp falloff of the transversity&generalized form factor $\tilde{F}_{TQO}(t)$. The isovector tensor anomalous magnetic moment is determined to be $\kappa_T = 1.051(94)$, which confirms a negative and large Boer-Mulders function, $h_T^+$, in the nucleon.

Introduction: Understanding the spin content of the nucleon is of paramount importance for hadron structure. While significant progress has been made in recent years revealing the longitudinal spin structure of the nucleon [1–3], the transverse spin structure remains lesser known from phenomenology [4–6], a situation that will improve with results from planned experiments (SoLID [7,8], Electron-Ion Collider [9]). In lattice QCD, theoretical progress [10,11] has enabled the extraction of the x-dependence of parton distribution functions (PDFs) at the physical pion mass [12–17], as well as first results on generalized parton distributions (GPDs) [13]. For a summary of these approaches we refer the reader to [18–22].

In this work, we use lattice QCD for the study of the transverse spin properties of the nucleon by considering the first two Mellin moments of the 3-dimensional (3D) probability densities $\rho(x, b_\perp, s_\perp, S_\perp)$, where $x$ is the longitudinal momentum fraction, $s_\perp$ the transverse quark spin, $b_\perp$ the transverse vector from the center of momentum of the nucleon, and $S_\perp$ the transverse spin of the nucleon. As discussed in Ref. [23], to access the transverse spin densities one needs to compute the twist-two matrix elements of the chiral-even unpolarized and chiral-odd transversity GPDs. The probability density [23] is then given as

$$
\rho(x, b_\perp, s_\perp, S_\perp) = \frac{1}{2} \left[ H(x, b_\perp^2) + \frac{b_\perp^i e^{i\theta}}{m_N} \left( S_\perp^i E'(x, b_\perp^2) + s_\perp^i E'(x, b_\perp^2) \right) + \frac{s_\perp^i s_\perp^j}{2m_N} \left( H_T(x, b_\perp^2) - \frac{\Delta_{ij}}{4m_N} \tilde{H}_T(x, b_\perp^2) \right) + s_\perp^i \left( 2b_\perp^i + \Delta_{ij} b_\perp^j \right) \tilde{H}_T(x, b_\perp^2) \right].$$

(1)

The GPDs $H, E, H_T, E_T, \tilde{H}_T$ involved in Eq. (1) are given in the impact parameter space for zero skewness by a Fourier transformation, $\Delta_\perp \leftrightarrow b_\perp$, where $\Delta_\perp$ is the transverse momentum transfer and $-t \equiv \Delta^2$. $m_N$ is the nucleon mass, $e^{i\theta}$ is the antisymmetric tensor, and the derivatives are denoted as $F' = \frac{\partial F}{\partial \theta}$ and $\Delta_{ij} F = 4 \frac{\partial^2}{\partial \theta^i \partial \theta^j} F$. The GPD $E_T$ is defined as a linear combination of two GPDs, namely $E_T = E_T + 2\tilde{H}_T$. The moments are then computed as an integral over the momentum fraction as

$$
\langle x^{n-1} \rangle_{\rho} (b_\perp, s_\perp, S_\perp) \equiv \int_{-1}^{1} dx \ x^{n-1} \rho(x, b_\perp, s_\perp, S_\perp), \n
(2)$$

where $n$ is a positive non-zero integer corresponding to the $n^{th}$-moment. The GPDs reduce to the generalized form factors (GFFs) if integrated over $x$. For the unpolarized
In this work, we are interested in GFFs that parameterize off-forward nucleon matrix elements of local vector and tensor quark operators, defined as

\[ O^\mu_V = \bar{q}(x)\gamma^\mu q(x), \quad O^\mu_{V,D} = \bar{q}(x)\gamma^\mu \hat{D}^\nu q(x), \quad (3) \]

\[ O^\mu_T = \bar{q}(x)\sigma^{\mu\nu} q(x), \quad O^\mu_{T,D} = \bar{q}(x)\sigma^{\mu\nu} \hat{D}^\nu q(x), \quad (4) \]

where \( \hat{D} \) is the symmetrized covariant derivative, \{\cdots\} denotes symmetrization and subtraction of the trace and \{\cdots\} antisymmetrization of the enclosed indices. For details on how the nucleon matrix elements of the operators in Eqs. (3) and (4) yield the GFFs we refer to Ref. [24].

**Lattice methodology**: We employ the twisted-mass fermion discretization scheme [25, 26], which provides automatic \( O(a) \)-improvement for both physical observables and renormalization constants [27]. The ensembles are generated with two mass-degenerate light, a strange, and a charm quark, referred to as \( N_f = 2 + 1 + 1 \). The bare light quark mass is tuned to reproduce the isosymmetric pion mass \( m_\pi = 0.135 \) MeV within 1-4 MeV while the heavy quark masses are tuned with inputs generated by the physical kaon and D-meson masses as well as the D-meson decay constant, following the procedure of Refs. [28, 29]. The parameters of the ensembles analyzed in this work can be found in Table I. We note that the lattice spacing has been determined from the nucleon mass as discussed in Ref. [30].

| Ensemble       | \( V/a^4 \) | \( \beta \) | \( a \) [fm] | \( m_sL \) | \# meas. |
|----------------|-------------|-------------|-------------|-----------|--------|
| cB211.072.64   | 64^4 × 128  | 1.778       | 0.07975(32) | 3.62      | 48,000 |
| cC211.06.80    | 80^4 × 160  | 1.836       | 0.06860(20) | 3.78      | 46,516 |
| cD211.054.96   | 96^4 × 192  | 1.900       | 0.05686(27) | 3.90      | 31,744 |

TABLE I: The parameters of the three \( N_f = 2 + 1 + 1 \) ensembles used in this work. In the first column we give the name of the ensemble, in the second column the lattice volume, in the third \( \beta = 6/g^2 \) where \( g \) the bare coupling constant, in the fourth the lattice spacing determined as discussed in Ref. [30], and in the fifth column the value of \( m_sL \). The last column is the number of measurements in the calculation of the three-point functions for \( t_s/a = 20 \).

To evaluate the nucleon matrix elements of the operators in Eqs. (3) - (4), we compute three- and two-point correlation functions. Gaussian smeared point sources are employed [31] to improve the overlap with the nucleon state. The connected three-point functions are computed using sequential propagators inverted through the sink, i.e. using the so-called fixed-sink method. In this work we restrict ourselves to the flavor non-singlet isovector combination where disconnected contributions vanish in the continuum limit. Connected three-point functions are computed using several time separations, \( t_s \), between the creation and annihilation nucleon interpolating operators, namely \( t_s \in [0.64, 1.6] \) fm for the cB211.072.64, \( t_s \in [0.55, 1.52] \) fm for the cC211.06.80 and \( t_s \in [0.46, 1.15] \) fm for the cD211.054.96 ensemble. This broad range of separations is necessary for a thorough investigation and elimination of excited state contribution. At constant statistics, the noise-to-signal ratio increases exponentially with \( t_s \) and the increase is exacerbated at the physical point. We thus increase the number of measurements with increasing \( t_s \) to compensate, yielding an approximately constant error for all \( t_s \).

The desired ground state matrix element is obtained by taking an appropriate ratio of three- to two-point functions (see Refs. [32, 33]), and analyzing its time dependence as explained below.

In general, the nucleon matrix elements of the operators in Eqs. (3) - (4) yield linear combinations of the GFFs in the non-forward limit depending on the insertion operator quantum numbers, the nucleon spin projection, and components of the momentum transfer. We follow a standard procedure, as described in Sec. C of Ref. [32], where we construct an overconstrained system of equations that is inverted through a Singular Value Decomposition (SVD) to obtain the individual GFFs. A delicate step in our analysis is to ensure that the ground state contribution is disentangled from the excited-states contamination. We follow the procedure of Ref. [32], comparing three methods, namely, the plateau, summation, and two-state fits. Both the plateau and summation fits take into account only contributions from the ground state, while in the two-state fit we consider contributions from the first excited state in both three- and two-point functions. An example analysis is shown in Fig. 1 for the \( A_{T20}(0) \) case. As can be seen, the ratio shows sizeable excited-states contamination. Including the first excited state in a two-state fit leads to a ground state matrix element that is significantly lower compared to the plateau method. For increasing \( t_s^{low} \) the summation fit agrees with the two-state fit, which is consistent for all \( t_s^{low} \). We therefore take the result of the two-state fit as the best determination of the ground state matrix element. This is done throughout our analysis of the GFFs.
scheme and results are converted to the $\overline{\text{MS}}$ scheme at a scale of 4 GeV$^2$. A significant improvement in the determination of these renormalization functions comes from subtracting the lattice artifact up to one-loop in perturbation theory [38].

Results: In Fig. 2 we show the continuum limit of a selection of GFFs in the forward limit. Since our physical observables are automatically $\mathcal{O}(a)$-improved, we perform a linear fit in $a^2$ to extrapolate the results to $a \to 0$. As can be seen, for most of the cases the extrapolation is rather mild, which means that discretization effects are small for those quantities, within the current statistical precision.

In Table I, we quote the values of the forward limit of the GFFs shown in Fig. 2 in the continuum limit. The quantity $g_T \equiv A_{T10}(0)$ is the tensor charge, which plays a crucial role in the search of beyond the Standard Model (SM) interactions [39] by experiments such as DUNE [40] and IsoDAR [41]. Namely, the individual quark flavor contributions to $g_T$ enter into the determination of the quark electric dipole moment contribution to the neutron electric dipole moment [42], which if non-zero would signal the existence of physics beyond the SM. Determination of $g_T$ from phenomenology is achieved through the transversity PDF. Recent results using a global analysis of electron-proton and proton-proton data have determined $g_T = 0.53(25)$ [43]. Although the central value is lower from our current determination, its error is large, leading to about two standard deviations effect. Furthermore, our determination is fully compatible with the recent FLAG report [43] and with our previous value [44] obtained using only the cB211.072.64 ensemble, which is at the coarsest lattice spacing.

Beyond $g_T$, another challenging quantity that is poorly known is the anomalous tensor magnetic moment $\kappa_T \equiv \vec{B}_{T10}(0)$. It is a fundamental quantity, perhaps more than $E_T$ and $\vec{H}_T$ [20], describing the deformation of the transverse polarized quark distribution in an unpolarized nucleon. First lattice results were presented in the pioneering work of the QCDSF/UKQCD collaboration [45], where a value $\kappa_T = 1.03(16)$ was reported obtained using chiral extrapolations from ensembles with
pion masses of $m_\pi > 400$ MeV. Our analysis, using physical point ensembles, agrees with their value. Other results for this quantity include $\kappa_T = 0.81$ and 1.24 from two approaches using the constituent quark model \[46\] and $\kappa_T = 1.73$ using the quark-soliton model \[47\]. Since $\kappa_T \sim -h^+_{\perp}$ \[48\], then all results suggest that the Boer-Mulders function, $h^+_{\perp}$, should be negative and sizeable. This conclusion has also been found in a lattice QCD study of the transverse momentum dependent PDFs \[49\].

There, an $N_f = 2 + 1$ mixed action scheme is used with domain wall valence fermions on Asqtad sea quarks and pion masses $m_\pi = 369, 518$ MeV.

| $A_{T10}(0)$ | $B_{T10}(0)$ | $A_{20}(0)$ | $B_{20}(0)$ | $J$ | $A_{T20}(0)$ | $B_{T20}(0)$ |
|---------------|---------------|--------------|--------------|-----|---------------|---------------|
| 0.924(54)     | 1.051(94)     | 0.126(32)    | 0.180(67)    | 0.156(46) | 0.168(44)     | 0.267(19)     |

TABLE II: Our values of the forward limit of GFFs presented in Fig. 2 in the continuum limit. We also include the value of the isovector light quark contribution to the nucleon angular momentum ($J$).

For the average momentum fraction, $\langle x \rangle \equiv A_{20}(0)$, our value is in agreement with the precise values from phenomenology \[50\]–\[52\]. While $\langle x \rangle$ is well-known, this is not the case for $B_{20}(0)$, which enters in the expression for the nucleon spin \[53\], $J = [A_{20}(0) + B_{20}(0)]/2$. Having determined both GFFs in the continuum limit we find $J = 0.156(46)$ for the isovector contribution which is compatible with our previous determination of 0.161(24) \[2\]–\[34\] obtained using only the cB211.072.64 ensemble. The slightly larger value obtained here can be attributed to the slightly negative slope of $B_{20}(0)$ towards $a \rightarrow 0$ observed in Fig. 2.

The second moment of the transversity PDF is $\langle x \rangle_{\delta u - \delta d} \equiv A_{T20}(0)$. Our finding is in agreement with our previous study using the cB211.072.64 ensemble \[33\] and also with the value by the RQCD collaboration \[34\]. $B_{T20}(0)$ is unknown from phenomenology. The lattice study by QCDSF/UKQCD \[45\], using ensembles with pion masses $m_\pi > 400$ MeV as discussed before, found $B_{T20}(0) = 0.160(39)$, which is about two standard deviations lower than our value.

The dependence of the GFFs on the momentum transfer squared, $-t$, is also extracted for each ensemble. Since in the lattice formulation $-t$ takes discrete values we employ the $p$-pole Ansatz \[23\]–\[55\],

$$F(t) = \frac{F(0)}{1 - t/m_p^2} p,$$

(5)
to fit the GFFs. There are three fit parameters, namely $F(0)$, the value of the GFF in the forward limit, the pole mass $m_p$, and the value of $p$. Varying all three parameters leads to significant instabilities, as also observed in Refs. \[45\]–\[54\]. We use Gaussian priors for $p$ centered at $p = 2$ with width 0.5. We find that this procedure leads to very stable results in all cases considered. Note that for $A_{10}(t)$ and $B_{10}(t)$, i.e., the Dirac and Pauli form factors respectively, we use a dipole fit to parameterize their momentum dependence, therefore fixing $p = 2$.

In Fig. 2 we show the vector and tensor GFFs in the continuum limit. With this information we can fully determine the first two moments of the transverse quark spin densities given in Eq. \[1\]. As can be seen, the GFFs are well determined, especially for the $n = 1$ case. As expected, for the higher moment, $n = 2$, the GFFs have smaller values as compared to the $n = 1$ GFFs. In addition, we observe that $A_{20}(t)$ and $A_{T20}(t)$ have a rather flat behavior. In impact parameter space, the fit function is given by \[23\]

$$F(b^2_{\perp}) = \frac{m_p^2 F(0)}{2p^2 \pi \Gamma(p)} (m_p b_{\perp})^{p-1} K_{p-1}(m_p b_{\perp}),$$

(6)

where $\Gamma(x)$ is the Euler gamma function and $K_{p-1}(x)$ the modified Bessel functions and $b_{\perp} = \sqrt{b^2_{\perp}}$.

In Fig. 2 we show the first moment of the probability density $\rho(x, b_{\perp}, s_{\perp}, s_{\perp})$. It is very interesting that for all the cases we observe a sizeable deformation. We consider four cases: i) For unpolarized quarks in a transversely polarized nucleon, we observe a large distortion towards the positive $b_y$ direction. This can be traced back to the GFF $B_{10}$, contributing to the term for $E'$ in Eq. \[1\], which from Fig. 3 we see is large and drops fast yielding a large derivative. The origin of this behavior is related to the Sivers effect \[56\], a connection that has already been made in Ref. \[57\]. ii) For transversely polarized
quarks in an unpolarized nucleon, we can also observe a
distortion, however, it is much milder compared to the
previous case. This is because in the isovector combination
the $\bar{B}T_{10}(b^2)$ term contributing here has a milder
behavior compared to the individual quark behavior ob-
erved in Ref. [15]. iii) Another interesting case is when
both quarks and the nucleon are transversely polarized.
In this situation, all the terms in Eq. (1) contribute de-
forming significantly the density. iv) If one chooses the
perpendicular polarization between the quarks and the
nucleon, the third term drops out and the fourth onecreates a significant impact, leading to a distortion also
in the $b_x$ direction.

$\rho_0(x_1, x_2, x_3) = b_0 \langle x \rangle_\rho.$

FIG. 4: Contours of the first moment of the probability
density defined in Eq. (1) $\langle x \rangle_\rho$ [fm$^{-2}$]. The notation is the same as in Fig. 2.

In Fig. 5 we show the second moment of the probability
densities for the same four cases discussed in Fig. 4. A
general observation is that the distortion is milder and
the densities are more localized around $b_\perp = 0$. One
reason is that $A_{20}(t)$ is relatively flat compared to $A_{10}(t)$,
leading to a rather localized density.

$\rho_0(x_1, x_2, x_3) = b_0 \langle x \rangle_\rho.$

Summary: A lattice QCD calculation of the ﬁrst two
Mellin moments of the isovector transverse quark spin
densities in the nucleon is presented. The calculation is
performed using three twisted-mass fermion ensembles
with lattice spacings $a \approx 0.057$, 0.069, 0.080 fm enabling
for the ﬁrst time a controlled continuum extrapolation
directly at the physical value of the pion mass. The ex-
trapolation shows that discretization effects are mild for
the targeted quantities. We conﬁrm the existence of a
sizeable Sivers and Boer-Mulders effect determining the
anomalous tensor magnetic moment $\kappa_T = 1.051(94)$. Re-
sults for the transverse quark spin densities demonstrate

that signiﬁcant deformations exist in the nucleon that
are more prominent for the ﬁrst moment. For the sec-
ond moment the densities are more localized around the
center of momentum of the proton.

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