Nucleon structure from Lattice QCD at nearly physical quark masses

Gunnar Bali for RQCD

with Sara Collins, Benjamin Gläßle, Meinulf Göckeler, Johannes Najjar, Rudolf Rödel, Andreas Schäfer, Wolfgang Söldner and André Sternbeck

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Proton structure	Lattice QCD set-up	Mass	Spin	Other charges	Momentum fraction	Summary
Outline						
o a time						

- Importance of proton structure beyond QCD
- Lattice QCD set-up
- Mass: σ-terms
- Spin: The Δq 's and g_A
- Other couplings
- Momentum fraction: $\langle x \rangle_{u-d}$
- Summary

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Other charges Mon

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Summary

Protons in use e.g. at the LHC



What is known about parton distribution functions?

The u and d PDFs are well-known from experiment, e.g., at DESY. Strangeness and gluonic PDFs have much larger uncertainties.

Generated using

http://hepdata.cedar.ac.uk/pdfs
from the NNPDF2.3 data set.
NNPDF: R D Ball et al,
NPB 867 (13) 244



Nucleons as dark matter probes: XENON1T at Gran Sasso



y-scale of shaded areas depends on scalar couplings $m_q \langle N | \bar{q}q | N \rangle$.

- ... essential to constrain beyond-the-Standard-Model (BSM) dark matter candidates, relating predictions to experimental limits.
- ... important to predict cross-sections for processes on the quark-gluon level. Experiment e.g. unable to directly measure strangeness and gluon PDFs.
- ... needed to relate QCD to low energy effective theories that are also relevant for precision experiments.

Here I concentrate on

- ▶ How is the mass distributed among the partons? (scalar couplings)
- How is the spin distributed? (axial couplings)
- ▶ Proton-neutron transition couplings. $(g_S, g_T, \tilde{g}_T, g_P, g_P^*)$
- ► How is the momentum distributed? (moments of PDFs)

Proton structure	Lattice QCD set-up	Mass	Spin	Other charges	Momentum fraction	Summary
Lattice C)CD					



typical values: $a^{-1} = 2-5$ GeV, Na = 2-7 fm continuum limit: $a \rightarrow 0$, Na fixed infinite volume: $Na \rightarrow \infty$

$$\langle \mathbf{O} \rangle = rac{1}{Z} \int [dU] \, [d\psi] [d\bar{\psi}] \, \mathbf{O}[U] e^{-S[U,\psi,\bar{\psi}]}$$

"Measurement": average over a representative ensemble of gluon configurations $\{U_i\}$ with probability $P(U_i) \propto \int [d\psi] [d\bar{\psi}] e^{-S[U,\psi,\bar{\psi}]}$

$$\langle \mathbf{O} \rangle = \frac{1}{n} \sum_{i=1}^{n} \mathbf{O}(U_i) + \Delta \mathbf{O} \qquad \Delta \mathbf{O} \propto \frac{1}{\sqrt{n}} \stackrel{n \to \infty}{\longrightarrow} 0$$

QCD

Proton structure Lattice QCD set-up Mass Spin Other charges Momentum fraction Summary

Input: discretized
$$\mathscr{L}_{QCD} = \frac{1}{16\pi\alpha_L(a)}FF + \bar{q}_f(\not\!\!D + m_f(a))q_f$$

$$m_N^{\text{latt}} = m_N^{\text{phys}} \longrightarrow a$$

 $m_\pi^{\text{latt}}/m_N^{\text{latt}} = m_\pi^{\text{phys}}/m_N^{\text{phys}} \longrightarrow m_u(a) \approx m_d(a)$

Output: hadron masses, matrix elements, decay constants, etc...

Required:

- 1. $L = Na \rightarrow \infty$: FSE suppressed with $\exp(-Lm_{\pi}) \Rightarrow Lm_{\pi} \gtrsim 4$.
- 2. $m_q^{\text{latt}} \rightarrow m_q^{\text{phys}}$: chiral perturbation theory (χ PT) helps for m_{ud} but m_{ud}^{latt} must be sufficiently small to start with ($m_\pi \lesssim 200 \text{ MeV}$?).
- 3. $a \to 0$: functional form known: $\mathcal{O}(a^2), \mathcal{O}(\alpha_s a) \Rightarrow \approx 4$ lattice spacings.

Other charges

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Momentum fraction Summary

Landscape of recent lattice simulations



Computational challenges

Cost of simulation is proportional to

- number of points: $(L/a)^4$
- condition number of linear system: $1/m_{\pi}^2$
- $L^{1/2}/m_{\pi}$ in (Omelyan) time integration within hybrid Monte Carlo
- $1/a^{\geq 2}$ critical slowing down (autocorrelations)

Adjusting $L \propto 1/m_{\pi}$ this means:

$$\mathrm{cost} \propto rac{1}{a^{\geq 6} \, m_\pi^{7.5}}$$

In addition: for baryonic observables at small m_{π} serious signal/noise problem.

State of the art: $64^3\times 128$ sites, corresponding to $\approx (4\times 10^9)^2$ (sparse) complex matrices.

Tremendous progress in Hybrid Monte Carlo, solver, noise reduction.



"Self-averaging" over many source points increases statistics. Becomes increasingly important towards small m_{π} .

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Nucleon structure

Three point functions

Evaluate $\langle N | \bar{q} \Gamma q | N \rangle$ (Lines: quark "propagators" M_{xy}^{-1} , $M = D + m_q$) $\mathcal{O} = \bar{q} \Gamma q$



 $q \in \{u, d\}$: both quark-line connected and disconnected terms. q = s: only the disconnected term.

"Connected" requires only 12 rows (spin × colour) of M^{-1} . "Disconnected" $12N^3$ rows (timeslice): stochastic "all-to-all" methods. "Disconnected" cancels ($m_u = m_d$, $Q \not = D$) from isovector combinations: "proton minus neutron", i.e. $\langle p | (\bar{u} \Gamma u - \bar{d} \Gamma d) | p \rangle = \langle p | \bar{u} \Gamma d | n \rangle$.

disconnected

- $N_f = 2$ NP improved Sheikholeslami-Wilson fermions, Wilson glue.
- Lm_{π} up to 6.7, *a* down to 0.06 fm, m_{π} down to 150 MeV.
- \blacktriangleright Two lattice spacings around $m_\pi \approx 290$ MeV, three around 425 MeV.
- 300–600 Wuppertal=Gauss smearing iterations on top of APE smearing.

#	β	<i>a</i> /fm	κ	V	$m_{\pi}/{ m MeV}$	Lm_{π}	n _{conf}	$t_{ m sink}/a$
Ι	5.20	0.081	0.13596	$32^3 \times 64$	280	3.69	1986(4)	13
П	5.29	0.071	0.13620	$24^{3} \times 48$	426	3.71	1999(2)	15
Ш			0.13620	$32^3 imes 64$	423	4.90	1998(2)	15,17
IV			0.13632	$32^3 imes 64$	295	3.42	2023(2)	7,9,11,13,15,17
V				$40^3 imes 64$	289	4.19	2025(2)	15
VI				$64^3 imes 64$	289	6.71	1232(2)	15
VII			0.13640	$48^3 imes 64$	160	2.78	3442(2)	15
VIII				$64^3 \times 64$	150	3.47	1593(3)	9,12,15
IX	5.40	0.060	0.13640	$32^3 \times 64$	490	4.81	1123(2)	17
Х			0.13647	$32^3 imes 64$	426	4.18	1999(2)	17
XI			0.13660	$48^3 imes 64$	259	3.82	2177(2)	17

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Ensembles II



Decomposition of the proton (and pion) mass I

$$m_{N} = \underbrace{\sum_{q \in \{u,d,s,\ldots\}}}_{\text{quarks}} m_{q} \langle N | \bar{q} \mathbbm{1} q | N \rangle}_{\text{quarks}} + \underbrace{\left\langle N \left| \frac{1}{8\pi\alpha_{L}} (\mathbf{E}^{2} - \mathbf{B}^{2}) + \sum_{q} \bar{q} \mathbf{D} \cdot \gamma q \right| N \right\rangle}_{\text{gluon interactions (Eucl. spacetime)}} + \underbrace{\frac{1}{4} \left(m_{N} - \sum_{q} m_{q} \langle N | \bar{q} \mathbbm{1} q | N \rangle \right)}_{\text{trace anomaly}}$$

VEV $\langle 0|\bar{q}q|0\rangle$ is understood to be subtracted from $\langle N|\bar{q}q|N\rangle$. Pion-nucleon σ -term: $\sigma_{\pi N} = m_u \langle N|\bar{u}u|N\rangle + m_d \langle N|\bar{d}d|N\rangle = \sigma_u + \sigma_d$. Scalar particles (Higgs, neutralino etc.) couple \propto quark matrix elements.



Decomposition of the proton (and pion) mass II

$$\sigma_{\pi} = m_{ud} \langle \pi | \bar{u}u + \bar{d}d | \pi \rangle = m_{ud} \frac{\partial m_{\pi}}{\partial m_{ud}} \quad \underbrace{= \frac{m_{\pi}}{2}}_{\text{GMOR}} + \mathcal{O}(m_{\pi}^3) \,.$$

Therefore:



 σ_{π} can be further decomposed into valence and sea quark contributions. Wilson fermions: singlet and non-singlet mass renormalization constants differ by $r_m > 1 \Rightarrow$ "valence" > "connected":

$$r := \frac{\langle \pi | \bar{u}u + \bar{d}d | \pi \rangle^{\text{sea}}}{\langle \pi | \bar{u}u + \bar{d}d | \pi \rangle} = r_m \left(\frac{\langle \pi | \bar{u}u + \bar{d}d | \pi \rangle^{\text{dis}}}{\langle \pi | \bar{u}u + \bar{d}d | \pi \rangle_{\text{lat}}} - 1 \right) + 1$$

Pion mass: σ_{π} compared to $m_{\pi}/2$



[S Collins, D Richtmann]

The theoretical expectation $\sigma_{\pi} \approx m_{\pi}/2$ is confirmed.



Pion mass: light sea quark and strange quark contribs.



Less than $\sim 10\%$ of σ_{π} (or $\sim 5\%$ of the mass) is due to sea quarks. Strange quarks are negligible too.

Nevertheless, $r_m = Z_m^{\rm singlet}/Z_m^{\rm nonsinglet} > 1$ means at $a \approx 0.071$ fm about 30% of the signal originates from the disconnected contribution. So this needs to be computed even for the valence quark contribution.



$\sigma_{\pi N}$ for the nucleon



The non-vanishing light quark masses are directly responsible for only ≈ 35 MeV of the nucleon mass but for 68 MeV of the pion mass! This may not be too surprising since $m_N \not\rightarrow 0$ as $m_{ud} \rightarrow 0$.

Chiral extrapolation of the nucleon mass





Proton structure Lattice QCD set-up Mass Spin Other charges Momentum fraction Summary

The scalar matrix elements $m_q \langle N | \bar{q}q | N \rangle$ determine the coupling of the nucleon to scalar particles at zero recoil:

$$\frac{f_N}{m_N} \approx \sum_{q \in \{u,d,s\}} f_{\mathcal{T}_q} \frac{\alpha_q}{m_q} + \frac{2}{33-6} f_{\mathcal{T}_G} \sum_{q \in \{c,b,t,\ldots\}} \frac{\alpha_q}{m_q}$$

Cross section $\propto |f_N|^2$. Higgs example: $\alpha_q \propto m_q/m_W$.

$$f_{T_q} \equiv rac{m_q \langle N | ar{q} q | N
angle}{m_N}$$

are the contributions of the light quark masses to the proton mass and

$$f_{\mathcal{T}_G} pprox 1 - \sum_{q \in \{u,d,s\}} f_{\mathcal{T}_q}$$
.

Little about f_{T_q} is known experimentally.



Scalar strangeness content



[QCDSF: GB et al, arXiv:1111.1600, RQCD: S Collins et al, in preparation]: NPI Wilson [M Engelhardt, arXiv:1210.0025]: domain wall on staggered [ETMC, C Alexandrou et al, arXiv:1309.7768]: twisted mass

Proton structure	Lattice QCD set-up	Mass	Spin	Other charges	Momentum fraction	Summary
Spin of t	he nucleon					

$$\frac{1}{2} = \frac{1}{2}\Delta\Sigma + \sum_{q,\bar{q}} L_q + J_g :$$

Ji decomposition into the contributions of the (longitudinal) quark spins

$$\Delta\Sigma = \Delta u + \Delta \bar{u} + \Delta d + \Delta \bar{d} + \Delta s + \Delta \bar{s} + \cdots,$$

the (longitudinal) quark and antiquark orbital angular momenta $L_q = J_q - \frac{1}{2}\Delta q$ and the (longitudinal) gluon total angular momentum J_g .

Naïve non-relativistic SU(6) quark model: $\Delta \Sigma = 1$, $L_q = J_g = \Delta s = 0$. Relativistic quark models: $\Delta \Sigma \sim 0.6$, $L_{\rm quarks} \sim 0.2$.

I will say nothing about the Jaffe and Manohar decomposition:

$$\frac{1}{2} = \frac{1}{2}\Delta\Sigma + \mathcal{L}_{\rm quarks} + \Delta G + \mathcal{L}_g \quad \left(J_g \neq \Delta G + \mathcal{L}_g, J_q \neq \frac{1}{2}\Delta q + \mathcal{L}_q\right) \,.$$



The total quark angular momenta $J_q = \frac{1}{2}\Delta q + L_q$ can be extracted from generalized form factors at $q^2 = 0$:

$$J_q + J_{\bar{q}} = rac{1}{2} \left[A^q_{20}(0) + B^q_{20}(0)
ight] \, ,$$

where $A_{20}^q(q^2)$ and $B_{20}^q(q^2)$ are obtained from matrix elements of local quark bilinears of the form

$$\left\langle N, s', p+q \left| \bar{q} \gamma^{\{\mu_1 \overleftrightarrow{D}^{\mu_2}\}} q \right| N, s, p \right\rangle$$
.

Then

$$L_q=J_q-rac{1}{2}\Delta q\,,\qquad J_g=rac{1}{2}-\sum_{q,ar{q}}J_q\,,$$

Individual quark spin contributions $(q \in \{u, d, s\})$

$$(\Delta q + \Delta \bar{q}) \; s_{\mu} = rac{1}{m_{\mathcal{N}}} \langle \mathcal{N}, s \left| \bar{q} \gamma_{\mu} \gamma_{5} q \right| \mathcal{N}, s
angle = \mathcal{F}_{\mathcal{A}}^{q}(0) = \tilde{\mathcal{A}}_{10}^{q}(0)$$

Axial charges:

а

$$\begin{split} a_{3} &= -s_{\mu} \frac{1}{m_{N}} \langle N, s | \bar{\psi} \gamma_{\mu} \gamma_{5} \lambda_{3} \psi | N, s \rangle = \Delta u - \Delta d = g_{A} \\ a_{8} &= -s_{\mu} \frac{\sqrt{3}}{m_{N}} \langle N, s | \bar{\psi} \gamma_{\mu} \gamma_{5} \lambda_{8} \psi | N, s \rangle \\ &= \Delta u + \Delta \bar{u} + \Delta d + \Delta \bar{d} - 2\Delta s - 2\Delta \bar{s} \\ a_{0}(Q^{2}) &= -s_{\mu} \frac{1}{m_{N}} \langle N, s | \bar{\psi} \gamma_{\mu} \gamma_{5} \mathbb{1} \psi | N, s \rangle \\ &= \Delta u + \Delta \bar{u} + \Delta d + \Delta \bar{d} + \Delta s + \Delta \bar{s} = \Delta \Sigma (Q^{2}) \,. \end{split}$$

 $\psi = (u, d, s)^t$, λ_j are Gell-Mann flavour matrices. $a_3 = g_A$ known from neutron β decay, assuming isospin symmetry. a_8 usually estimated from hyperon β decay, assuming SU(3)_F symmetry.

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Nucleon structure



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Extraction of the Δq 's from experiment

DIS gives spin structure functions of proton and neutron $g_1^{p,n}(x, Q^2)$. First moment related to a_i 's via OPE (leading twist):

$$\begin{split} \Gamma_1^{p,n}(Q^2) &= \int_0^1 \mathrm{d}x \, g_1^{p,n}(x,Q^2) &= \frac{1}{36} \left[(a_8 \pm 3a_3) C_{NS} + 4a_0 C_S \right] \\ \text{Use models to extrapolate } g_1 \text{ from experimental } x_{\min} \text{ to } x = 0! \\ C_{S/NS} &= C_{S/NS}(\alpha_s(Q^2)). \end{split}$$

Combinations of a_i give Δq 's, e.g., $(\Delta s + \Delta \bar{s})(Q^2) = \frac{1}{3}[a_0(Q^2) - a_8]$

SIDIS allows for direct measurements of the $\Delta q(x)$ but requires fragmentation functions.

[COMPASS, arXiv 1001.4654]

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DSSV: [de Florian et	al, arXiv:0904.3821]	
$(\Delta s + \Delta \overline{s})(5 { m GeV}^2)$	$-0.02\pm0.02\pm0.02$	$-0.10 \pm 0.02 \pm 0.02$
	Naive Extrap.	combined with DSSV

Proton structure

No continuum limit, $m_{\pi} \approx 290$ MeV \Rightarrow add 20 % systematic error.



 $\Delta s = -0.020(10)(4)$

Other charges

Comparison of recent lattice calculations



Consistency between different determinations: small $\Delta s + \Delta \bar{s}$. ETMC result shows statistical accuracy that is possible. Systematics! [QCDSF: GB et al, 1112.3354; M Engelhardt, 1210.0025; ETMC: A Abdel-Rehim et al, 1310.6339; χ QCD: Y Yang et al, unpublished.] Gunnar Bali (Regensburg) Nucleon structure Rec. 2

$\overline{J_q + J_{\bar{q}}} = \frac{1}{2} \left(A_{20}^q(0) + B_{20}^q(0) \right)$

From Lattice 14 review [M Constaninou, 1411.0078]



 ∇ : disconnected contribution included.

[LHPC: S Syritsyn et al, 1111.0718 ($N_f = 2 + 1$); QCDSF/UKQCD: A Sternbeck et al, 1203.6579 ($N_f = 2$); ETMC: C Alexandrou et al, 1104.1600, unpublished ($N_f = 2$); ETMC: C Alexandrou et al,

1303.5979 ($N_f = 2 + 1 + 1$).]



Spin Other charges

$g_A = \Delta u - \Delta d$



Finite volume effects predicted by χ PT similar for g_A and F_{π} \implies follow QCDSF: R Horsley et al, arXiv:1302.2233 and plot ratio



Extrapolation to physical point: $g_A/F_{\pi} = 13.88(29) \text{ GeV}^{-1}$ Expt: $g_A/F_{\pi} = 13.797(34) \text{ GeV}^{-1}$.

Using $F_{\pi}(\text{expt}) = 92.21$ MeV we obtain $g_A = 1.280(27)(35)$ Expt: $g_A = 1.2670(35)$.

g_A: summary of recent lattice results



QCDSF: 1302.2233 Mainz: 1311.5804 ETMC 2: 1312.2874 LHPC: 1209.1687 RBC/UKQCD: 1309.7942 ETMC 2+1+1: 1303.5979 PNDME: 1306.5435 RQCD: 1412.7336



Isovector scalar charge



LHPC: 1206.4527, PNDME: 1306.5435, ETMC: 1411.3494, RQCD: 1412.7336

Isovector tensor charge



ETMC 2: 1311.4670, RBC: 1003.3387, LHPC: 1206.4527, PNDME: 1306.5435, ETMC 2+1+1: 1311.4670, RQCD: 1412.7336

General remark: we vary a^2 only by a factor $1.8 \Rightarrow$ we cannot exclude lattice spacing effects of up to $0.071^2/(0.081^2 - 0.060^2) \cdot \Delta g \approx 1.7 \cdot \Delta g$.

Isovector electromagnetic formfactors

$$\langle p | \bar{u} \gamma_{\mu} d | n \rangle = \bar{u}_{p} (\mathbf{p}_{f}) \bigg[g_{V}(q^{2}) \gamma_{\mu} + \frac{\tilde{g}_{T}(q^{2})}{2m_{N}} i \sigma_{\mu\nu} q^{\nu} \bigg] u_{n}(\mathbf{p}_{i})$$

Dirac FF: $g_{V}(q^{2}) = F_{1}^{p}(q^{2}) - F_{1}^{n}(q^{2}) \xrightarrow{q^{2} \to 0} 1$
Pauli FF: $\tilde{g}_{T}(q^{2}) = F_{2}^{p}(q^{2}) - F_{2}^{n}(q^{2}) \xrightarrow{q^{2} \to 0} \kappa_{p} - \kappa_{n} \approx 3.7058901(5)$
 $g_{V}(Q^{2}) = 1 - \frac{r_{1}^{2}}{6}Q^{2} + \mathcal{O}(Q^{4}), \quad \tilde{g}_{T}(Q^{2}) = \tilde{g}_{T}(0) \left[1 - \frac{r_{2}^{2}}{6}Q^{2} + \mathcal{O}(Q^{4}) \right]$

Proton radius:

$$r_p^2 pprox r_1^2 + rac{3 ilde{g}_T(0)}{2 m_N^2} \, .$$

Dipole fit to determine the induced tensor charge $\tilde{g}_T = \tilde{g}_T(0)$:

$$ilde{g}_{\mathcal{T}}(Q^2) = rac{ ilde{g}_{\mathcal{T}}(0)}{\left(1 + r_2^2 Q^2 / 12\right)^2}$$

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Nucleon structure

Extrapolation of the Pauli formfactor at $m_{\pi} = 290 \text{ MeV}$

Difference between magnetic moment anomalies $\tilde{g}_T(0) = \kappa_p - \kappa_n$.



Extrapolation error decreases with smaller $Q_{\min}^2 = \pi^2/L^2$. Therefore, invisible FSE for $Lm_{\pi} > 3.4$ at $m_{\pi} = 290$ MeV (L > 2.3 fm) do not necessarily imply they are irrelevant within the smaller statistical errors at $m_{\pi} = 150$ MeV (L > 4.5 fm).

Induced isovector tensor charge

Extrapolating in the usual way... however, FSE are unquantifiable at the lightest mass point and O(a) improvement is not yet included.



QCDSF: 1106.3580, Mainz: 1311.5804 + 1411.4804, ETMC 2: 1102.2208, LHPC: 1404.4029, RBC: 0904.2039, ETMC 2+1+1: 1303.5979, PNDME: 1306.5435, RQCD: 1412.7336

Isovector quark momentum fraction: $\langle x \rangle_{u=d}^{MS}(2 \text{ GeV})$



 $Lm_{\pi} \approx 6.7$: $Lm_{\pi} > 4.1$: $Lm_{\pi} > 3.4: * * *$ $Lm_{\pi} \approx 2.8$: \triangle

Mild dependence on V, m_{π} . Renormalised non-perturbatively. $\mathcal{O}(a)$ leading errors, a varied from 0.08 to 0.06 fm.

Improvement on earlier calculations which suffered from excited state contamination $\langle x \rangle_{\mu=d}^{MS} (2 \text{ GeV}) \sim 0.25$.

Near physical point but more work needs to be done — lattice spacing dependence?



$\langle x \rangle_{u-d}^{MS}$ (2 GeV): summary of recent lattice results



PDFs from

S Alekhin et al, 1310.3059; CT10: J Gao et al, 1302.6246; NNPDF: R Ball et al 1207.1303; A Martin et al 0905.3531.

[ETMC, arXiv:1410.8761]: disconnected contributions small \Rightarrow predictions for $\langle x \rangle_q^{\overline{\text{MS}}}(2 \,\text{GeV})$ soon. Mixing between quarks and glue!

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Nucleon structure

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Summary	1					

- ► Lattice can contribute to many quantities that are hard to constrain by experiment, e.g., $\sigma_{\pi N}$, f_{T_s} , g_S , g_T .
- Lattice calculations are important to determine the spin content of the nucleon: Δq, ΔΣ, J_q, ⟨x⟩_{Δq},
- In the past disconnected quark line diagrams were often omited and differences quoted: g_A, ⟨x⟩_{u-d}, ..., but no Δs, ΔΣ, J_q, ⟨x⟩_q etc.
- Improved methods now allow for the calculation of these contributions.
- g_A seems to approach the physical value, once $Lm_{\pi} > 4$.
- ► ⟨x⟩_{u-d} comes out 20% bigger than expected. lattice spacing effects? Renormalization?
- ► Precision physics requires an extrapolation a → 0. For quite a few quantities however errors of 20% are acceptable.
- ► High Mellin moments almost impossible to compute ⇒ recent interest also in "quasi" parton distribution functions.

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Nucleon structure

