

Extracting parton distribution functions from lattice quantum chromodynamics

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William & Mary

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DOE Early Career Award DE-SC0023047

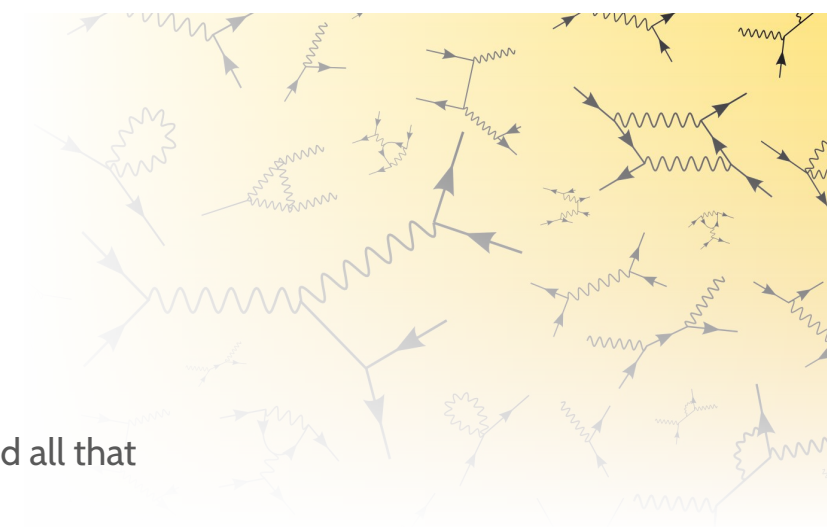
Overview

1. Introduction:

- Parton distribution functions
- Lattice quantum chromodynamics
- LaMET, quasi-distributions, pseudo-distributions and all that

2. Recent progress and results

- Quark distributions
- Gluon distributions

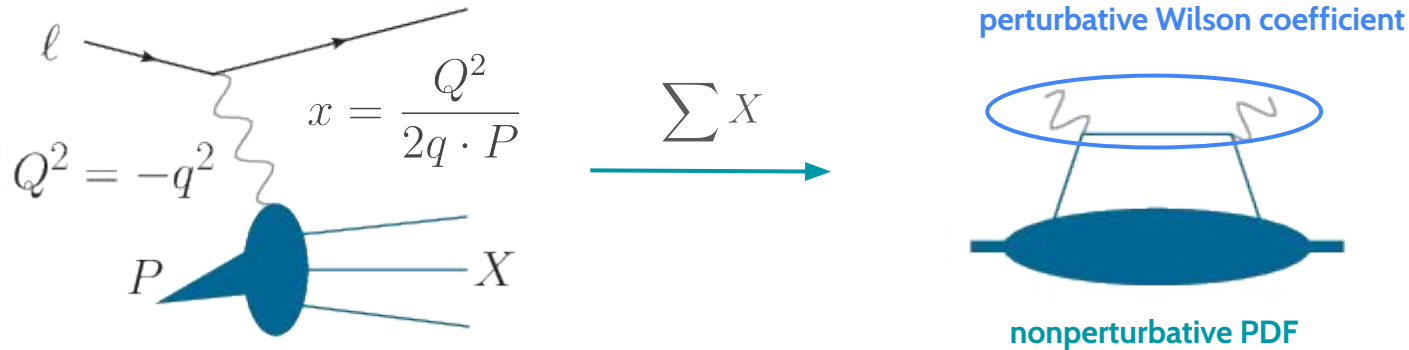


Parton distribution functions and inclusive scattering processes

Parton distribution functions (PDFs) encode longitudinal partonic structure of hadrons

- Directly connect the standard model to nuclear physics
- Important source of systematic uncertainties at hadron colliders

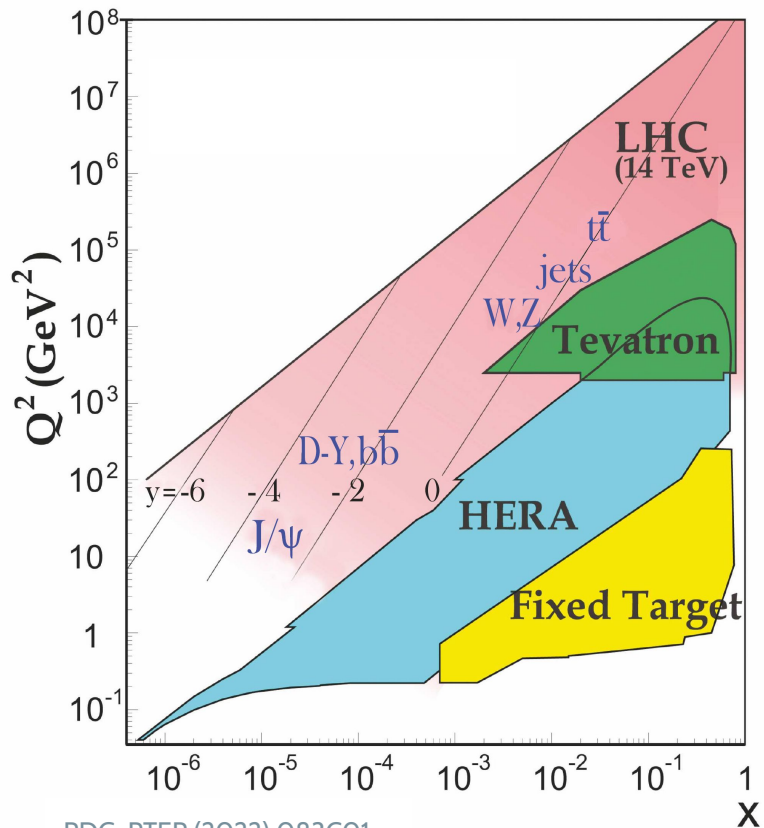
Deep inelastic scattering is the primary theoretical and experimental probe of PDFs



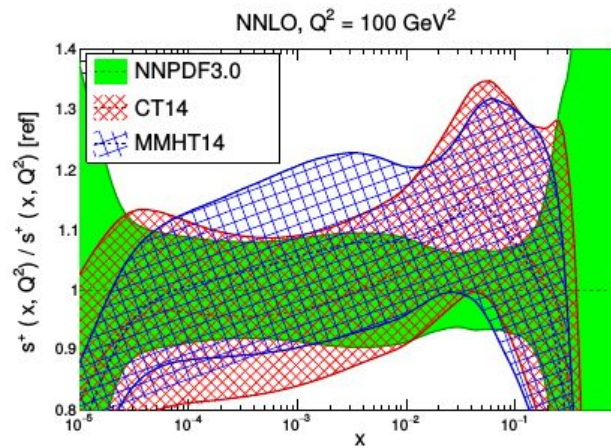
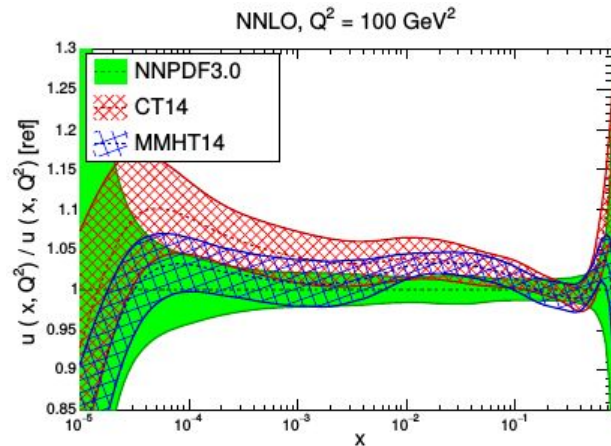
In QFT, PDFs are defined through matrix elements of fields at light-like separations

- Lattice QCD provides the primary method for systematic, first-principles calculations of QCD
- Lattice can only compute matrix elements of fields at space-like separations
- Until a decade ago, first principles' calculations of parton distribution functions were impractical

Phenomenological solution

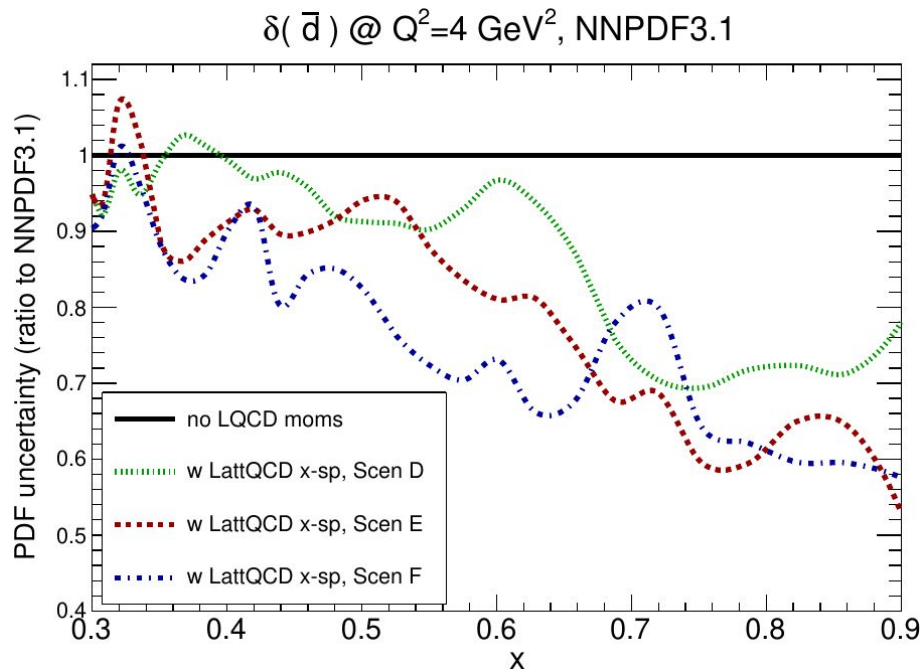


PDG, PTEP (2022) O83C01

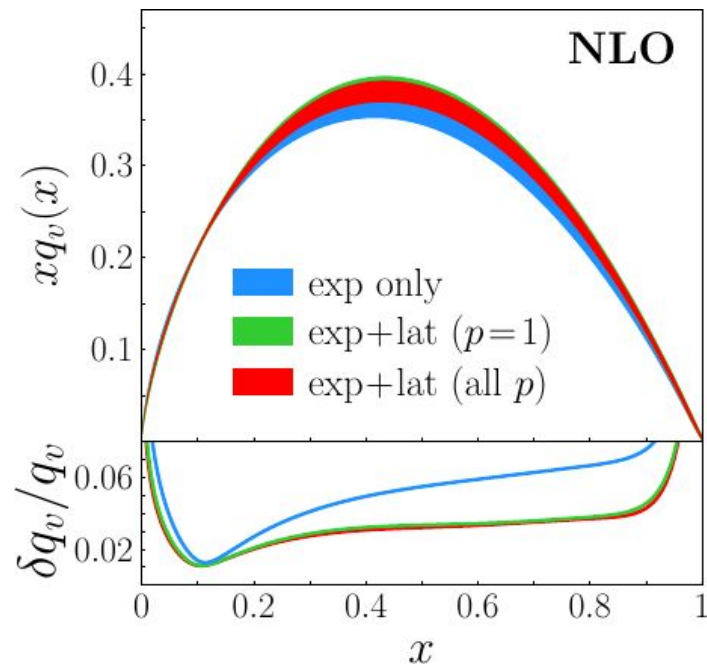


PDFs from QCD

First principles calculations complement, and inform, JLab 12 GeV, the LHC and the EIC



Lin et al., Prog. Nucl. Part. Phys. 100 (2018) 107



Barry et al., PRD 105 (2022) 114051

Lattice QCD

Provides a rigorous, nonperturbative, gauge-invariant definition of QCD

Formulated in the path integral representation of quantum field theory

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D} [\bar{\psi}, \psi, A] \mathcal{O} [\bar{\psi}, \psi, A] e^{iS_{\text{QCD}}[\bar{\psi}, \psi, A]}$$

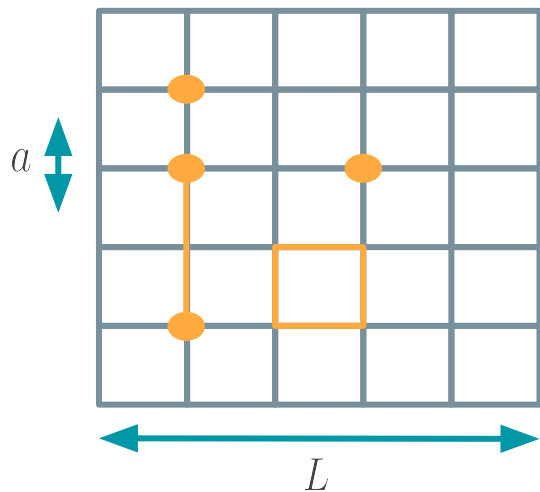
“Wick rotate” to Euclidean spacetime

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D} [\bar{\psi}, \psi, A] \mathcal{O} [\bar{\psi}, \psi, A] e^{-S_{\text{QCD}}[\bar{\psi}, \psi, A]}$$

Integral computed stochastically using Markov Chain Monte Carlo methods

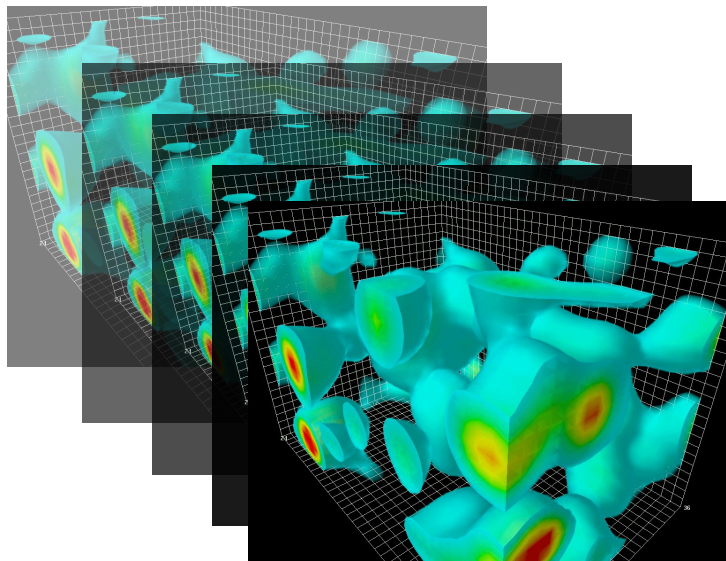
$$\langle \mathcal{O} \rangle \approx \frac{1}{\mathcal{Z}} \sum \mathcal{O} [\bar{\psi}, \psi, A] \Big|_{e^{-S_{\text{QCD}}[\bar{\psi}, \psi, A]}}$$

Lattice QCD: the numerical recipe



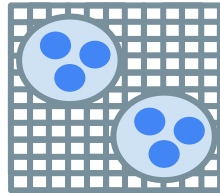
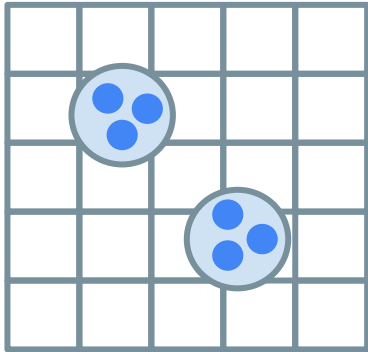
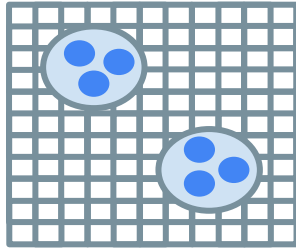
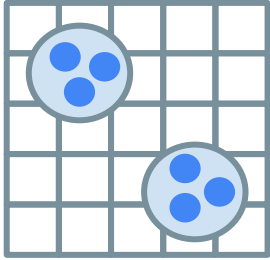
1. Take a small box of Euclidean spacetime and discretise the box to form a hypercubic spacetime lattice
2. Distribute quarks and gluons in the box - quarks on the nodes, gluons on the links

Lattice QCD: the numerical recipe



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3. Generate many copies (ensemble) of this QCD vacuum, with Boltzmann probability distribution $\exp[-S_{\text{QCD}}]$

Lattice QCD: the numerical recipe



1. Take a small box of Euclidean spacetime and discretise the box to form a hypercubic spacetime lattice
2. Distribute quarks and gluons in the box - quarks on the nodes, gluons on the links
3. Generate many copies (ensemble) of this QCD vacuum
4. On each copy, “measure” your correlation function and average
5. Repeat at finer lattice spacings and larger volumes and extrapolate to the continuum and infinite volume limits

Lattice QCD: the numerical costs

Finite volume effects

Discretisation effects

Excited state contamination at short times

Statistical uncertainty

Signal-to-noise issues in long Euclidean time limit

Renormalisation prescription

1. Take a small box of Euclidean spacetime and discretise the box to form a hypercubic spacetime lattice

2. Distribute quarks and gluons in the box - quarks on the nodes, gluons on the links

3. Generate many copies (ensemble) of this QCD vacuum

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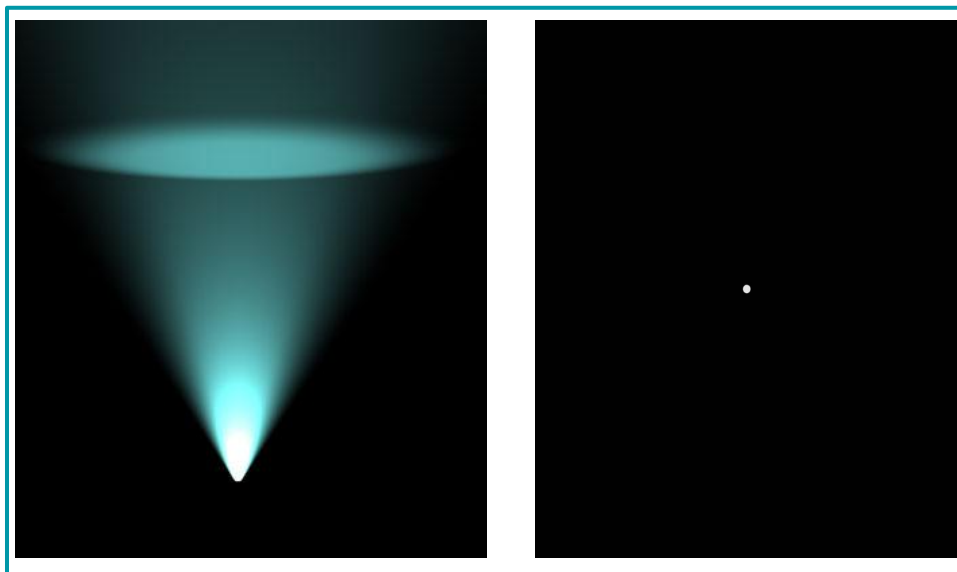
5. Repeat at finer lattice spacings and larger volumes and extrapolate to the continuum and infinite volume limits

Model dependency

Parton distribution functions: the challenge

Lattice QCD is formulated in a finite volume on a discretised Euclidean spacetime lattice

Lightcone not accessible



Parton distribution functions: the challenge

Lattice QCD is formulated in a finite volume on a discretised Euclidean spacetime lattice

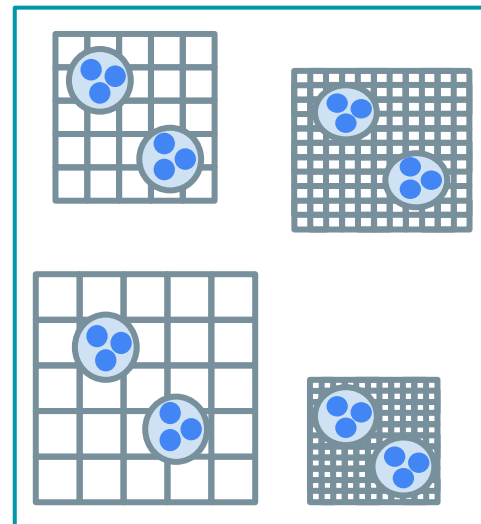
- Light cone not accessible

Path integral is sampled stochastically via Markov chain Monte Carlo

- Infinite momentum not accessible numerically!

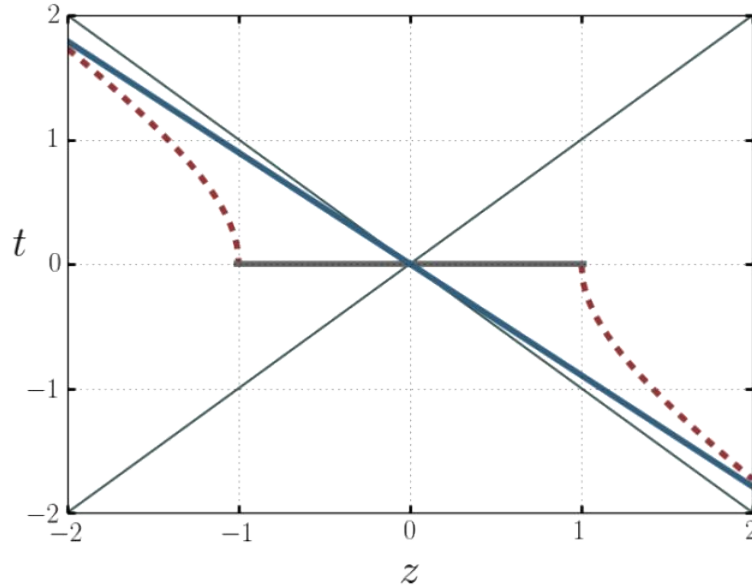
Static quantities extracted in the long Euclidean-time limit

- Noise-to-signal ratio increases exponentially with Euclidean time
- Particularly challenging for gluons



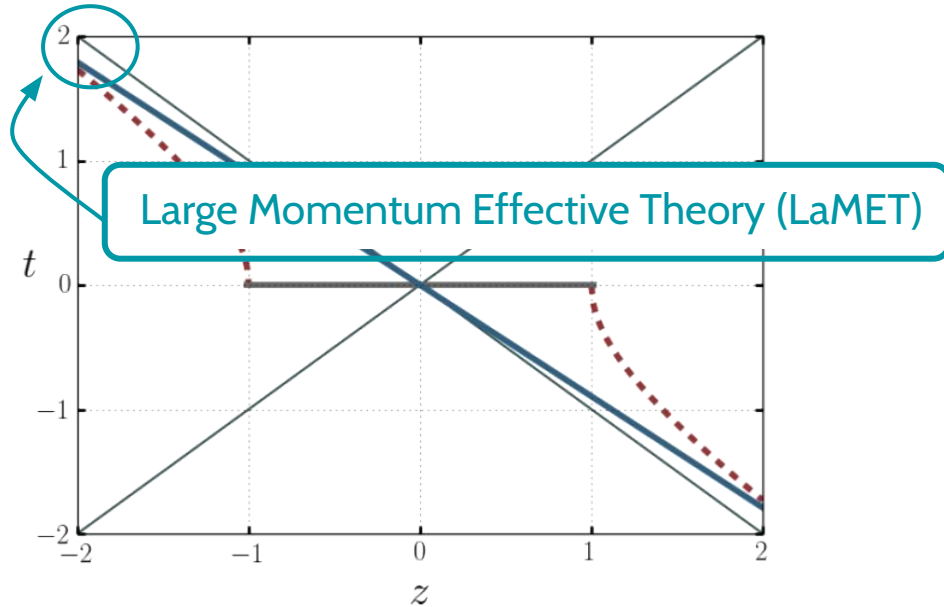
Large-momentum effective theory (LaMET)

Intuitive picture for PDFs - defined through operators of light-like separated fields



Large-momentum effective theory (LaMET)

Intuitive picture for PDFs - defined through operators of light-like separated fields



Large momentum effective theory (LaMET)

Framework to relate lattice-calculable to infinite-momentum quantities

Ji et al., PRL 111 (2013) 112002

- originally introduced to enable the calculation of the gluon spin contribution
- now a general framework for first principles' calculations

Effective theory: infinite momentum limit does not commute with removing the regulator

Relies on perturbative matching

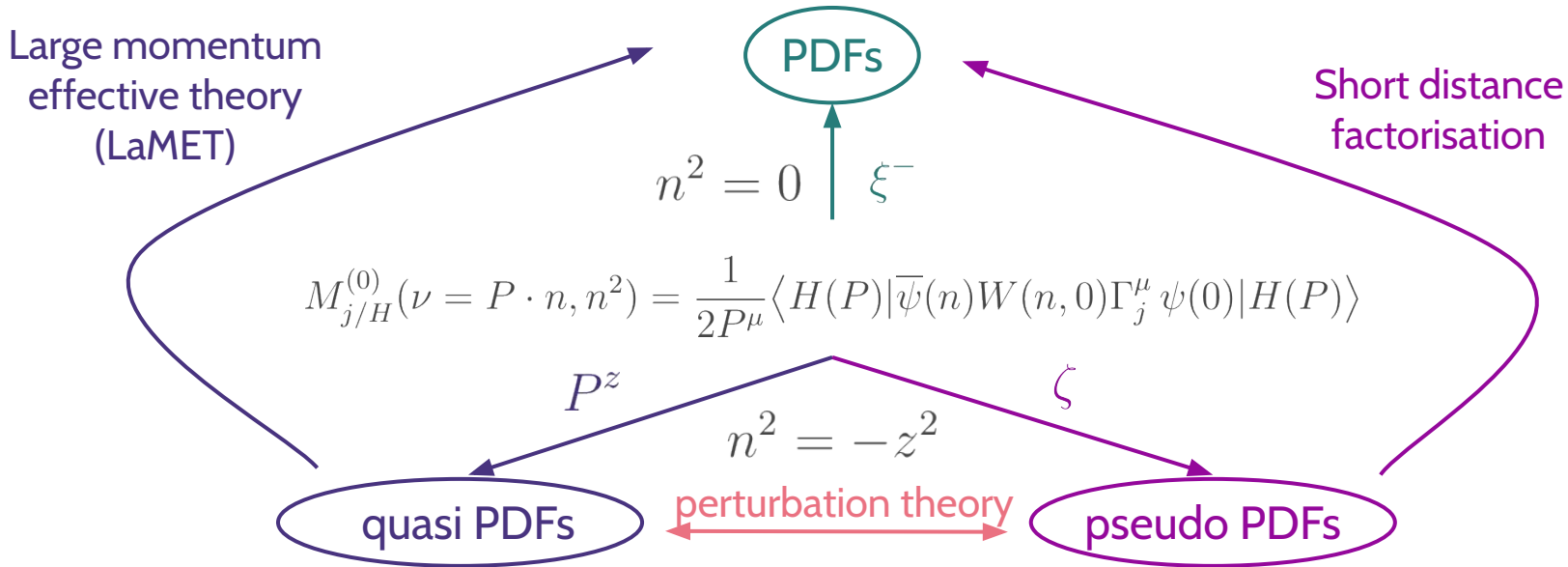
- Quantities required to have the same infrared behaviour
- For example, at one loop in the $\overline{\text{MS}}$ -bar scheme

$$\Delta G^{\overline{\text{MS}}}(\mu) = \frac{\alpha_s}{3\pi} \left[3 \ln \frac{\mu^2}{m^2} + 7 \right]$$

$$\Delta G^{\overline{\text{MS}}}(\mu, P_z) = \frac{\alpha_s}{3\pi} \left[\frac{5}{3} \ln \frac{\mu^2}{m^2} - \frac{1}{9} + \frac{4}{3} \ln \frac{P_z}{m^2} \right]$$

A panoply of distributions

$$f_{j/H}^{(0)}(\xi) = \int_{-\infty}^{\infty} \frac{d\omega^-}{4\pi} e^{-i\xi P^+ \omega^-} \langle H(P) | \bar{\psi}(0, \omega^-, \mathbf{0}_T) W(\omega^-, 0) \Gamma_j \psi(0) | H(P) \rangle$$

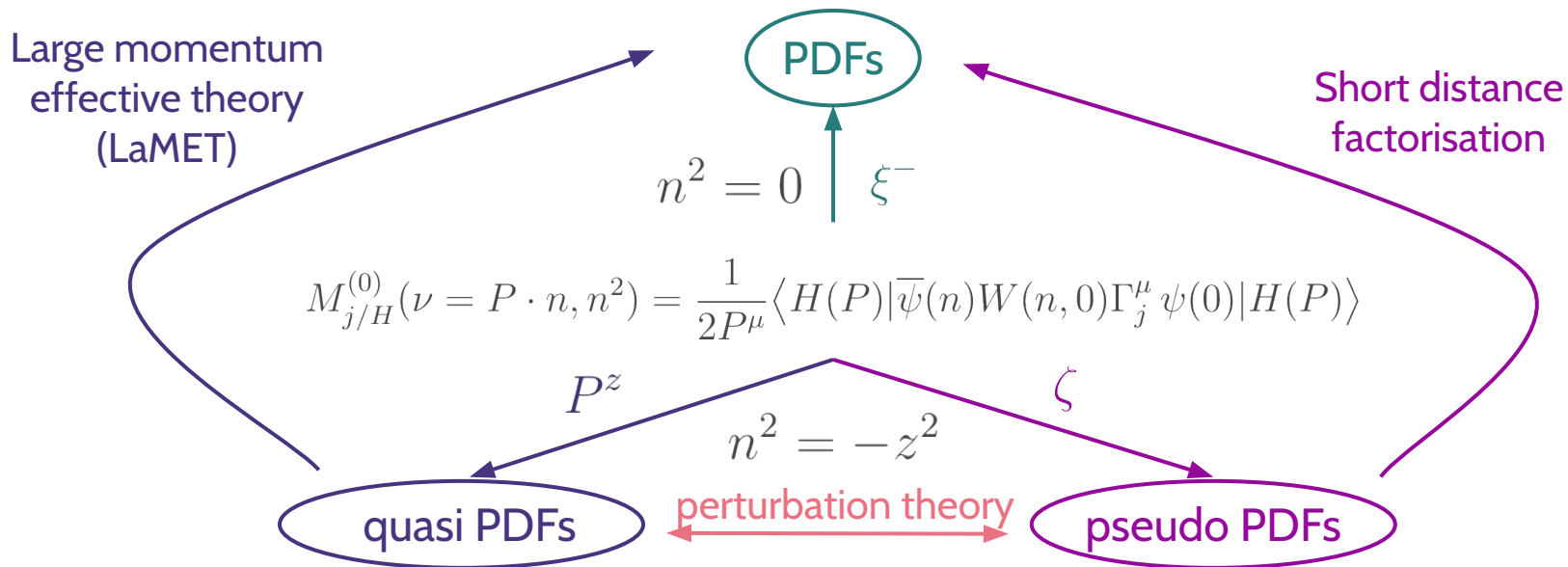


$$\tilde{f}_{j/H}^{(0)}(\xi, P^z) = \int_{-\infty}^{\infty} \frac{dz}{4\pi} e^{i\xi P_z z} \langle H(P) | \bar{\psi}(0, z, \mathbf{0}_T) W(z, 0) \Gamma_j \psi(0) | H(P) \rangle \quad \tilde{p}_{j/H}^{(0)}(\xi, z^2) = \int_{-\infty}^{\infty} \frac{d\zeta}{4\pi} e^{i\xi \zeta} \langle H(P) | \bar{\psi}(0, z, \mathbf{0}_T) W(z, 0) \Gamma_j \psi(0) | H(P) \rangle$$

A panoply of distributions

Lin et al., PNP 100 (2018) 107
 CJM, POS(LATTICE2018) 018
 Zhao, IMJPA 33 (2019) 1830033

Cichy & Constantinou, AHEP (2019) 3036904
 Constantinou et al., PNP 121 (2021) 130908
 Ji et al., RMP 93 (2021) 035005
 Constantinou et al., 2202.07193



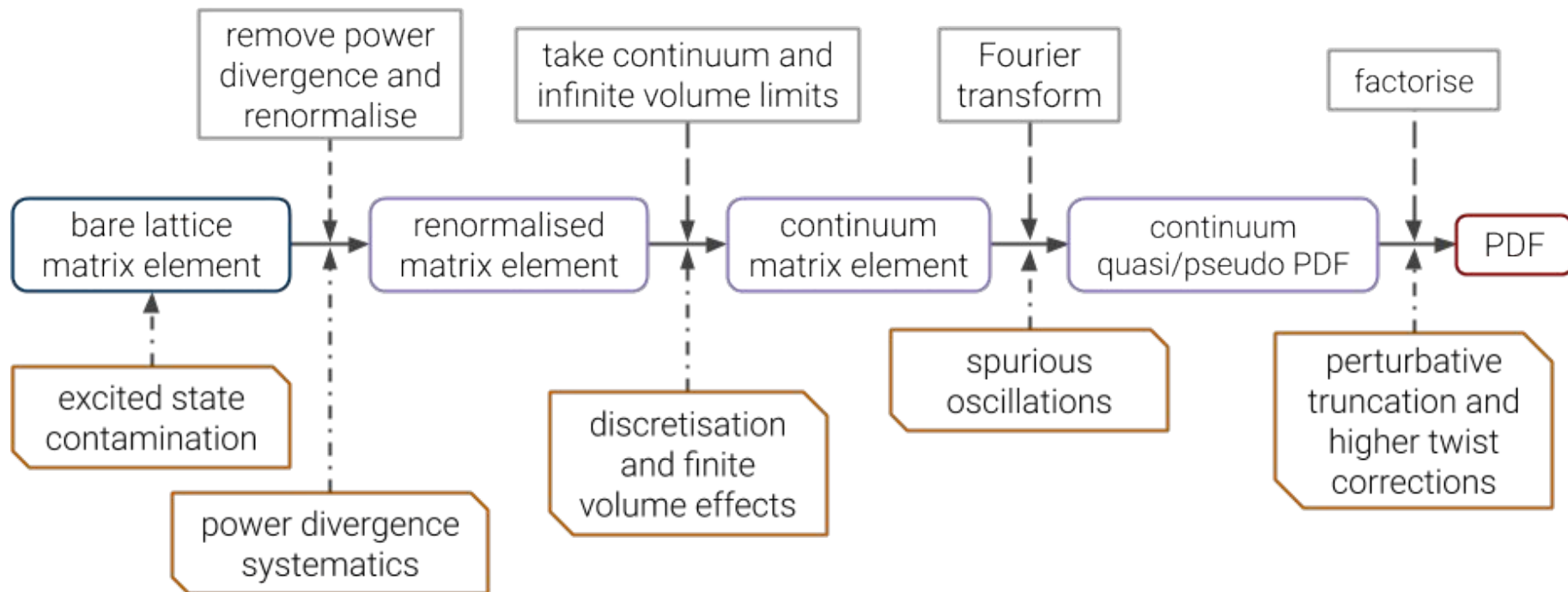
“Lattice cross-sections” factorisable matrix elements

$$\sigma_{j/H}(\xi, \dots) \in \left\{ \tilde{f}_{j/H}^{(0)}(\xi, P^z), \tilde{p}_{j/H}^{(0)}(\xi, z^2), \dots \right\}$$

Note: Davoudi & Savage, PRD 86 (2012) 054505
 Musch et al., PRD 83 (2011) 094507
 Braun & Müller, EPJC 55 (2008) 349
 Detmold & Lin, PRD 73 (2006) 014501
 Liu & Dong, PRL 72 (1994) 1790

In practice

CJM, POS(LATTICE2018) 018



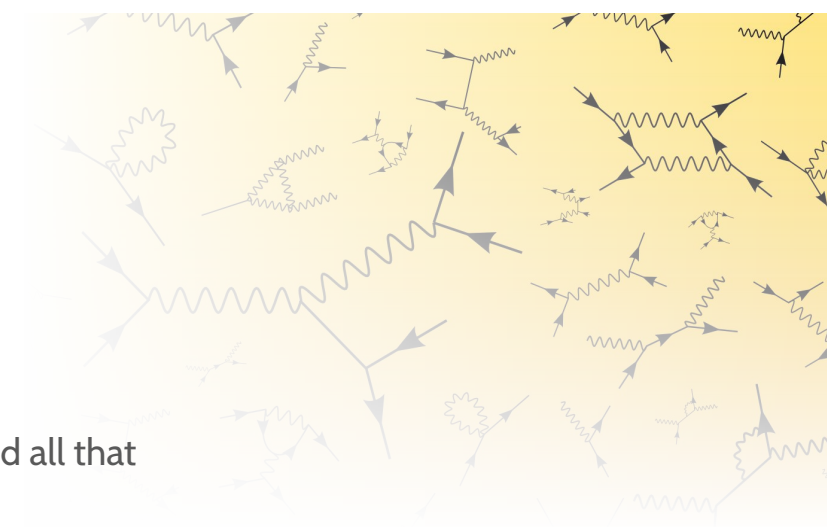
Overview

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2. Recent progress and results

- Quark distributions
- Gluon distributions



Current landscape of lattice calculations

Lattice determinations currently **innovative** but on the cusp of becoming **industrial**

Gao et al., PRD 107 (2023) 074509
Edwards et al., JHEP 03 (2023) 086
Bhat et al., PRD 106 (2022) 054504

Multiple collaborations investigating multiple theoretical approaches

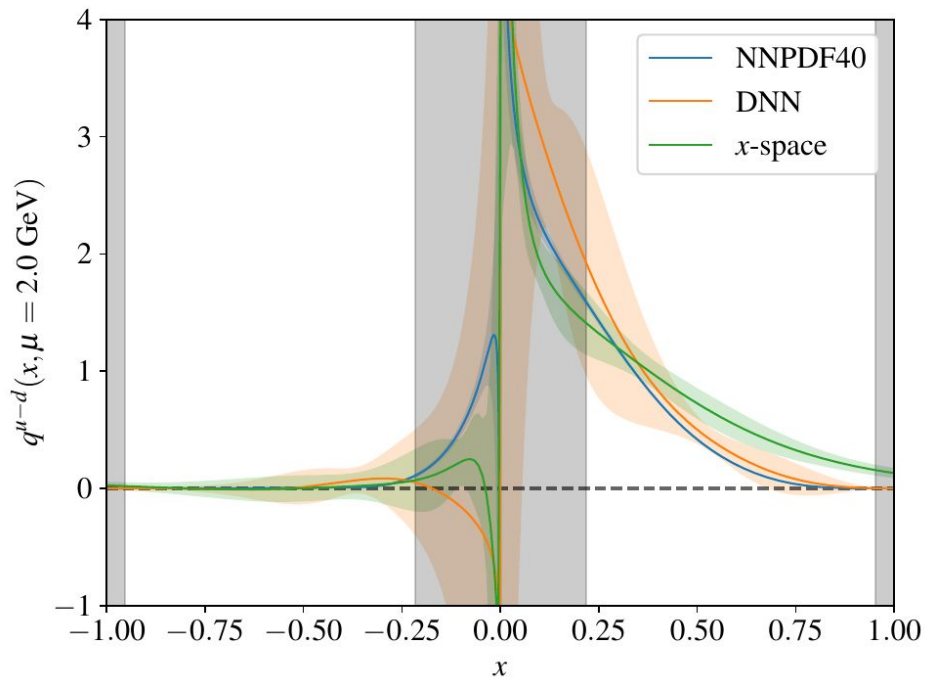
- Benchmark calculations of well-known valence quark PDFs of nucleons and pions
 - state-of-the-art calculations with multiple lattice spacings and volumes at physical pion masses
 - identifying, quantifying and reducing systematic uncertainties
- Exploratory calculations of poorly-known parton distribution functions
 - gluon and quark-singlet PDFs of nucleons
 - quark parton distribution functions of other mesons and baryons
 - calculations of distributions beyond leading twist
 - systematic uncertainties of **20%** will have **significant phenomenological impact**
- Exploratory calculations of poorly-known three-dimensional structure
 - valence quark GPDs
 - Collins-Soper kernel for rapidity evolution of TMDs
 - systematic uncertainties of **50%** will have **very significant phenomenological impact**

Gao et al., PRD 106 (2022) 074505
Gao et al., PRD 106 (2022) 114510
Gao et al., PRL 128 (2022) 142003
Egerer et al., PRD 105 (2022) 034507

Fan et al., PRD 108 (2023) 014508
Salas-Chavira et al., PRD 106 (2022) 0945110
Bhattacharya et al., PRD 104 (2021) 114510

Bhattacharya et al., PRD 106 (2022) 114512
Lin, PLB 824 (2022) 136821

Isvector unpolarised PDF of the nucleon



Gao et al., PRD 107 (2023) 074509

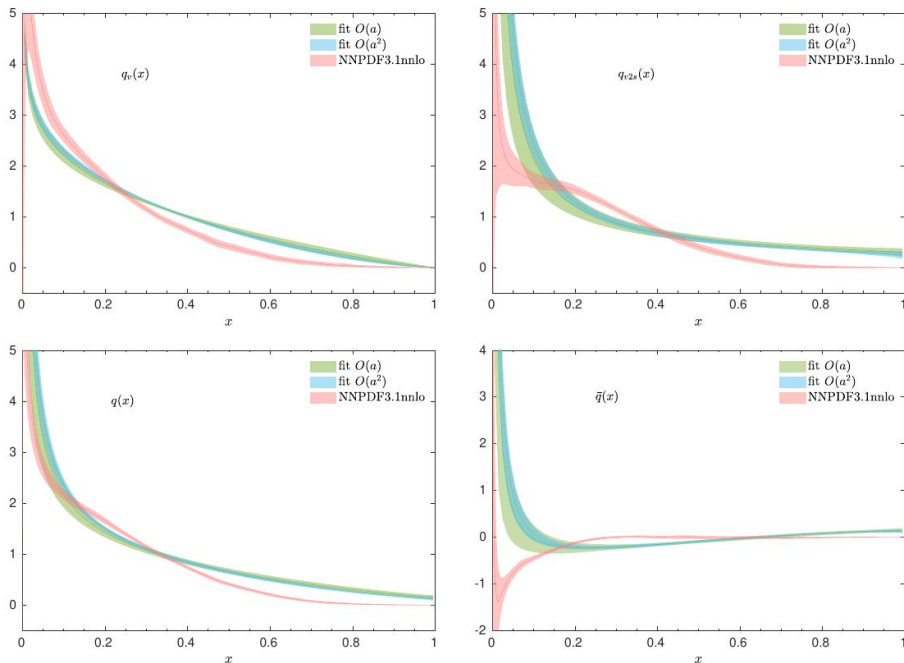
First determination using NNLO matching at physical pion mass

- $a = 0.076 \text{ fm}$, pion mass of 140 MeV
- $N_f = 2+1$ HISQ fermions
- maximum momentum of 1.53 GeV
- NNLO perturbative matching

Comparison of methods:

- fit to first four moments
- pseudo-PDF with deep neural network
- quasi-PDF with hybrid renormalization

Isvector unpolarised PDF of the nucleon



Bhat et al., PRD 106 (2022) 5 054504

First determination using NNLO matching with continuum extrapolation

- $a = 0.064, 0.082, 0.093$ fm,
- pion mass of 370 MeV
- $N_f = 2+1+1$ twisted mass fermions
- maximum momentum of 1.8 GeV
- NNLO perturbative matching
- pseudo-PDF approach

Comparison of reconstruction methods

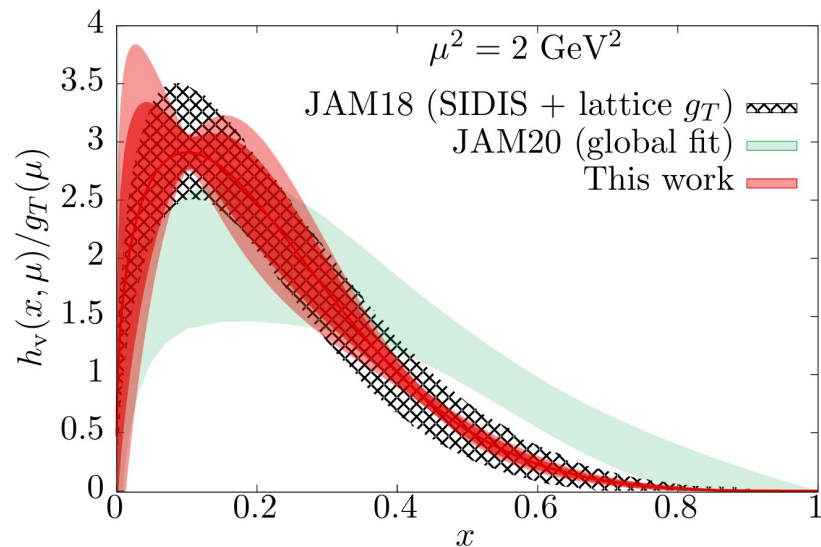
- naive Fourier transform
- Backus-Gilbert method
- model ansatz

Investigation of continuum limit

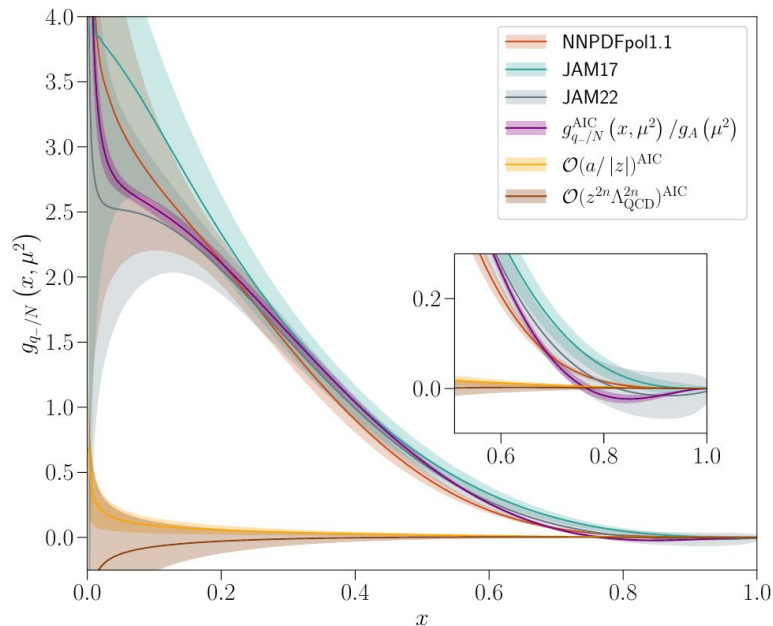
Transversity and helicity distributions of the nucleon

Determined via pseudo-PDF approach

- $a = 0.094$ fm and pion mass of 358 MeV
- $N_f = 2+1$ clover-Wilson fermions
- maximum momentum of 2.47 GeV

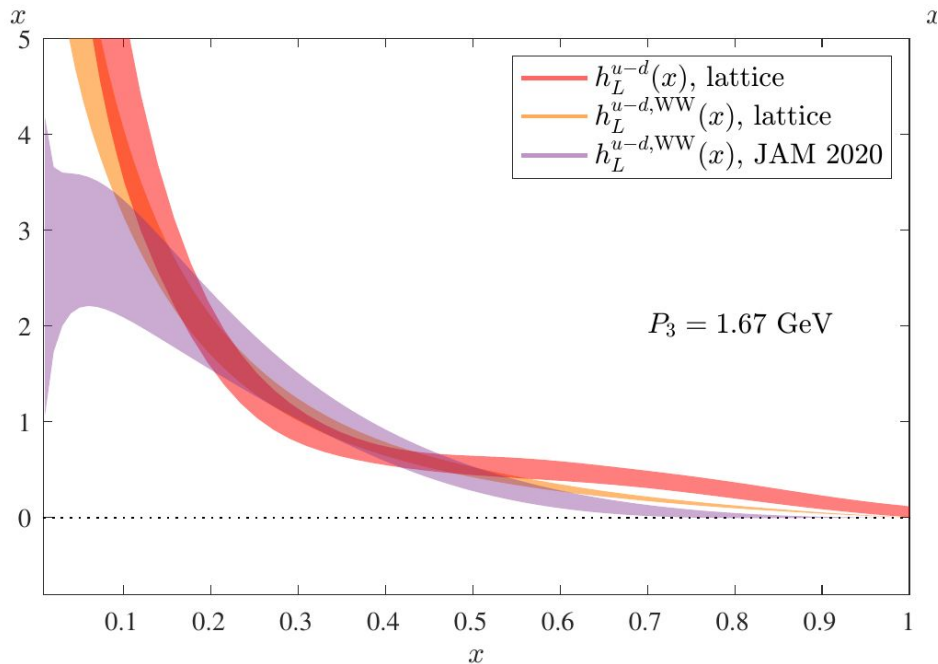


Egerer et al. (HadStruc), PRD 105 (2022) 034507



Edwards et al. (HadStruc), JHEP 03 (2023) 086

Isovector chiral-odd twist-3 PDF of the nucleon

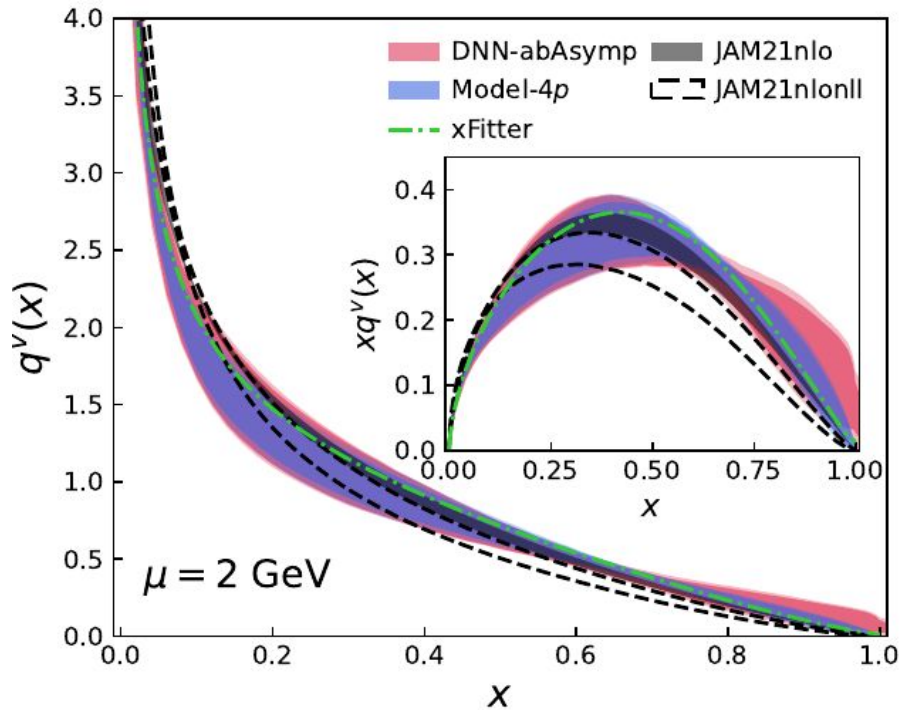


First determination of a twist-3 PDF

- $a = 0.093 \text{ fm}$, pion mass of 260 MeV
- $N_f = 2+1+1$ twisted mass fermions
- maximum pion momentum of 1.67 GeV
- quasi-PDF method

Comparison of Wandzura-Wilczek approximation to lattice data and global fit

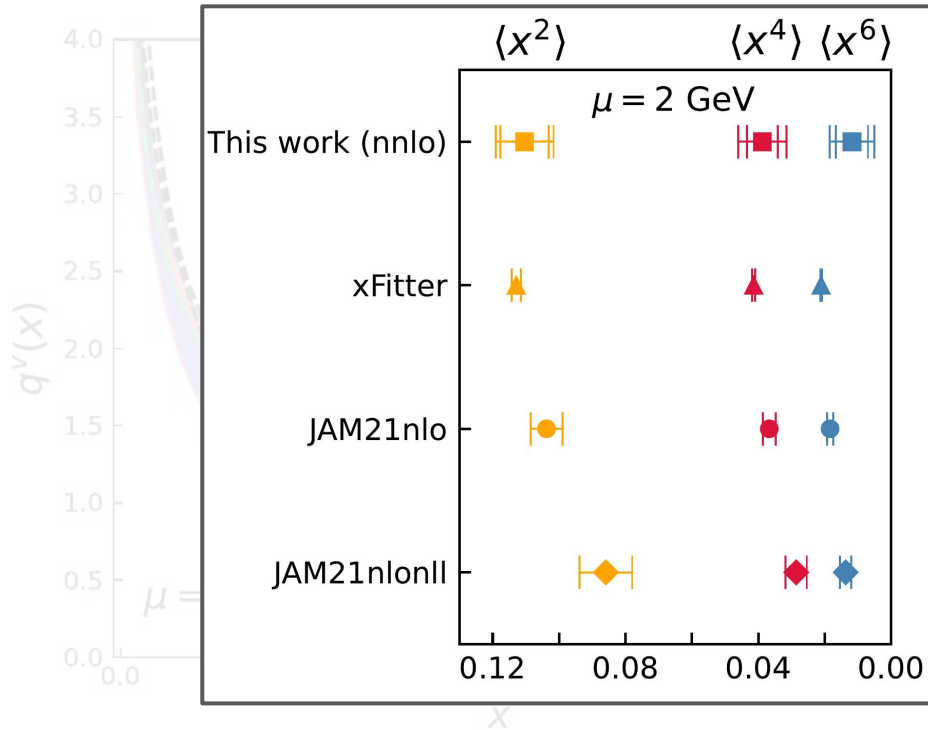
Isvector unpolarised light quark PDFs of the pion



First determination of continuum-extrapolation at physical pion mass

- $a = 0.04, 0.06, 0.075 \text{ fm}$,
- pion masses of 140 and 300 MeV
- $N_f = 2+1$ HISQ fermions
- maximum pion momentum of 2.42 GeV
- NNLO perturbative matching

Isovector unpolarised light quark PDFs of the pion



First determination of continuum-extrapolation at physical pion mass

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Gluons!

Gluons are key to understanding the visible universe

- Dominant contribution to mass of the visible universe
- Significant contribution to the spin of hadrons
- Fundamental to understanding a new form of matter: color glass condensate

Complete tomography of hadrons* needs detailed understanding of gluon structure

*a central goal of the largest US-based collider effort (EIC) for the next 20 years

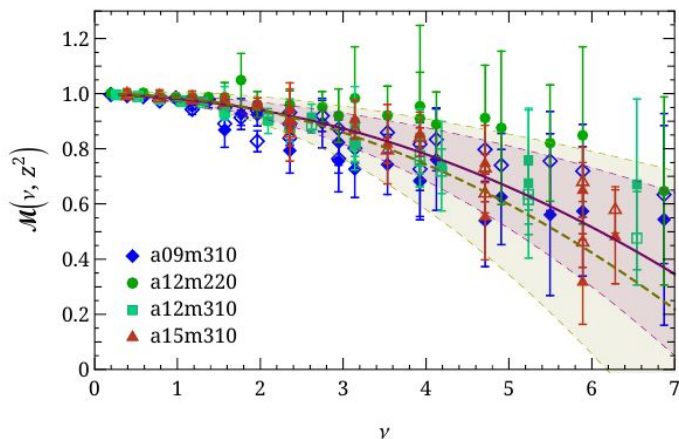
Opportunity for collaboration and interplay between theory and experiment

Exploratory calculations (one lattice spacing and pion mass)

Nucleons: Fan et al., PRL 121 (2018) 242001
Fan et al., IJMP A 36 (2021) 2150080
Khan et al. (HadStruc), PRD 104 (2021) 094516
Egerer et al. (HadStruc), PRD 106 (2022) 094511

Mesons: Fan et al., PLB 823 (2021) 136778
Salas-Chavira et al., PRD 106 (2022) 9 0945110

Unpolarised gluon distribution of the nucleon



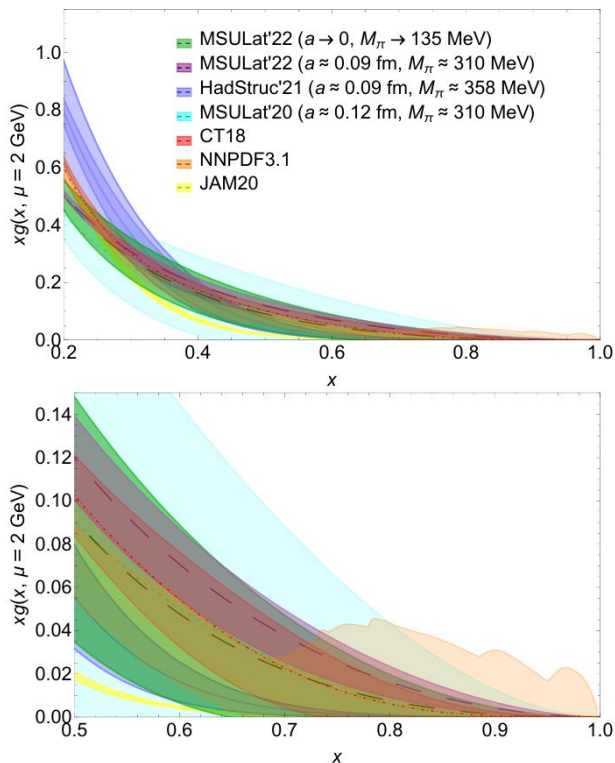
First determination of unpolarized gluon distribution in continuum and physical pion mass limits

Steps towards a precision calculation

- pseudo-distribution approach
- three lattice spacings and three pion masses
- clover-Wilson on $N_f = 2+1+1$ HISQ
- maximum nucleon momentum of 2.14 GeV

Demonstrates steps towards full quantitative control of systematic uncertainties for lattice calculations of gluon distributions

Unpolarised gluon distribution of the nucleon



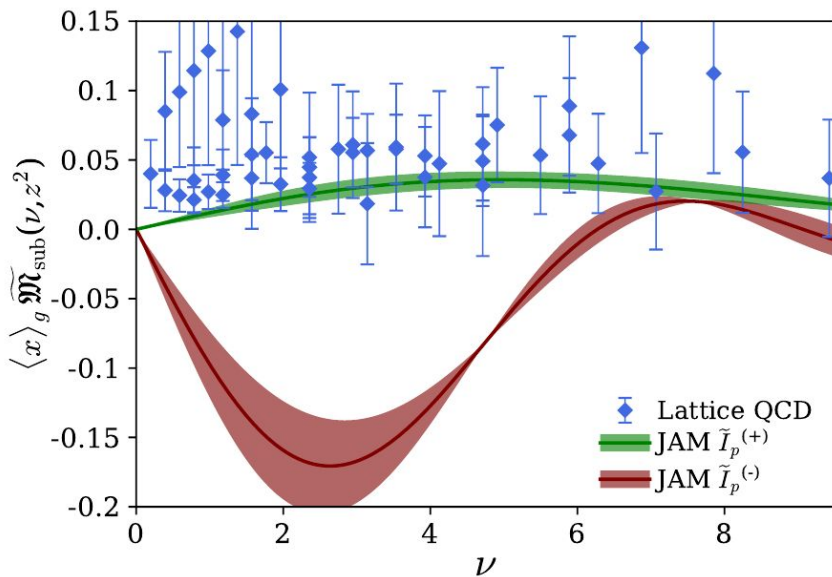
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- maximum nucleon momentum of 2.14 GeV

Demonstrates steps towards full quantitative control of systematic uncertainties for lattice calculations of gluon distributions

Polarised gluon distribution of the nucleon



Egerer et al. (HadStruc), PRD 106 (2022) 094511

First determination of polarized gluon distribution

Very poorly constrained from experiment

Proof-of-principle calculation

- one lattice spacing and one pion mass
- $N_f = 2+1$ clover-Wilson
- maximum nucleon momentum of 2.29 GeV

Demonstrates potential of lattice calculations, at the level of 20-50% precision, to understand poorly-constrained distributions

Lattice inputs for global analyses

QCD factorization: PDFs are universal hadronic quantities, independent of probe

- Extract from experimental cross-sections
- Extract from lattice matrix elements

JAM-HadStruc approach:

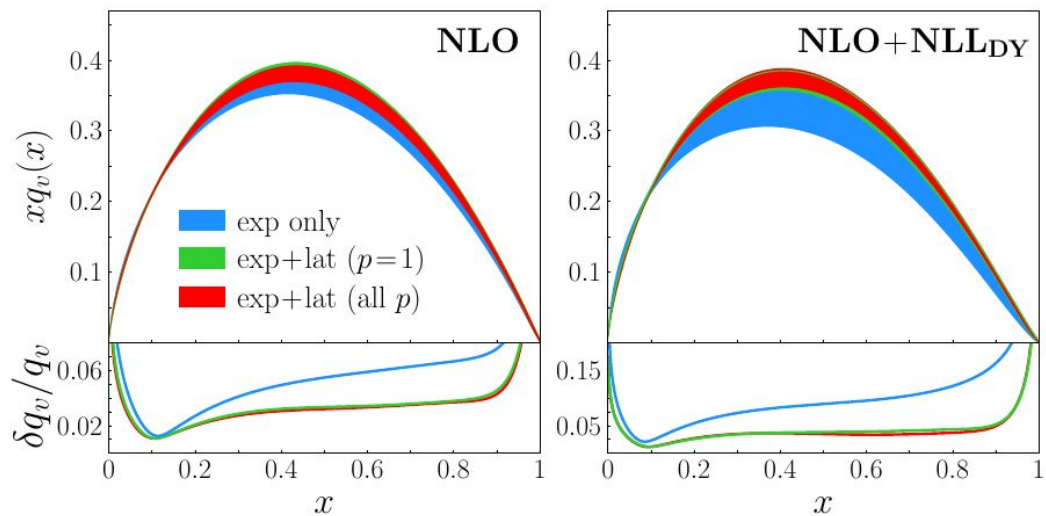
- Lattice matrix elements provide first principles' priors for global analysis framework

Lattice results and experimental data complementary

- For example, lattice QCD sensitive to $x > 0.2$, where experimental data are less constraining

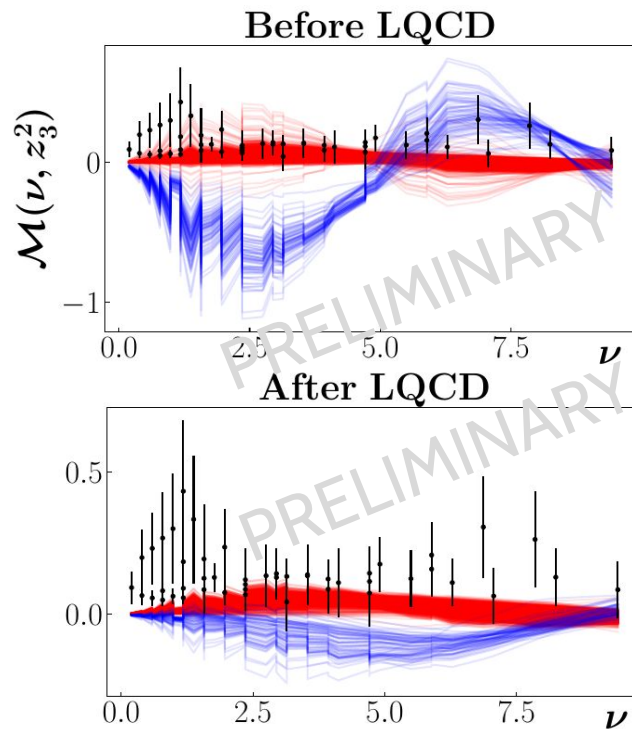
Lattice inputs for global analyses

Isvector quark PDF of the pion



Barry et al. (HadStruc & JAM), PRD 105 (2022) 114051

Polarised gluon PDF of the nucleon



(HadStruc & JAM), in progress

Summary

Multiple efforts worldwide to extract PDFs from lattice QCD calculations

Challenging calculations, but significant theoretical and computational progress

Benchmark calculations of well-known valence quark PDFs of nucleons and pions

- state-of-the-art calculations with multiple lattice spacings and volumes at physical pion masses
- identifying, quantifying and reducing systematic uncertainties

Exploratory calculations of poorly-known parton distribution functions and three-dimensional structure

- gluon and quark-singlet PDFs of nucleons
- quark parton distribution functions of other mesons and baryons
- valence quark GPDs
- Collins-Soper kernel for rapidity evolution of TMDs

Ongoing efforts to incorporate lattice data as Bayesian priors in global analysis

Outlook

Current and near-term: 0-5 years

- Fully-controlled calculations of isovector quark PDFs at large x
- Calculations of isoscalar quark and unpolarised gluon PDFs
- Proof-of-principle calculations of TMDs
- Calculations of GPDs mapped over a range of momentum transfers and skewness
- Continued theoretical and algorithmic development to enable long-term goals
- Pipelines for global analyses of 3D structure incorporating lattice data

Longer term: 5-10 years

- Fully-controlled precision calculations of isovector quark PDFs at large x
- Fully-controlled calculations of isoscalar quark and unpolarised gluon PDFs
- Calculations of TMDs at a range of transverse momenta
- Controlled calculations of GPDs over a broader kinematic range
- Global analyses of 3D structure that include lattice data, tightly coupled to EIC program

Thank you!

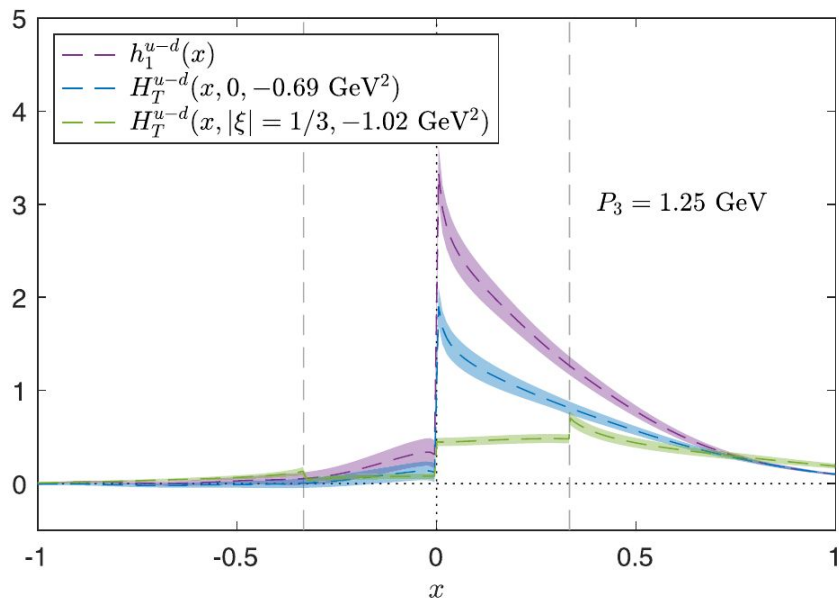
Chris Monahan

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Back-up slides

GPDs of the nucleon



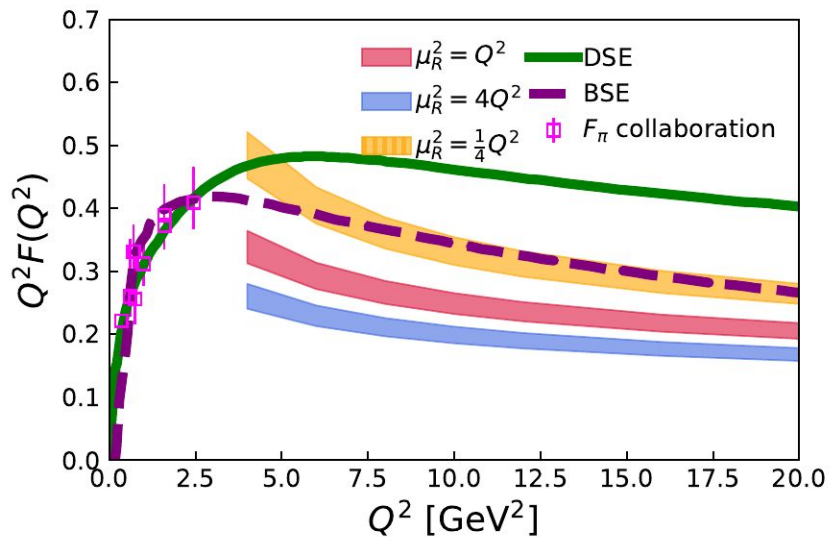
Alexandrou et al. (ETM), PRD 105 (2022) 034501

First determination of quark transversity GPDs of the nucleon

- Nf = 2+1+1 twisted mass clover-Wilson fermions with one lattice spacing and pion mass
- Maximum nucleon momentum = 1.67 GeV
- Maximum momentum transfer = -1.02 GeV²
- Zero and nonzero skewness

Demonstrates feasibility for lattice QCD calculations to map the three-dimensional structure of hadrons!

Distribution amplitude of the pion



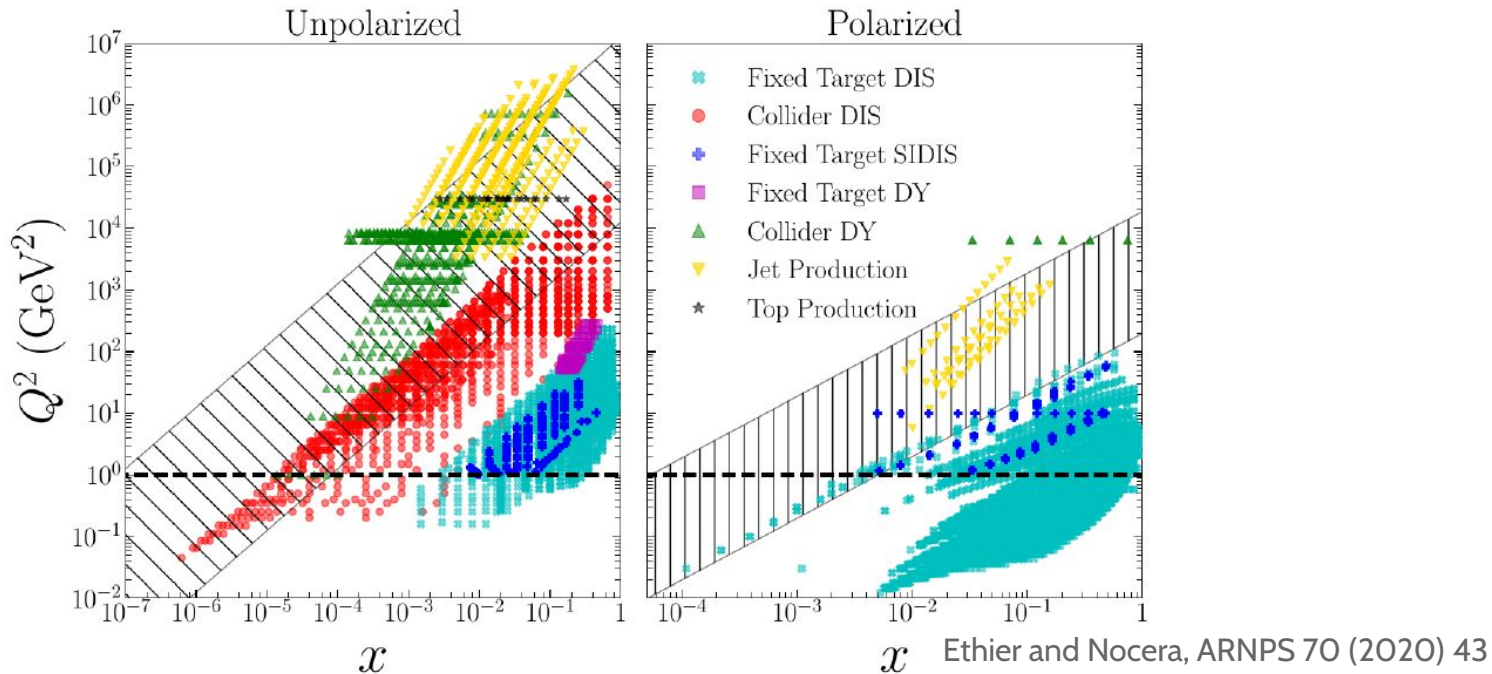
Determination of pion distribution amplitude

- $a = 0.076$ fm and pion mass of 140 MeV
- Wilson-clover on $N_f = 2+1$ HISQ fermions
- maximum pion momentum of 1.78 GeV
- NNLO perturbative matching

Gao et al., PRD 106 (2022) 074505

Gluon PDFs from experimental data

PDFs: How much of the momentum of a fast-moving hadron is carried by its constituent gluons?

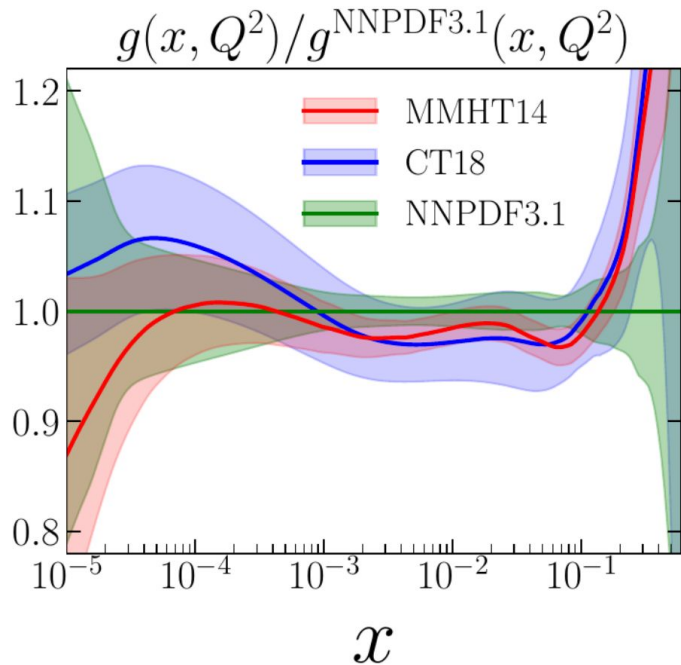


LHC has considerably improved our knowledge of gluon PDFs

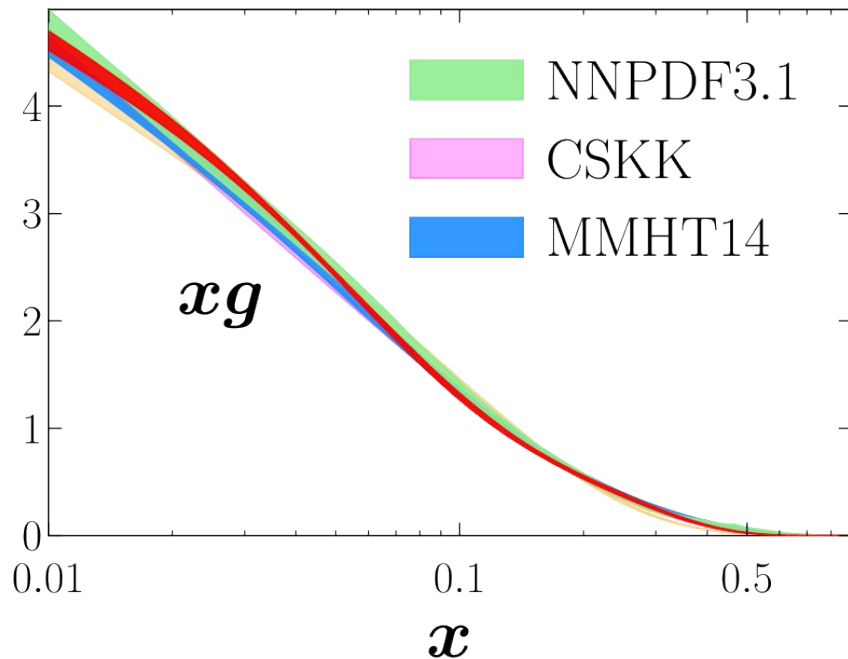
EIC and LHeC will expand this significantly

Gluon PDFs from experimental data

PDFs: How much of the momentum of a fast-moving hadron is carried by its constituent gluons?



Ethier and Nocera, Ann.Rev.Nucl.Part.Sci. 70 (2020) 43

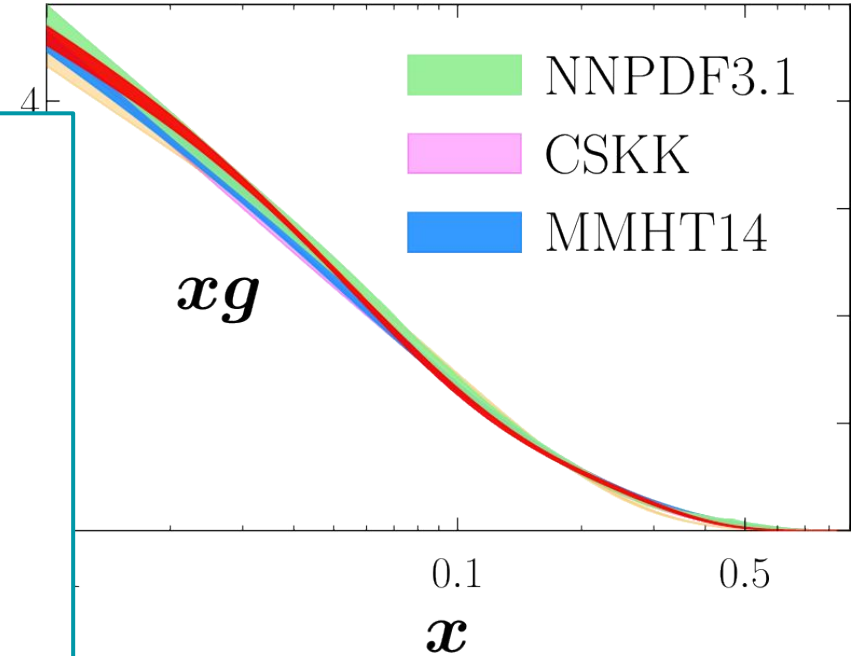
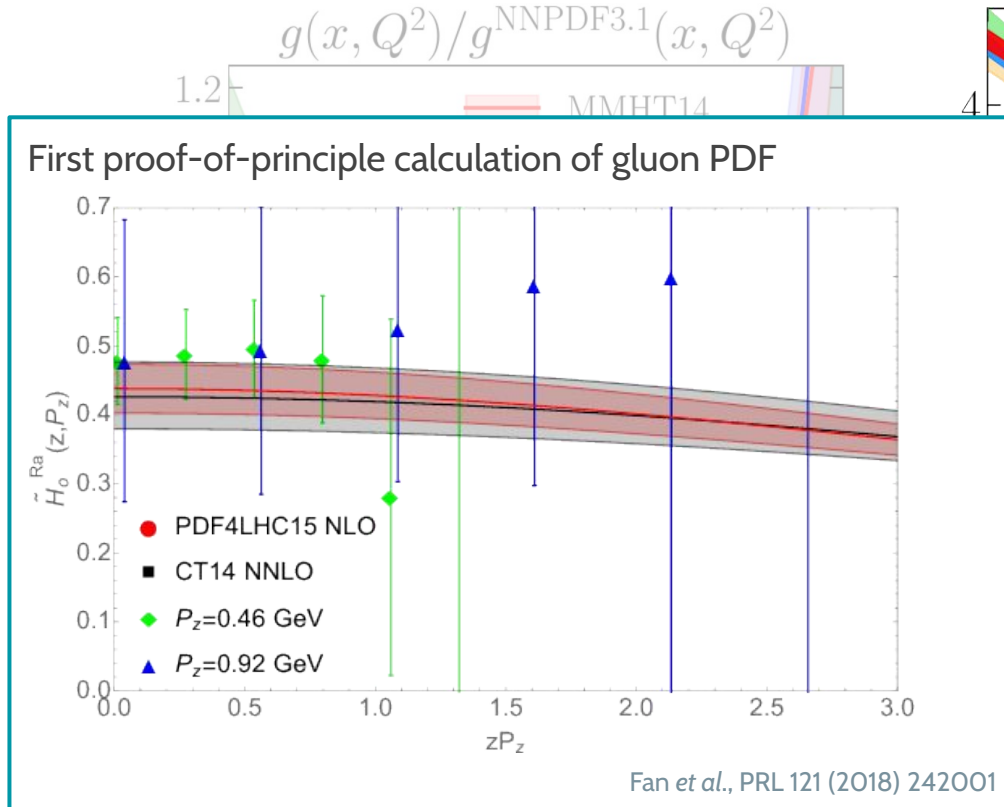


Zhou et al., PRD 105 (2022) 074022

Large uncertainties remain at large and small Bjorken-x

Gluon PDFs from experimental data

PDFs: How much of the momentum of a fast-moving hadron is carried by its constituent gluons?

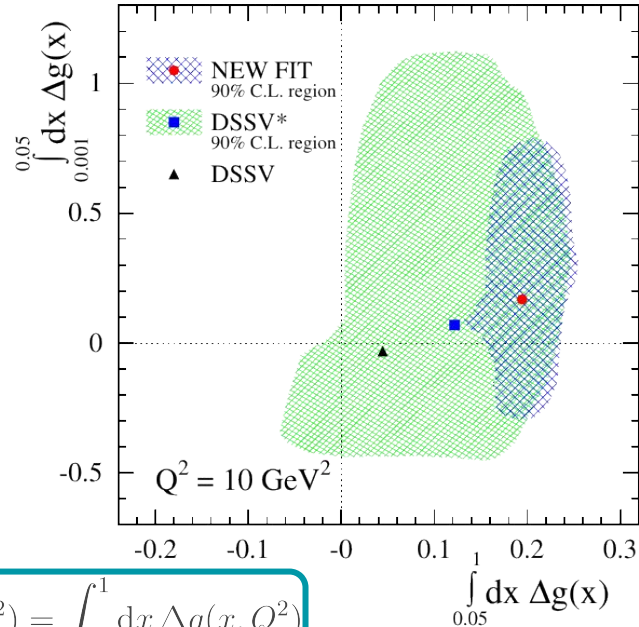


The origin of hadron spin

30 years after the EMC experiment precipitated the “proton spin crisis”, experimental picture still unclear

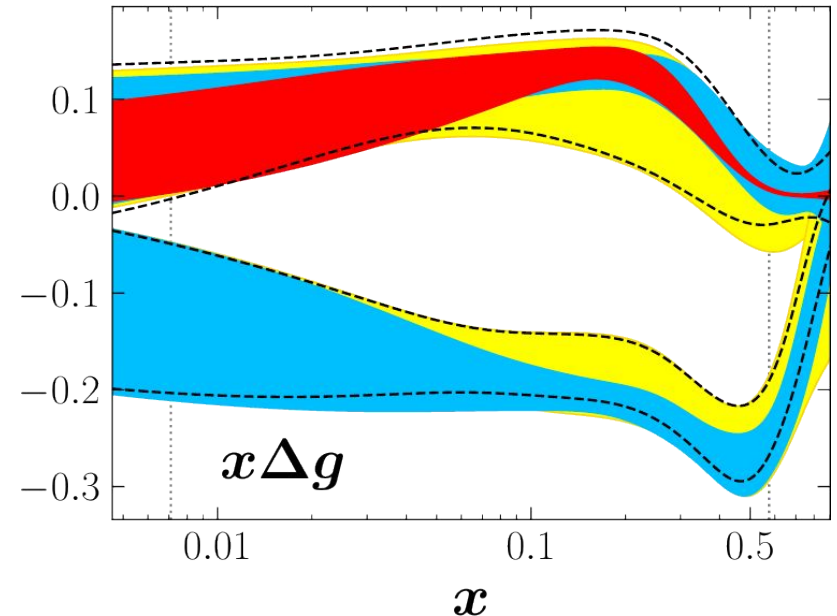
Quarks carry approximately 30% of the proton’s spin, gluon picture is much less clear

de Florian et al., PRL 113 (2014) 012001



$$\Delta G(Q^2) = \int_0^1 dx \Delta g(x, Q^2)$$

Zhou et al., PRD 105 (2022) 074022



See positivity bound discussion: Collins et al., PRD 105 (2022) 076010 ⁴²

The origin of hadron spin

Broadly speaking - two approaches to first principles calculations of these contributions

“Ji sum rule”

$$\frac{\Delta\Sigma}{2} + L_q + J_g = \frac{1}{2}$$

Obtained from the axial current

Defined through TMDs or through form factors of the energy-momentum tensor

Obtained from the axial current

$$\frac{\Delta\Sigma}{2} + \Delta G + \ell_q + \ell_g = \frac{1}{2}$$

“Jaffe-Manohar sum rule”

Defined through the local operator in the infinite-momentum frame

$$S_G = \int d^3x \text{Tr} [\mathbf{E} \times \mathbf{A}_{\text{phys}}]$$

Defined through local operators in IMF or through TMDs

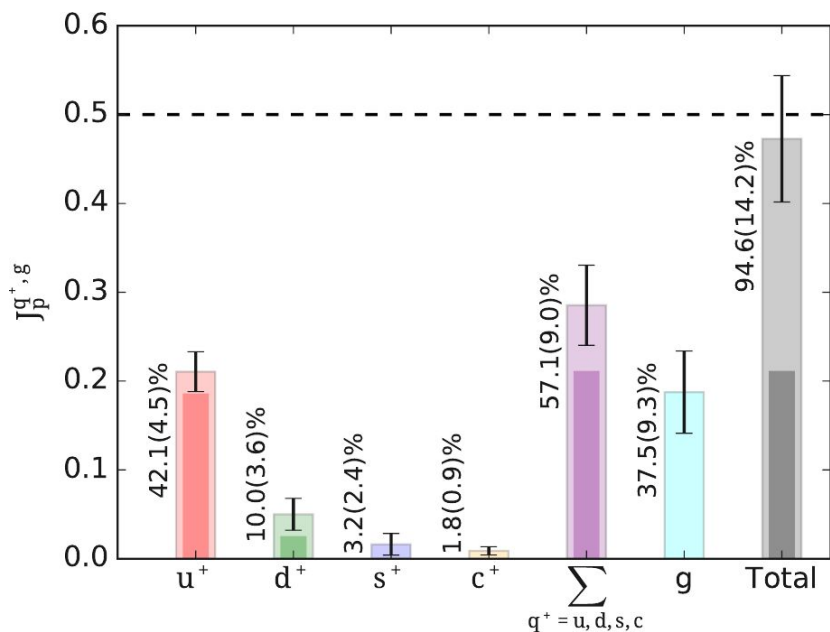
Defined through the integral of the helicity PDF

$$\Delta G(Q^2) = \int_0^1 dx \Delta g(x, Q^2)$$

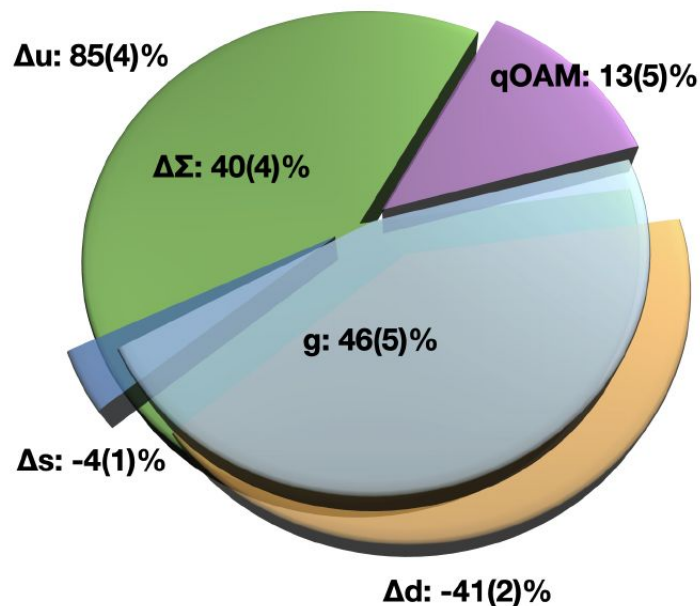
Both challenging for lattice QCD!

First calculations of the spin of the proton

Two state-of-the-art decompositions from lattice QCD



Alexandrou et al., PRD 101 (2020) 094513



Wang et al., PRD 106 (2022) 014512

Gluon PDFs: pseudo-distribution formalism

Starting point:

Balitsky, Morris and Radyushkin, PLB 808 (2020) 135621

$$M_{\mu\nu\rho\sigma;H}^{(0)}(P, n) = \langle H(P) | G_{\mu,\nu}(n^\alpha) W^{(A)}(n^\alpha, 0) G_{\rho\sigma} | H(P) \rangle$$

$$W^{(A)}(n^\alpha, 0) = \mathcal{P} \exp \left\{ ig \int_0^n dy^\mu A_\mu^{(A)}(y) \right\}$$

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$n^2 = 0$ \rightarrow

$$\mathcal{M}_{g/H}^{(0)}(\nu, 0) = \frac{1}{2(P^+)^2} [M_H^{(0)}(P, z^-)]^{+\mu}_{+\mu}$$

PDFs

ξ^-

$$x f_{g/H}^{(0)}(x) = \int_{-1}^1 d\nu e^{ix\nu} \mathcal{M}_{g/H}^{(0)}(\nu, 0)$$

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$$\mathcal{M}_{g/H}^{(0)}(\nu, z^2) = \frac{1}{2E_P^2} [M_{0ii0;H}^{(0)}(P, z) - M_{jijj;H}^{(0)}(P, z)]$$

PDFs

$$\xi^- \downarrow$$

$$x f_{g/H}^{(0)}(x) = \int_{-1}^1 d\nu e^{ix\nu} \mathcal{M}_{g/H}^{(0)}(\nu, 0)$$

$$\mathcal{M}_{g/H}^{(\text{red.})}(\nu, z^2) = \left(\frac{\mathcal{M}_{g/H}^{(0)}(\nu, z^2)}{\mathcal{M}_{g/H}^{(0)}(\nu, 0)|_{z=0}} \right) / \left(\frac{\mathcal{M}_{g/H}^{(0)}(0, z^2)|_{p=0}}{\mathcal{M}_{g/H}^{(0)}(0, 0)|_{p=0, z=0}} \right)$$

$\zeta \downarrow$ pseudo PDFs

$$\mathcal{M}_{g/H}^{(\text{red.})}(\nu, z^2) = \int_0^1 \frac{d\xi \xi}{\langle \xi \rangle^2(\mu)} \left[c_{gg}(\xi\nu, \mu^2 z^2) f_{g/H}(\xi, \mu^2) + \frac{Pz}{E_P} c_{gq}(\xi\nu, \mu^2 z^2) f_{S/H}(\xi, \mu^2) \right]$$

Gluon PDFs: pseudo-distribution formalism

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$\zeta \downarrow$ pseudo PDFs

what we want

neglect mixing

$$\mathcal{M}_{g/H}^{(\text{red.})}(\nu, z^2) = \int_0^1 \frac{d\xi \xi}{\langle \xi \rangle^2(\mu)} \left[c_{gg}(\xi\nu, \mu^2 z^2) f_{g/H}(\xi, \mu^2) + \frac{Pz}{E_P} c_{gq}(\xi\nu, \mu^2 z^2) f_{S/H}(\xi, \mu^2) \right]$$

Gluon PDFs: pseudo-distribution formalism

Starting point:

$$M_{\mu\nu\rho\sigma;H}^{(0)}(P, z) = \langle H(P) | G_{\mu\nu}(0, z, \mathbf{0}_T) W^{(A)}(z, 0) \tilde{G}_{\rho\sigma}(0) | H(P) \rangle$$

$$M_{\mu\nu\rho\sigma;H}^{(0)}(P, n) = \langle H(P) | G_{\mu,\nu}(n^\alpha) W^{(A)}(n^\alpha, 0) G_{\rho\sigma} | H(P) \rangle$$

$$n^2 = -z^2 \downarrow$$

$$M_{0i;0i}^{(0)}(P, z) + M_{ij;ij}^{(0)}(P, z) = -2P^z E_H \mathcal{M}_{\Delta g/H}(\nu, z^2) + 2E_H^3 z \mathcal{M}_{pp}(\nu, z^2)$$

what we want

$$\mathcal{M}_{g/H}^{(0)}(\nu, z^2) = \frac{1}{2E_P^2} \left[M_{0ii0;H}^{(0)}(P, z) - M_{jii j;H}^{(0)}(P, z) \right]$$

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ζ ↓ pseudo PDFs

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HadStruc lattice implementation

Glueballs provide significant signal-to-noise challenges for lattice calculations, mitigated through:

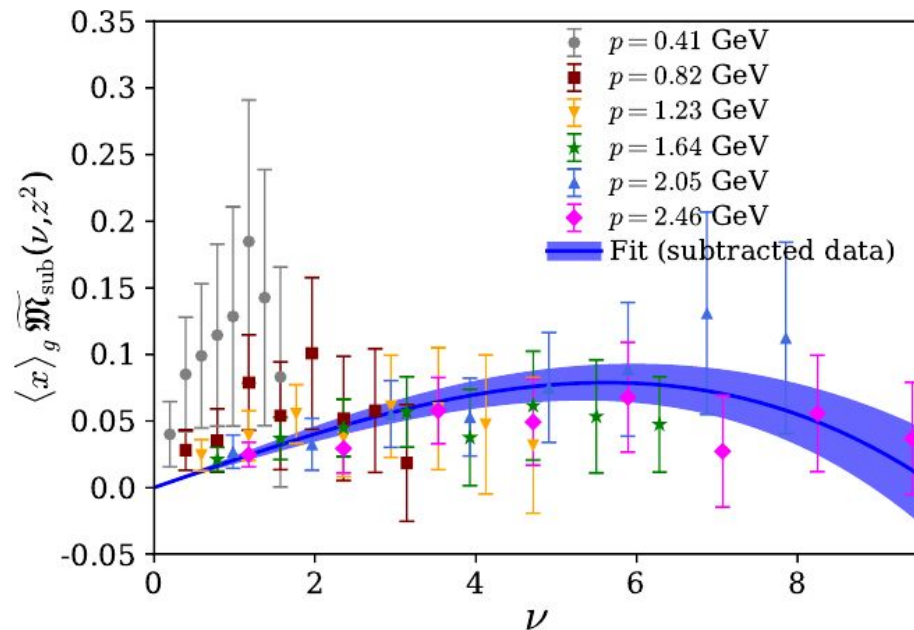
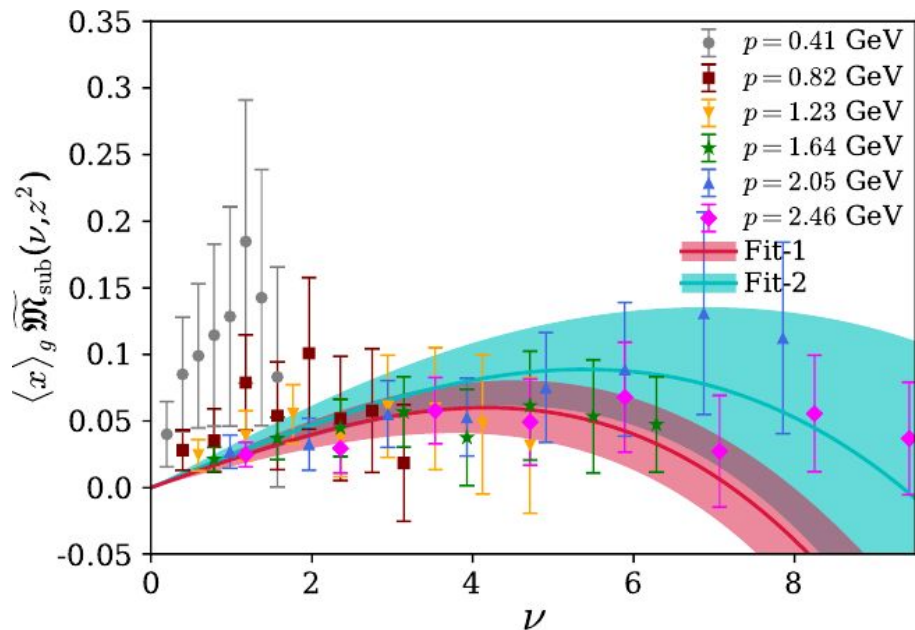
1. Gradient flow smearing reduces ultraviolet fluctuations
2. Distillation and summed GEVP method improves operator overlap and reduces excited state contamination
3. Reduced Ioffe-time distribution reduces correlated uncertainties through ratio

We neglect mixing with scalar quark distribution

Results calculated on a single lattice ensemble of 2+1 stout-smearred Wilson-improved clover fermions and tree-level tadpole-improved Symanzik gauge action, with Wilson flow, momentum-smearred nucleon interpolating operators and unimproved gauge field tensor

ID	a (fm)	M_π (MeV)	$L^3 \times N_t$	N_{cfg}	N_{srCs}
<i>a094m358</i>	0.094(1)	358(3)	$32^3 \times 64$	349	64

Polarised gluon pseudo-distribution



Egerer et al. (HadStruc), PRD 106 (2022) 094511