# The NNLO unpolarized isovector quark PDF of the nucleon at the physical point from lattice QCD

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# Outline

- Motivations and formalism
- Lattice setup
- Analysis of two-point and three-point functions
- Model-independent extraction of lowest Mellin moments
- *x*-dependent PDF from model fits, deep neural network, and LaMET

All results are preliminary!

### Motivations

- Test methods against experimental data
- Extract nucleon PDFs using various methods
  - Leading-twist OPE
  - Model-dependent fits
  - $\circ$  Deep neural network
  - $\circ$  x-space matching with Hybrid renormalization
- When does short-distance factorization break down?
- Check perturbative uncertainty by including NNLO matching

# Light-cone PDFs from lattice QCD

- Cannot calculate matrix elements separated along the light cone in lattice QCD
- Instead, calculate equal-time spatiallyseparated matrix element of highly-boosted hadron

 $h^{B}(z,P_{z}) = \langle N; P_{z} | \overline{\psi}(z) \Gamma W(z,0) \psi(0) | N; P_{z} \rangle$ 

• Can be matched to light-cone PDF through Large-momentum Effective Theory or short-distance factorization

Theoretical Framework: [V. Braun, D. Müller '07] [X. Ji '13] [A. Radyushkin '17]



[X. Ji et al., Rev. Mod. Phys. 93, 035005, arXiv: 2004.03543]

#### **Correlation functions**

Use standard nucleon operator:  $N_{\alpha}^{(s)}(x,t) = \varepsilon_{abc} u_{a\alpha}^{(s)}(x,t) (u_b^{(s)}(x,t)^T C \gamma_5 d_c^{(s)}(x,t))$ 

For two-point functions: 
$$C^{2\text{pt}}(\vec{p}, t_{\text{sep}}; \vec{x}, t_0) = \sum_{\vec{y}} e^{-i\vec{p}\cdot(\vec{y}-\vec{x})} \mathcal{P}^{2\text{pt}}_{\alpha\beta} \langle N_{\alpha}(\vec{y}, t_{\text{sep}}+t_0) \overline{N}_{\beta}(\vec{x}, t_0) \rangle$$

And three-point functions:

$$C^{3\text{pt}}(\vec{p}_{f}, \vec{q}, t_{\text{sep}}, t_{\text{ins}}; \vec{x}, t_{0}) = \sum_{\vec{y}, \vec{z}} e^{-i\vec{p}_{f} \cdot (\vec{y} - \vec{x})} e^{-i\vec{q} \cdot (\vec{x} - \vec{z})} \mathcal{P}_{\alpha\beta}^{3\text{pt}} \langle N_{\alpha}(\vec{y}, t_{\text{sep}} + t_{0}) \mathcal{O}^{\Gamma}(\vec{z}, \hat{\mathcal{L}}, t_{\text{ins}} + t_{0}) \overline{N}_{\beta}(\vec{x}, t_{0}) \rangle$$
$$\mathcal{O}^{\Gamma}(\vec{z}, \hat{\mathcal{L}}, t_{\text{ins}} + t_{0}) = \overline{q}(\vec{z}, t_{\text{ins}} + t_{0}) \Gamma \tau_{3} W(\vec{z}, t_{\text{ins}} + t_{0}; \vec{z} + \hat{\mathcal{L}}, t_{\text{ins}} + t_{0}) q(\vec{z}, + \hat{\mathcal{L}}, t_{\text{ins}} + t_{0})$$

For unpolarized distribution:  $\mathcal{P}^{2\text{pt}} = \mathcal{P}^{3\text{pt}} = \frac{1}{2}(1 + \gamma_t)$ ,  $\Gamma = \gamma_t, \gamma_z$ Smeared-smeared (SS) and smeared-point (SP) two-point correlators **No mixing** Only smeared-smeared three-point correlators

# Calculation setup

- Mixed fermion action
  - $\circ~$  Sea quark action:  $N_f=2{+}1~{\rm HISQ}$  with physical quark masses,  $L^3\times T=64^3\times 64,$   $a=0.076~{\rm fm}$
  - $\circ~$  Valence quark action:  $\rm N_f=2+1$  Wilson-Clover with physical quark masses, 1-HYP smeared gauge links
- Calculations done with Qlua, which utilizes the multigrid solver in QUDA
- Use momentum smearing for quarks to achieve better overlap with boosted hadrons
- Included four momentum projections to  $P_x^{(f)}$  at the sink for three-point functions

$P_x^{(f)}$	$k_x$	$t_{\rm sep}$	$N_{\mathrm{samp}}$
0	0	6	16
0	0	$8,\!10$	32
0	0	12	64
1	0	$6,\!8,\!10,\!12$	32
4	2	6	32
4	2	$8,\!10,\!12$	128
6	3	6	20
6	3	8	100
6	3	$10,\!12$	140

### Analysis of two-point functions

• Fit two-point functions to 
$$C_N^{\text{2pt}}(\vec{p}, t_{\text{sep}}) = C_0 e^{-E_0 t_{\text{sep}}} \left[ 1 + \sum_{i=1}^{N-1} R_i \prod_{i=1}^{i} e^{-\Delta_{j,j-1} t_{\text{sep}}} \right]$$

- Use SP and SS correlators to help control excited states
- All energies below largest energy are priored
- Three states required to fit full  $t_{sep}$



# Three-point function analysis

• Fit ratio of three-point to two-point data

$$R(\vec{p}_f, t_{\rm ins}, t_{\rm sep}) = \frac{C^{\rm 3pt}(\vec{p}_f, \vec{q} = 0, t_{\rm ins}, t_{\rm sep})}{C^{\rm 2pt}(\vec{p}_f, t_{\rm sep})}$$

- Two-state fits to three-point ratio priored with 'effective' energy gap and amplitudes from two-state fits to two-point SS correlators
- Reasonable agreement between two-state and other fit strategies, like summation fits

$$R_{\rm sum}(\vec{p}_f,t_{\rm sep}) = \sum_{t_{\rm ins}=n_{\rm exc}a}^{t_{\rm sep}-n_{\rm exc}a} R(\vec{p}_f,t_{\rm ins},t_{\rm sep})$$



### **Ratio-scheme renormalization**

• The operator  $\mathcal{O}_{\Gamma}(z)$  is multiplicatively renormalizable

 $h_{\Gamma}^B(z,P_z,a) = e^{-\delta m(a)|z|} Z_O(a) h_{\Gamma}^R(z,P_z,\mu)$ 

• Can form renormalization-group invariants with the double ratio (z = 0 for exact normalization)

$$\mathcal{M}(\lambda, z^{2}; P_{z}^{0}, a) = \frac{h^{B}(z, P_{z}, a)}{h^{B}(z, P_{z}^{0}, a)} \Big/ \frac{h^{B}(0, P_{z}, a)}{h^{B}(0, P_{z}^{0}, a)} \quad , \lambda \equiv z P_{z}$$

- Consider  $\mathcal{M}(\lambda, z^2; P_z^0 = 0, a)$ , referred to as the reduced Ioffe Time Distribution (rITD)
- rITD can be perturbatively matched to light-cone ITD  $~Q(\lambda,\mu^2)$



#### Lowest moments from leading-twist OPE

The lowest few moments can be extracted from the rITD by fits to

$$\mathcal{M}(\lambda, z^2; \lambda^0 \equiv z P_z^0) = \frac{\sum_{n=0}^{\infty} c_n (\mu^2 z^2) \frac{(-i\lambda)^n}{n!} \langle x^n \rangle(\mu) + \mathcal{O}(\Lambda_{\text{QCD}}^2 z^2)}{\sum_{n=0}^{\infty} c_n (\mu^2 z^2) \frac{(-i\lambda^0)^n}{n!} \langle x^n \rangle(\mu) + \mathcal{O}(\Lambda_{\text{QCD}}^2 z^2)}$$

where  $c_n(\mu^2 z^2) \equiv C_n(\mu^2 z^2)/C_0(\mu^2 z^2)$ , and  $C_n(\mu^2 z^2)$  are Wilson coefficients, which have been computed up to next-to-next-leading-order (NNLO)



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### Model dependent fits

- Model the PDF  $q_{\text{model}}(x)$  and evaluate the moments  $\langle x^n \rangle_{\text{model}} = \int_0^1 dx \, x^n q_{\text{model}}(x)$
- Substitute  $\langle x^n \rangle_{\text{model}}$  into leading-twist OPE to obtain  $\mathcal{M}_{\text{model}}(\lambda, z^2; \lambda^0)$

• Fit by minimizing,  

$$\chi^2 = \sum_{P_z > P_z^0} \sum_{z_{\min}}^{z_{\max}} \frac{(\mathcal{M}(\lambda, z^2; \lambda^0) - \mathcal{M}_{\text{model}}(\lambda, z^2; \lambda^0))^2}{\sigma^2(z, P_z, P_z^0)}$$

• Real and Imaginary part of rITD related to

$$q^{-}(x) \equiv q^{u}(x) - q^{d}(x) - (q^{\overline{u}}(x) - q^{\overline{d}}(x)), \quad q^{+}(x) \equiv q^{u}(x) - q^{d}(x) + (q^{\overline{u}}(x) - q^{\overline{d}}(x)), \quad x \in [0, 1]$$

respectively, and can be expressed via a simple model

$$q^{-}(x;\alpha,\beta) = \frac{\Gamma(2+\alpha+\beta)}{\Gamma(1+\alpha)\Gamma(2+\beta)} x^{\alpha}(1-x)^{\beta}, \qquad q^{+}(x;\alpha,\beta,A) = Ax^{\alpha}(1-x)^{\beta}$$

#### Isovector PDF from model fits

- Include all  $P_z$  and  $z \in [2a, z_{\max}]$  for fit
- Use  $q^{f}(-x) = -q^{\overline{f}}(x)$  to form isovector PDF from

$$q^{u-d}(x) = \begin{cases} \frac{q^{-}(x)+q^{+}(x)}{2}, & x > 0\\ \frac{q^{-}(-x)-q^{+}(-x)}{2}, & x < 0 \end{cases}$$



# Deep Neural Network

• Use leading-twist factorization formula

• Consider modifications to model fits with a function represented by a deep neural network

 $q^{-}(x;\alpha,\beta,\theta) \equiv A^{-}x^{\alpha}(1-x)^{\beta}[1+\delta\sin(f_{\rm DNN}^{-}(x,\theta))],$ 

$$q^+(x;\alpha,\beta,A,\theta) \equiv A^+ x^\alpha (1-x)^\beta [1+\delta \sin(f^+_{\rm DNN}(x,\theta))].$$

• Minimize loss function

$$J(\boldsymbol{\theta}) \equiv \frac{\eta}{2} \boldsymbol{\theta} \cdot \boldsymbol{\theta} + \frac{1}{2} \chi^2(\boldsymbol{\theta}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \dots)$$



# Hybrid renormalization

- Need full range of *z* for Fourier transform
  - $\circ$   $\,$  Must be careful about renormalization at large z
- Determine  $\delta m$  from static  $q-\overline{q}$  potential, and change scheme to  $\overline{MS}$  with

 $e^{\delta m(z-z_0)} \frac{h^B(z,0,a)}{h^B(z_0,0,a)} = e^{-\overline{m}_0(z-z_0)} \frac{C_0(\mu^2 z^2) - \Lambda z^2}{C_0(\mu^2 z_0^2) - \Lambda z_0^2}$ 

• Ratio scheme at short distances and include Wilson-line mass correction at large distances

$$\tilde{h}^{R}(z, z_{S}, P_{z}, \mu) = \begin{cases} N \frac{h^{B}(z, P_{z}, a)}{h^{B}(z, 0, a)} \frac{C_{0}(z^{2}\mu^{2}) + \Lambda z^{2}}{C_{0}(z^{2}\mu^{2})}, & z \leq z_{S} \\ N \frac{h^{B}(z, P_{z}, a)}{h^{B}(z_{S}, 0, a)} \frac{C_{0}(z_{S}^{2}\mu^{2}) + \Lambda z_{S}^{2}}{C_{0}(z_{S}^{2}\mu^{2})} e^{\delta m'(z-z_{S})}, & z > z_{S}. \end{cases}$$

• Extrapolate with exponential decay model  $\frac{Ae^{-m_{\rm eff}\lambda/P_z}}{|\lambda|^d}$ 



#### *x*-space matching

• Obtain quasi-PDF from Fourier transform

$$\tilde{q}^{v}(x,\lambda_{S},P_{z},\mu) = \int \frac{dz}{2\pi} e^{ixP_{z}z} \,\tilde{h}^{R}(z,z_{S},P_{z},\mu)$$

• Match quasi-PDF to PDF

$$q^{v}(x,\mu) = \int_{-\infty}^{\infty} \frac{dy}{|y|} C^{-1}\left(\frac{x}{y}, \frac{\mu}{yP_{z}}, |y|\lambda_{S}\right) \tilde{q}^{v}(y,\lambda_{S}, P_{z},\mu)$$
$$+ \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}^{2}}{(xP_{z})^{2}}, \frac{\Lambda_{\text{QCD}}^{2}}{((1-x)P_{z})^{2}}\right)$$

- Need to estimate valid range of *x* 
  - $\circ \qquad \text{Use DGLAP evolution to remove } \ln \frac{\mu^2}{4x^2 P_z^2} ,$ which breaks down at  $2xP_z \sim \Lambda_{\text{QCD}}$



# **Conclusions and Outlooks**

- Conclusions
  - Excited-state contamination at the physical point can be controlled
  - $\circ$  % = Leading-twist OPE can describe the proton ratio data for  $z\sim0.8~{\rm fm}$ 
    - First four moments extracted
    - $\langle x \rangle$  is above result from NNPDF40
  - Some tension between various extraction methods
  - Perturbative convergence appears to have been achieved
- Future work/Outlooks
  - $\circ$  ~ More statistics and source-sink separations would be helpful
  - Larger  $P_{z}$  would also be useful if possible
  - $\circ$  Helicity and transversity distributions

