Improved parton distribution functions at the physical pion mass

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(Received 30 August 2017; revised manuscript received 30 April 2018; published 5 September 2018)

We present the first lattice results on isovector unpolarized and longitudinally polarized parton distribution functions (PDFs) at physical pion mass. The PDFs are obtained using the large-momentum effective field theory (LaMET) framework where the full Bjorken-*x* dependence of finite-momentum PDFs, called "quasi-PDFs," can be calculated on the lattice. The quasi-PDF nucleon matrix elements are renormalized nonperturbatively in the RI/MOM-scheme. However, the recent renormalized quasi-PDFs suffer from unphysical oscillations that alter the shape of the true distribution as a function of Bjorken-*x*. In this paper, we propose two possible solutions to overcome this problem and demonstrate the efficacy of the methods on the 2 + 1 + 1-flavor lattice data at physical pion mass with lattice spacing 0.09 fm and volume (5.76 fm)³.

DOI: 10.1103/PhysRevD.98.054504

Parton distribution functions (PDFs) are universal nonperturbative properties of the nucleon which describe the probability densities of quarks and gluons seen by an observer moving at the speed of light relative to the hadron. The unpolarized PDFs can be used as inputs to predict cross sections in high-energy scattering experiments, one of the major successes of QCD. These distributions can be extracted through global analysis using multiple experiments by factorizing the hard-scattering cross sections into the PDFs and short-distance matrix elements that are calculable in perturbation theory. Today, multiple collaborations provide regular updates concerning the phenomenological determination of the PDFs [1–6] using the latest experimental results, from medium-energy QCD

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experiments at Jefferson Lab in the U.S. to high-energy collisions at the LHC in Europe. Progress has also been made in polarized PDFs using data from RHIC at Brookhaven National Lab and the COMPASS experiment at CERN; further progress would also be made at the proposed electron-ion collider (EIC). After the past half century of effort in both theory and experiment, our knowledge of PDFs has greatly advanced. However, as the experiments get more precise, the precision needed in PDFs to make standard model (SM) predictions has increased significantly too. Current and planned experiments (such as the EIC) will go further into unexplored or less-known regions, such as sea-quark and gluonic structure. We would like to explore these unknown regions using a first-principles calculation from the standard model in lattice QCD.

A new approach for the direct computation of the x-dependence of PDFs on the lattice was proposed by Ji [7,8]: large-momentum effective theory (LaMET), where lightcone PDFs can be obtained by approaching the infinite-momentum frame (IMF). Prior to this development, lattice QCD was limited to calculating charges and various leading moments of nucleon matrix elements, integrals

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of the PDFs, through the operator product expansion (OPE). In LaMET on the lattice, we start by calculating the "quasi-PDF" \tilde{q} with a nucleon moving along the *z* direction with finite momentum P_z . The quasi-PDF is an integral over matrix elements *h* with a spatial correlation of partons,

$$\tilde{q}(x, P_z, \tilde{\mu}) = \int_{-\infty}^{\infty} \frac{dz}{2\pi} e^{ixP_z z} h(z, P_z, \tilde{\mu}), \qquad (1)$$

where $\tilde{\mu}$ is the renormalization scale in a chosen renormalization scheme. The boosted-nucleon matrix elements are

$$h(z, P_z, \tilde{\mu}) = \frac{1}{2} \langle P | \bar{\psi}(z) \Gamma \exp\left(ig \int_0^z dz' A_z(z')\right) \psi(0) | P \rangle,$$
(2)

for $\Gamma = \gamma_z$ or γ_t for the unpolarized case. To obtain polarized PDFs, $\Delta \tilde{q}$, we calculate $\Delta h(z)$ as in Eq. (2) with $\Gamma = \gamma_5 \gamma_z$. Note that the quasi-PDF depends nontrivially on the nucleon momentum P_z , unlike the lightcone PDF. Within LaMET framework, the lightcone PDFs can be matched to the quasi-PDF through a factorization formula [7,8],

$$\begin{split} \tilde{q}(x, P_z, \tilde{\mu}) &= \int_{-1}^{+1} \frac{dy}{|y|} C\left(\frac{x}{y}, \frac{\tilde{\mu}}{P_z}, \frac{\mu}{P_z}\right) q(y, \mu) \\ &+ \mathcal{O}\left(\frac{M_N^2}{P_z^2}, \frac{\Lambda_{\text{QCD}}^2}{P_z^2}\right), \end{split}$$
(3)

where M_N is the nucleon mass, C is the matching kernel, and the $\mathcal{O}(M_N^2/P_z^2, \Lambda_{\text{OCD}}^2/P_z^2)$ terms are power corrections suppressed by the nucleon momentum. Here, $q(y, \mu)$ for negative y corresponds to the antiquark contribution. References [7–9] show \tilde{q} and q have the same infrared (IR) divergences; therefore, the matching kernel C only depends on ultraviolet (UV) physics and can be calculated in perturbative QCD [9,10]. Since Ji's proposal in 2013, there have been many follow-up works concerning the quasi-PDFs. On the lattice side, there have been many lattice-QCD calculations of the nucleon isovector quark distributions [11-18] including the unpolarized, polarized, and transversity cases and variations of the quasi-PDF methods. The renormalization properties of quasi-PDFs have also been intensively studied [17-25], and they were shown to be multiplicatively renormalizable to all loop orders. The multiplicative renormalization involves an exponential mass renormalization for the Wilson line and two renormalization factors associated with its end points where the quark fields are situated. This finding motivated the lattice analysis of nonperturbative renormalization of the quasi-PDF in the regularization-independent momentum subtraction (RI/MOM) scheme [17]. The RI/MOM renormalization constant is defined by sandwiching the quasi-PDF operator in Eq. (2) between a highly off-shell quark state with a given momentum, such that the renormalization factor absorbs the radiative corrections completely. The renormalization factor defined this way can then be used to renormalize the nucleon matrix element.

Recent renormalized quasi-PDF studies have shown oscillatory behavior [17,18] that significantly distorts the true distribution, especially in the antiquark region. This happens due to the renormalization constants' enhancement of the large-z matrix elements through exponential counterterm; in the bare quasi-PDF, it is less severe. This issue was briefly mentioned in Ref. [17], where the z-truncated and inverse Fourier-transformed central value of the PDFs [26], nucleon matrix elements h(z), are compared with the RI/MOM-renormalized lattice ones $h(z)^{\text{lattice}}$. The global fit parametrizes xf(x), where f is the valence up or down distribution $\{u, d\}^v(x)$ with f(x) parametrized as $x^{a_n}(1-x)^{b_n}P(x)$ and P(x) a polynomial in x; when one takes the isovector combination, x(u(x) - d(x)) (or the antiquark combination), it does not necessarily go to zero. However, it is important to bear in mind that the divergence in u(x) - d(x) for x near 0 is an extrapolation from larger x results rather than a result from direct measurement. The large size of u(x) - d(x) at small x gives its Fourier transform nonvanishing values at z far beyond the size of the largest currently available lattices. Similarly, the matrix elements h(z) near z = 0 correspond to the large-x region, where most global analyses either rely on extrapolation or have to handle nuclear corrections; this introduces theory uncertainty to the global analysis. It was suggested in Ref. [17] that the lattice data may have mixing with highertwist operators in the large-z region and that going to higher nucleon boosted momenta P_z would reduce the z range needed to reconstruct the quasi-PDFs.

In this paper, we take the CT14 NNLO PDF [4] where the errors for the isovector quark distribution have been properly taken into account and investigate these issues. First, we transform the CT14 PDF without any mass correction to $h(z)^{CT14}$ using momenta $P_z = \{4, 8, 12, 24\}\pi/L$ with L = 5.76 fm, the lattice spatial length. Figure 1 shows the error in the PDF propagated accordingly, and we see the expected nonvanishing matrix elements at large z, especially for the imaginary matrix elements. In the bottom rows of Fig. 1, we show the matrix elements plotted as a function of zP_z (as in Ref. [17]); since there is no nucleonmass correction nor higher-twist effects here, the data points all lie on top of each other. If the small-x region of the PDF is really as divergent as the global PDF extrapolation, we will need an alternative approach to be able to calculate small-x PDFs in lattice calculations.

Using the ideal pseudodata $h(z)^{CT14}$, we can start to investigate the sources of the unphysical oscillations in the lattice quasi-PDFs and seek ways to improve or remove them. First, we study the oscillatory behavior as functions of the boosted momentum inputs. The left-hand side of



FIG. 1. The real (top left) and imaginary (top right) pseudonucleon matrix elements derived from CT14 PDFs as functions of z with nucleon boosted momenta $P_z = \{4, 8, 12, 24\}\pi/L$. (Bottom) Similar plots as the top row but plotted along the horizontal axis in dimensionless units of zP_z .

Fig. 2 shows the transform of $h(z, P_z)^{\text{CT14}}$ using the quasi-PDF formulation with a *z* cutoff of 32, half of the lattice spatial size we used at the physical pion mass. One can clearly see that the oscillatory behavior worsens as the P_z used in the calculation increases. This also indicates that the oscillations are purely an artifact coming from the truncation of the Fourier transformation. Let us focus on the oscillatory behavior of the PDFs at the largest $P_z = 24\pi/L$ here. We transform the $h(z, P_z = 24\pi/L)^{\text{CT14}}$ using the quasi-PDF formulation with different z_{max} cutoffs {10, 20, 40, 80}, as shown in the right-hand side of Fig. 2. The smaller-z cutoffs have milder oscillatory contamination of the resulting PDFs; however, the larger-z cutoff recovers the small-x region better. We need a way to recover as much of the true distribution as possible.

One solution proposed here is to remove these oscillations by means of a low-pass filter. Note that such a filter should be P_z dependent, and one can carefully tune the function that best recovers the true PDF using a selected set of PDFs as guidelines. Here, we demonstrate one possible filter formulation; one should keep in mind that there are many possible solutions, and we should continue exploring



FIG. 2. (Left) The quasi-PDFs obtained from the matrix elements shown in Fig. 1 with $z_{max} = 32$. The unphysical oscillations worsen as the nucleon momentum P_z increases. This presents a serious problem: we need larger P_z to recover the lightcone limit, but the unphysical oscillations alter the PDF shape. (Right) The quasi-PDFs obtained from the matrix elements with $P_z = 24\pi/L$ with different values of z_{max} . The larger values of z_{max} have worse oscillations but possess the information needed to reach the smaller-x region.

to find the most robust way to remove the unphysical oscillations from the quasi-PDFs. We propose a hat-shaped filter in z constructed using the sigmoidal error functions:

$$F(z_{\rm lim}, z_{\rm wid}) = \frac{1 + \operatorname{erf}(\frac{z + z_{\rm lim}}{z_{\rm wid}})}{2} \frac{1 - \operatorname{erf}(\frac{z - z_{\rm lim}}{z_{\rm wid}})}{2}.$$
 (4)

For F(36, 24), the filter shape is shown in the upper-left corner of Fig. 3. For comparison, we show in orange the filter F(32, 1), which is close to a simple z_{max} cutoff in the quasi-PDFs transformation. The lower rows of Fig. 3 show how the filter alters the matrix elements; the smoother transition to zero at larger z plays an important role in removing the unphysical oscillation. The quasi-PDFs corresponding to these filtered matrix elements are shown in the upper-right of Fig. 3. There is a definite reduction in the oscillatory behavior and significant improvement in recovering the medium- to large-x region of the PDFs. One can recover the PDFs in the |x| > 0.1 region.

We expect to test the filter function on the known PDFs through similar exercises in this work, then use the same function on lattice data; the mismatch region between the original PDFs and the quasi-PDFs tells us where lattice systematics are present.

Another idea is the "derivative" method; this should not only remove the unphysical oscillation but also allow us to reach smaller x for the PDFs. This is essential, since the current knowledge of the x < 0.001 region may not be reliable; if there is indeed a divergence in the true distribution, the lattice data should be able to address it without compromising the predictive power. To take into account the potential nonvanishing of h(z) at infinite values of z, we take the derivative of the nucleon matrix elements h'(z) = (h(z+1) - h(z-1))/2. The Fourier expansion of this derivative differs from the original in a known way:

$$q(x) = \int_{-z_{\text{max}}}^{+z_{\text{max}}} dz \frac{-1}{2\pi} \frac{e^{ixP_z z}}{iP_z x} h'(z).$$
(5)

The upper row of Fig. 4 shows the real (left) and imaginary (right) parts of h'(z) as functions of the nucleon momentum P_z . Here, we drop the error propagation of the PDFs, since the correlations introduced by transforming the pseudodata become degenerate when taking the derivative. This does not affect our investigation, since we know the central value of our final quasi-PDF will reproduce the original CT14 one. It is expected that the real (imaginary) derivative matrix elements are antisymmetric (symmetric) with respect to z = 0. The peaks are sharper for larger P_z .

The quasi-PDFs using the derivative method [and a filter F(32, 1)] are shown in the bottom-left of Fig. 4. The derivative-method PDFs have no unphysical oscillation



FIG. 3. (Top left) The filter shapes proposed to apply to h(z) with $\{z_{max}, z_{wid}\} = \{36, 24\}$ (blue) and $\{32, 1\}$ (orange); the latter is the same as a hard z cutoff. The real (bottom left) and imaginary (bottom right) matrix elements before (purple) and after (blue) applying the F(36, 24) filter. (Top right) The soft-filtered PDF (blue) has significant improvement in recovering the original PDF (gray) while the hard cutoff (orange) suffers from significant unphysical oscillations throughout the entire x range.



FIG. 4. The real (top left) and imaginary (top right) components of h'(z) as a function of z with $P_z = \{4, 8, 12, 24\}\pi/L$. (Bottom left) The original CT14 PDF (gray) along with the new PDFs obtained from the "derivative" method with $P_z = \{4, 8, 12, 24\}\pi/L$ using F(32, 1). The oscillatory behavior is gone and positive x is mostly recovered for $P_z > 4\pi/L$. However, for the antiquark (negative x) region, with $P_z = 24\pi/L$ one can trust up to $|x| \approx 0.05$. (Bottom right) The original CT14 PDF (gray) in comparison with the recovered PDF with $P_z = 24\pi/L$ using the filter method described earlier (blue) and derivative method (red). Both methods recover the distribution in the |x| > 0.1 region; only the derivative method can recover the divergence in the small-x region with $z_{max} = 32$.

without any filter function needed, and also recover most of the positive-x region parton distribution for $P_z > 4\pi/L$. For the antiquark region, however, we find a sensitive P_z dependence in recovering the small-x PDFs. With the largest nucleon momentum $P_z = 24\pi/L$, we can recover the antiquark distribution up to x = -0.05. If we apply a soft filter or increase z_{lim} , it does not make noticeable changes in the distribution with $P_z > 4\pi/L$. Lastly, we compare the PDF obtained from the filter and derivative methods, shown in the bottom-right of Fig. 4 using $P_z = 24\pi/L$. The derivative method (slightly more complicated to implement) recovers the smaller-x region better: 0.1 vs 0.05. Since real lattice data will have worse signal-tonoise ratios than these pseudodata, one in principle should try both approaches to see which one works better with the data qualities, reliability of matrix elements obtained in larger z regions, and other issues to address.

We apply the improved PDF methods to the lattice nucleon matrix elements from clover-on-HISQ lattices [27,28] and concentrate on the a = 0.09 fm 135-MeV pion-mass ensemble with lattice spatial length 5.76 fm. The nucleon matrix elements are generated using $P_z = \{4, 8, 12\}\pi/L$ with a 2 × 2 matrix of standard Gaussian sources and statistics of 2562 measurements each. Two values of source-sink separation, 0.9 fm and 1.08 fm, are

used to account for the excited-state contamination using two-state fits [29,30]. The rest of the unpolarized and polarized lattice calculations and RI/MOM-scheme setup are similar to our previous calculations [11,13,17]. Figure 5 shows results from the quark density (unpolarized) and helicity (polarized) distributions along with selected PDFs, CT14 NNLO [4] at 2 GeV, NNPDFpol1.1 [31] and JAM [32] at 1 GeV. To demonstrate that these two methods work for real lattice data, we use the derivative (filter) method for unpolarized (polarized) PDFs separately; the oscillation behavior in the earlier works [17,18] is indeed no longer present. Note that there are systematics that we are not currently addressing here: (1) The power correction and matching are currently not applied to emphasize the Fourier transformation truncation effect. (2) There will be a systematic introduced by applying either method to lattice data; given the statistical error on the current data, we omit it here. We will study the parameter dependence here, along with all the corrections, and quote them in a future study with larger boost momentum and high statistics.

In this paper, we propose two ideas to remove the current biggest systematic uncertainty in the LaMET approach to studying *x*-dependent hadron structure: Fourier transformation truncation. Without assuming a parametrization form, such a determination of the shape of the PDF. We apply these



FIG. 5. The unpolarized (left) and polarized (right) isovector nucleon PDFs as functions of x; in both cases, a comparison with globalfit PDFs of the corresponding distribution from largest nucleon boosted momentum $P_z = \{8, 12\}\pi/L$. The unpolarized distribution is plotted using the derivative method while the helicity distribution is obtained from the filter method; both results look promising. Higher momenta are needed to achieve more consistent results.

methods to lattice quasi-PDFs at physical pion mass for both unpolarized and polarized distribution and show the method works well on lattice data. The two approaches proposed here have their own parameter dependence, just like the current distribution in this paper has P_z , lattice spacing and possible finite-volume effects. One should carefully study these dependences in future precision calculations with larger boost momentum and high statistics.

ACKNOWLEDGMENTS

We thank the MILC Collaboration for sharing the lattices used to perform this study. The LQCD calculations were performed using the CHROMA software suite [33]. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231; facilities of the USQCD Collaboration, which are funded by the Office of Science of the U.S. Department of Energy and supported in part by Michigan State University through computational resources provided by the Institute for Cyber-Enabled Research. H. W. L. thanks Tie-Jiun Hou from CTEQ Collaboration for providing the CT14 NNLO isovector PDFs. We thank Luchang Jin, Yi-Bo Yang and Yong Zhao for useful discussions. The work of H.W.L. is supported by the U.S. National Science Foundation under Grant No. PHY 1653405 "CAREER: Constraining Parton Distribution Functions for New-Physics Searches." J. W. C. is partly supported by the Ministry of Science and Technology, Taiwan, under Grants No. 105-2112-M-002-017-MY3 and No. 104-2923-M-002-003-MY3, the Center for Advanced Study in Theoretical Sciences (CASTS) of National Taiwan University (NTU), the Kenda Foundation, and DFG and NSFC (CRC 110). T. I. is supported by the Science and Technology Commission of Shanghai Municipality (Grant No. 16DZ2260200) and in part by the Department of Energy, Laboratory Directed Research and Development (LDRD) funding of BNL, under Contract No. DE-EC0012704. J. H. Z. is supported by the Sonderforschungsbereich (SFB)/TRR-55 grant "Hadron Physics from Lattice QCD" and National Science Foundation of China (Grant No. 11405104).

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