Lattice QCD Determination of the Bjorken-x Dependence of Parton Distribution Functions at Next-to-Next-to-Leading Order

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We report the first lattice QCD calculation of pion valence quark distribution with next-to-next-to-leading order perturbative matching correction, which is done using two fine lattices with spacings $a = 0.04$ and 0.06 fm and valence pion mass $m_\pi = 300$ MeV, at boost momentum as large as 2.42 GeV. As a crucial step to control the systematics, we renormalize the pion valence quasidistribution in the recently proposed hybrid scheme, which features a Wilson-line mass subtraction at large distances in coordinate space, and develop a procedure to match it to the $\overline{\mathrm{MS}}$ scheme. We demonstrate that the renormalization and the perturbative matching in Bjorken-x space yield a reliable determination of the valence quark distribution for $0.03 \lesssim x \lesssim 0.80$ with 5%–20% uncertainties.

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Understanding the hadron inner structure remains one of the top fundamental questions in nuclear and particle physics. As the lightest hadrons in nature, pions are the Nambu-Goldstone bosons of quantum chromodynamics (QCD), and their quark and gluon structures can help us to understand the origins of hadron mass and dynamical chiral symmetry breaking. The parton distribution functions (PDFs), which describe 1D momentum densities of quarks and gluons in a hadron, are the simplest and most important quantities that have been extensively studied from global high-energy scattering experiments and will be probed at unprecedented precision at the future Electron-Ion Collider [1,2]. Besides the experimental efforts, the first-principles calculations of PDFs using lattice QCD are also expected to provide useful predictions.

Computation of the PDFs on a Euclidean lattice has been extremely difficult because they are defined from light-cone correlations with real-time dependence in Minkowski space. For a long time, only the lowest moments of the PDFs were calculable as they are matrix elements of local gauge-invariant operators. For reviews see Refs. [3,4]. Less than a decade ago, a breakthrough was made by large-momentum effective theory (LaMET) [5–7], which starts from a Euclidean "quasi-PDF" (qPDF) in a boosted hadron and obtains the PDF through a large-momentum expansion and perturbative matching of the qPDF in Bjorken-x (longitudinal momentum fraction) space. Over the years, LaMET has led to much progress in the calculation of PDFs and other parton physics [4,7], which reinvigorated the field as other proposals [8–13] are also being studied and implemented.

Despite substantial progress, lattice calculation of the PDF x dependence has yet to achieve essential control of the systematic uncertainties [14]. In the LaMET approach, lattice renormalization is one of the most important sources of error. The nonlocal quark bilinear operator $O_\Gamma(z) \equiv \bar{\psi}(z)\Gamma W(z,0)\psi(0)$, where Γ is a Dirac matrix and $z^\mu = (0,0,0,z)$, which defines the qPDF, suffers from a linear power divergence in the Wilson line $W(z,0)$ that must be subtracted before taking the continuum limit. The most popular methods so far are the regularization independent momentum subtraction scheme [15–18] and other ratio schemes [19–22], which use the matrix element of $O_\Gamma(z)$ in an off-shell quark [15–18], a static or boosted hadron [19,22], or the vacuum state [20,21] as the renormalization factor. At small z the matrix elements in these schemes satisfy a factorization relation to the light-cone correlation [13,23–25]. However, at large z they introduce nonperturbative effects [26] that propagate to the qPDF via Fourier transform (FT) of the matrix elements, which contaminates the LaMET matching in x

space. To overcome this limitation, the hybrid scheme [27] was proposed to subtract the linear divergence at large z and match the result to the $\overline{\mathrm{MS}}$ scheme, thus preserving the LaMET matching after FT. To date, the hybrid scheme has not been used in calculating the PDFs, except for a recent work on meson distribution amplitudes [28]. Apart from renormalization, the accuracy of perturbative matching also controls the precision of the calculation. In all the existing lattice calculations, the matching was done at only next-to-leading order (NLO), and it is not until recently that the next-to-next-to-leading order (NNLO) matching was derived for the nonsinglet quark qPDF in the $\overline{\mathrm{MS}}$ scheme [21,29].

In this Letter we present a state-of-the-art calculation of pion valence quark PDF using high-statistics, superfine-spacing, and large-momentum lattice data [26], with an adapted hybrid-scheme renormalization and the first-time implementation of NNLO matching. The pion valence PDF has been extracted from global fits [30–33] and studied in lattice QCD [26,34–40], with both at NLO accuracy. In this work, we subtract the linear divergence in $O_\Gamma(z)$ with subpercent precision, and develop a procedure to match the lattice subtraction scheme to $\overline{\mathrm{MS}}$, a crucial step in the hybrid scheme to reduce the power corrections [27]. We derive the NNLO hybrid-scheme matching and apply it to the qPDF, showing good perturbative convergence and reduced scale-variation uncertainty compared to NLO matching. Finally, we demonstrate that our analysis yields a reliable determination of the PDF for $0.03 \lesssim x \lesssim 0.80$ with 5%–20% uncertainties.

Our lattice data was produced using gauge ensembles in $2+1$ flavor QCD generated by the HotQCD Collaboration [41] with highly improved staggered quarks [42], including two lattice spacings $a = 0.04$ and 0.06 fm, and volumes $L_s^3 \times L_t = 64^4$ and $48^3 \times 64$, respectively. We use tadpole-improved clover Wilson valence fermions on the hypercubic (HYP) smeared [43] gauge background, with a valence pion mass $m_\pi = 300$ MeV. Furthermore, the Wilson line in $O_\Gamma(z)$ is constructed from HYP-smeared gauge links. We use pion momenta $P^z = (2\pi n_z)/(L_s a)$ with $0 \le n_z \le 5$, resulting in P^z as large as 2.42 GeV.

The qPDF $\tilde{f}_v(x, P^z, \mu)$ is defined in a boosted pion state $|P\rangle$ with four-momentum $P^\mu = (P^t, 0, 0, P^z)$:

$$\tilde{f}_v(x, P^z, \mu) = \int \frac{dz}{2\pi} e^{ixP^z z} \tilde{h}(z, P^z, \mu), \tag{1}$$

where $\tilde{h}(z, P^z, \mu) \equiv \langle P|O_{\gamma^t}(z)|P\rangle/(2P^t)$, and μ is the $\overline{\mathrm{MS}}$ scale. The operator $O_\Gamma(z)$ can be renormalized under lattice regularization as [44–46]

$$O_\Gamma^B(z, a) = e^{-\delta m(a)|z|} Z_O(a) O_\Gamma^R(z), \tag{2}$$

where "B" and "R" denote bare and renormalized quantities. The factor $Z_O(a)$ includes all the logarithmic ultraviolet (UV) divergences which are independent of z, while the Wilson-line mass correction $\delta m(a)$ includes the linear UV divergence $\propto 1/a$ and can be expressed as

$$\delta m(a) = \frac{m_{-1}(a)}{a} + m_0, \tag{3}$$

where $m_{-1}(a)$ is a series in the strong coupling $\alpha_s(1/a)$, and m_0 is an $\mathcal{O}(\Lambda_{\mathrm{QCD}})$ constant originating from the renormalon ambiguity in $m_{-1}(a)$ [47].

The hybrid scheme is implemented as follows: For $0 \le z \le z_S$ with $a \ll z_S \ll 1/\Lambda_{\mathrm{QCD}}$, we form the ratio $\tilde{h}(z, P^z, a)/\tilde{h}(z, 0, a)$ to cancel the UV divergences and the cutoff effects from $z \sim a$ [19]; at $z > z_S$ we subtract $\delta m(a)$ and determine $Z_O(a)$ by imposing a continuity condition of the renormalized matrix elements at $z = z_S$. There are different ways to calculate $\delta m(a)$ [27,46,48–51]. We determine $\delta m(a)$ from the combination of the static quark-antiquark potential, $V^{\mathrm{lat}}(r)$ [41,52], and the free energy of a static quark at nonzero temperature [53–55], with the following normalization scheme,

$$V^{\mathrm{lat}}(a, r = r_0) + 2\delta m(a) = 0.95/r_0, \tag{4}$$

where $r_0 = 0.469$ fm is the Sommer scale for $2+1$ flavor QCD [41], and the constant 0.95 defines the scheme. The linear divergence $m_{-1}(a)/a$ does not depend on the scheme, while m_0 does. The results are $a\delta m = 0.1586(8)$ and 0.1508 (12) for $a = 0.06$ and 0.04 fm, respectively.

Since m_0 is scheme dependent, a factor of $e^{\bar{m}_0|z|}$ with $\bar{m}_0 \sim \mathcal{O}(\Lambda_{\mathrm{QCD}})$ is needed to match the lattice scheme to $\overline{\mathrm{MS}}$, otherwise the LaMET expansion of the qPDF will include a power correction $\propto \bar{m}_0/P^z$ [27], which slows down convergence to the PDF as P^z grows. It was proposed that $\bar{m}_0$ can be obtained by comparing the subtracted matrix elements of $O_\Gamma(z)$ [51] or $W(z,0)$ [49] with their $\overline{\mathrm{MS}}$ operator product expansion (OPE), whose accuracy requires $z \lesssim 0.2$ fm [27]. But because of discretization effects, the window of z that can be used is actually narrow.

Our new procedure for the hybrid scheme is distinct by the determination of $\bar{m}_0$. In order to use larger z, we construct the following ratio and compare it to a form motivated by the OPE of $\tilde{h}(z, 0, \mu)$,

$$\lim_{a\to 0} e^{\delta m(a)(z-z_0)} \frac{\tilde{h}(z, 0, a)}{\tilde{h}(z_0, 0, a)} = e^{-\bar{m}_0(z-z_0)} \frac{C_0(\mu^2 z^2) + \Lambda z^2}{C_0(\mu^2 z_0^2) + \Lambda z_0^2}, \tag{5}$$

where $z, z_0 \gg a$, and the parameter $\Lambda \sim \mathcal{O}(\Lambda_{\mathrm{QCD}}^2)$. The Wilson coefficient C_0 is known to NNLO [21,25,29], and $\bar{m}_0$ and Λz^2 originate from the leading UV and infrared renormalons in C_0 [20]. According to Eq. (2), the left-hand side of Eq. (5) must have a continuum limit if $\delta m(a)$ includes all the linear divergences, which is renormalization group (RG) invariant. We choose $z \ge z_0 = 0.24$ fm and find agreement between the $a = 0.04$ fm and $a = 0.06$ fm ratios at subpercent level up to $z \sim 1$ fm. Then we extrapolate the lattice ratios to the continuum with a^2 dependence [26], and fit the result to the right-hand side of Eq. (5). For $z_0 \leq z \leq 0.4$ fm, we obtain decent plateaus and χ^2 values for both $\bar{m}_0$ and Λ with the NNLO C_0. By definition $\bar{m}_0$ cancels the lattice scheme dependence of $\delta m(a)$, as changing the scheme only shifts $\delta m(a)$ by a constant, but $\bar{m}_0$ will inherit the $\mathcal{O}(\Lambda_{\rm QCD})$ ambiguity in the $\overline{\rm MS}$ scheme. Since C_0 is at fixed order, both $\bar{m}_0$ and Λ depend on μ, which we vary to estimate the related uncertainty in the final result. At $\mu = 2.0$ GeV, $\bar{m}_0 = 0.137(2)$ GeV and $\Lambda = -0.058(1)$ GeV^2, so the power correction is not negligible. Therefore, we modify the hybrid scheme by correcting the Λz^2 term in $\tilde{h}(z, 0, \mu)$ at short z as

$$\begin{aligned}\tilde{h}(z, z_S, P^z, \mu, a) = {} & N \frac{\tilde{h}(z, P^z, a)}{\tilde{h}(z, 0, a)} \frac{C_0(z^2\mu^2) + \Lambda z^2}{C_0(z^2\mu^2)} \theta(z_S - z) \\ & + N e^{\delta m'(z - z_S)} \frac{\tilde{h}(z, P^z, a)}{\tilde{h}(z_S, 0, a)} \frac{C_0(z_S^2\mu^2) + \Lambda z_S^2}{C_0(z_S^2\mu^2)} \\ & \times \theta(z - z_S), \end{aligned} \tag{6}$$

where $\delta m' = \delta m + \bar{m}_0$, and $N = \tilde{h}(0, 0, a)/\tilde{h}(0, P^z, a)$ normalizes $\tilde{h}(z, z_S, P^z, \mu, a)$ to one at $z = 0$. Since C_0 is at fixed order, $\tilde{h}(z, z_S, P^z, \mu, a)$ depends on μ despite the fact that it should be RG invariant. Such a renormalization is performed through bootstrap loops so that the correlation between different P^z and z is taken care of.

The hybrid-scheme matrix elements are shown in Fig. 1. At small z, $\tilde{h}(z, P^z)$ is dominated by the leading-twist contribution. At large z, the spacelike correlator for pion valence quarks will exhibit an exponential decay $\propto e^{-m_{\rm eff}|z|}$ where $m_{\rm eff}$ is an effective mass related to the system [56]. When plotted as a function of $\lambda = zP^z$, $\tilde{h}(\lambda, P^z)$ should scale in P^z at small λ, with slight violation due to QCD evolution. Its exponential decay will emerge at a larger λ with greater P^z and with decay rate $m_{\rm eff}/P^z$. In the $P^z \to \infty$ limit, the exponential decay vanishes at finite λ ($z \to 0$), and only the leading-twist contribution remains, which almost scales in P^z and features a power-law decay at large λ that corresponds to small-x PDF [27]. This picture is consistent with Fig. 1.

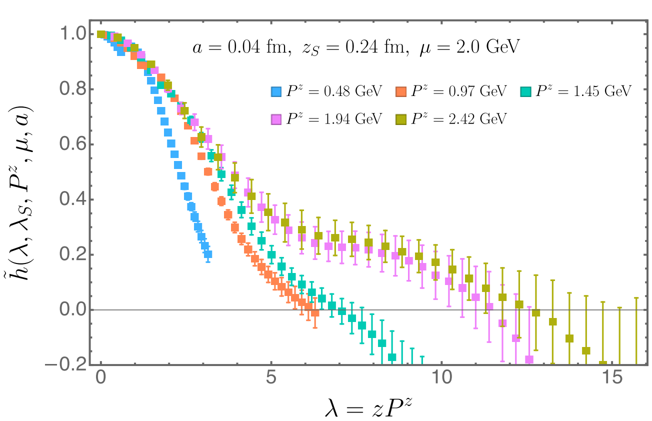

FIG. 1. Renormalized matrix elements in the hybrid scheme.

The next step is a FT. We truncate the matrix elements at z_L or $\lambda_L = z_L P^z$ where $\tilde{h}(\lambda_L) \sim 0$, and extrapolate to ∞ to remove the unphysical oscillations from a truncated FT [27]. The extrapolation form is $Ae^{-m_{\rm eff}|z|}/|\lambda|^d$, where A, $m_{\rm eff}$, and d are the parameters. Since $m_{\rm eff}$ is independent of P^z, by fitting to the $P^z = 0$ matrix elements we find that it is around 0.1 GeV, which is not far from the phenomenological estimate of 0.2–0.5 GeV in HQET [57]. Therefore, we impose $m_{\rm eff} > 0.1$ GeV, as well as $A > 0$ and $d > 0$, to ensure a convergent FT on each bootstrap sample. Since the FT converges fast with the exponential decay, the extrapolation mainly affects the small-x region apart from removing the unphysical oscillations. To verify this we vary z_L, which turns out to have little impact, and use different $m_{\rm eff}$ bounds and extrapolation forms, which lead to consistent qPDFs down to $x \sim 0.05$.

Then, we match the qPDF $\tilde{f}_v(x, \lambda_S, P^z, \mu)$ to the $\overline{\rm MS}$ PDF $f_v(x, \mu)$ through LaMET [25,27,58,59]:

$$\begin{aligned} f_v(x, \mu) = {} & \int_{-\infty}^{\infty} \frac{dy}{|y|} C^{-1}\left(\frac{x}{y}, \frac{\mu}{yP^z}, |y|\lambda_S\right) \tilde{f}_v(y, \lambda_S, P^z, \mu) \\ & + \mathcal{O}\left(\frac{\Lambda_{\rm QCD}^2}{(xP^z)^2}, \frac{\Lambda_{\rm QCD}^2}{((1-x)P^z)^2}\right), \end{aligned} \tag{7}$$

where $\lambda_S = z_S P^z$, $z_S = 0.24$ fm, and the power corrections are controlled by the parton and spectator momenta xP^z and $(1-x)P^z$ [27]. Here C^{-1} is the inverse of the hybrid-scheme matching coefficient C, which we derive at NNLO [60] by conversion from the $\overline{\rm MS}$ result [21,29]. Based on Eq. (7), we can directly calculate the PDF with P^z-controlled power corrections for $x \in [x_{\rm min}, x_{\rm max}]$.

In Fig. 2 we show the results of perturbative matching. The matching drives the qPDF to smaller x and reduces the

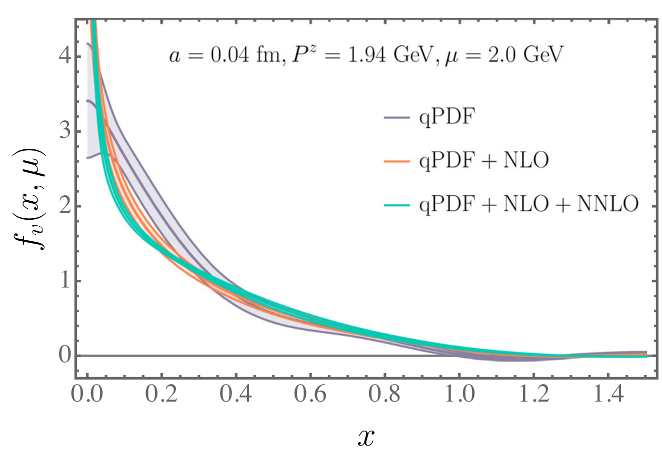

FIG. 2. Comparison of PDFs obtained from the qPDF with NLO and NNLO matching corrections.

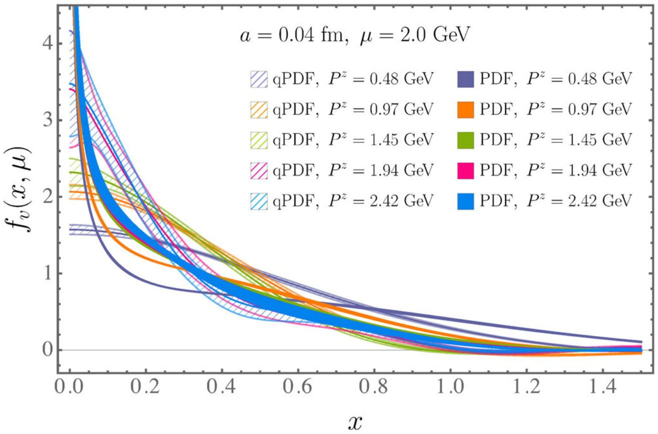

FIG. 3. The PDFs obtained from the qPDFs with NNLO matching at different P^z.

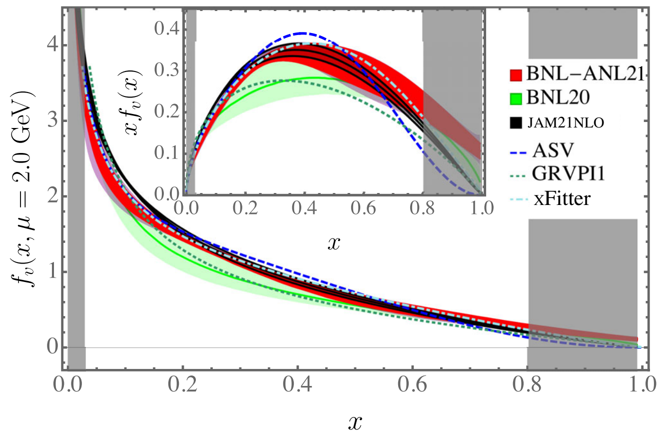

FIG. 4. Comparison of our prediction of $f_v(x)$, BNL-ANL21, to global fits and BNL20. The shaded regions $x < 0.03$ and $x > 0.8$ are excluded by requiring that estimates of $\mathcal{O}(\alpha_s^3)$ and power corrections be smaller than 5% and 10%, respectively.

statistical errors at moderate x, because matching effectively relates the qPDF from finite P^z to infinity, and the qPDF evolves to smaller x as P^z increases. The NNLO correction is generally smaller than the NLO correction, which indicates good perturbative convergence, a crucial criterion for precision calculation. Besides, by varying μ and evolving the matched results to the same μ, we find that the scale-variation uncertainty is reduced at NNLO, which is further evidence of improved precision. The matching correction diverges as $x \to 0$, implying that resummation of small-x logarithms is needed. A resummation is also necessary as $x \to 1$ [40], but these resummations are not needed for moderate x.

We compare the PDFs obtained at different P^z with NNLO matching in Fig. 3. At moderate x, the P^z dependence is remarkably reduced, and the results appear to converge for $P^z \geq 1.45$ GeV, which strongly indicates the effectiveness of LaMET matching. At $x \gtrsim 1$, each PDF curve has a small nonvanishing tail due to the power corrections in Eq. (7), but they decrease with larger P^z. To estimate the size of the power corrections, we fit the PDFs obtained at $a = 0.04$ fm, $P^z = \{1.45, 1.94, 2.42\}$ GeV, and $a = 0.06$ fm, $P^z = \{1.72, 2.15\}$ GeV to the *ansatz* $f_v(x) + \alpha(x)/P_z^2$ for each fixed x, where we ignore the a dependence as it has been found that the matrix elements have $\mathcal{O}(a^2 P_z^2)$ effects that are less than 1% [26]. Since this fit is mainly affected by the datasets at lower P^z with smaller statistical errors, which have larger power corrections, we use the result at $P^z = 2.42$ GeV instead of the fitted $f_v(x)$ as our final prediction. The power correction at $P^z = 2.42$ GeV is estimated to be $\alpha(x)/[P_z^2 f_v(x)] < 0.10$ for $0.01 < x < 0.80$. It is surprising that the results are insensitive to P^z for x as small as 0.01, nor do they show dependence on the extrapolation form in the FT as we have checked. This can be explained by that, under matching, the qPDF contributes to the PDF at larger x which has less dependence on P^z or the extrapolation. Nevertheless, it must be pointed out that the smallness here is only relative, as $\alpha(x)/P_z^2$ still diverges as $x \to 0$.

Our final prediction for the pion valence quark PDF (BNL-ANL21) is shown in Fig. 4, which is obtained from the qPDF at $a = 0.04$ fm, $z_S = 0.24$ fm, $z_L = 0.92$ fm, $\mu = 2.0$ GeV, and $P^z = 2.42$ GeV with exponential extrapolation and NNLO matching. The red band represents the statistical error, and the light purple band includes the error from scale variations, which is obtained by repeating the same analysis for $\mu = 1.4$ and 2.8 GeV and evolving the PDFs to $\mu = 2.0$ GeV with the NLO Dokshitzer–Gribov–Lipatov–Altarelli–Parisi kernel. Since the hybrid-scheme parameter $\bar{m}_0$ depends on μ, the small scale variation in the final result demonstrates that the renormalization uncertainty is well under control. We require that the $\mathcal{O}(\alpha_s^3)$ matching correction at $\mu = 2.0$ GeV be smaller than 5%, which propagates geometrically to <37% at NLO and <14% at NNLO, thus excluding $x < 0.03$ and $x > 0.88$. A list of the above uncertainties at selected x is shown in Table I. We neglect the FT uncertainty as it is extremely small. As for m_π dependence, our associated calculation of the second PDF moment at $m_\pi = 140$ MeV [61] shows consistency within 5% statistical uncertainty, which will be validated by a direct comparison in the future. Previous studies [62,63] also suggest that the finite volume correction is less than 1% for our lattice setup. At last, by limiting the estimated power corrections to be less than 10%, we determine the PDF at $0.03 \lesssim x \lesssim 0.80$ with 5%–20% uncertainties. See all analysis details in Ref. [64]. Our result is in great agreement with the recent global fits by xFitter [31] and

TABLE I. Statistical and systematic uncertainties at given x.

x	Statistical	Scale	$\mathcal{O}(\alpha_s^3)$	Power corrections	$\mathcal{O}(a^2P_z^2)$
0.03	0.10	0.04	<0.05	<0.01	<0.01
0.40	0.07	<0.01	<0.05	0.04	<0.01
0.80	0.15	0.03	<0.05	0.10	<0.01

JAM21NLO [32] for $0.2 < x < 0.6$, but deviates from the earlier GRVPI1 [30] and ASV [33] fits. When compared to a previous analysis of the same lattice data (BNL20) [26], which used a short-distance factorization of the matrix elements at NLO, and a parametrization of the PDF, our new result has shifted central values and considerably reduced uncertainties at moderate x, but still agrees within errors. With finite P^z and statistics, lattice QCD can only make predictions for $x \in [x_{\min}, x_{\max}]$. The PDF parametrization correlates the information at all $x \in [0, 1]$, so the larger uncertainties at moderate x in BNL20 could be propagated from the uncontrolled errors in the end-point regions. Besides, there is no practical estimate of the model uncertainty in the parametrization. Therefore, the LaMET calculation for $x \in [x_{\min}, x_{\max}]$ is more reliable as it does the power expansion and matching directly in x space.

In summary, we have performed a state-of-the-art lattice QCD calculation of the x dependence of pion valence quark PDF, where we developed a procedure to renormalize the qPDF in the hybrid scheme and match it to the $\overline{\mathrm{MS}}$ PDF at NNLO. The final results show reduced perturbation theory uncertainty and converge at moderate x with pion momenta greater than 1.45 GeV, which allows us to reliably estimate the systematic errors. This calculation can be improved with physical pion mass, continuum extrapolation, and higher statistics for the matrix elements at long distances and at larger boost momenta.

Our renormalization procedure can also be incorporated into the lattice calculations of gluon PDFs, distribution amplitudes, generalized parton distributions and transverse momentum distributions. With the systematics under control, we can expect lattice QCD to provide reliable predictions for these quantities in the future.

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Correction: The values for $\bar{m}_0$ and Λ contained errors in the second sentence before Eq. (6) and have been fixed. In the Supplemental Material, the first full paragraph after Eq. (C10) has been modified.