Extraction of Next-to-Next-to-Leading-Order PDFs from Lattice QCD Calculations

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We define quark correlation functions that are not only calculable in lattice QCD, but also factorizable into parton distribution functions with coefficients perturbatively calculable to all orders in QCD with a proper regularization. We present for the first time the complete next-to-next-to-leading-order calculation of valence-quark coefficient functions. We find that theoretical uncertainties are improving with higher order coefficients. Our method of calculations can be readily generalized to evaluate gluon correlation functions, and high order sea-quark matching coefficients, putting the program to extract partonic structure of hadrons from lattice QCD calculations to be comparable with that from experimental measurements.

I. INTRODUCTION

Parton distribution functions (PDFs) encode important nonperturbative information of strong interactions, and they are crucial for understanding all phenomena at the Large Hadron Colliders (LHC) [1]. In terms of QCD factorization [2], a typical hadronic cross section with a large momentum transfer Q and collision energy $\sqrt{S}$ at the LHC can be factorized as

$$d\sigma_{hh'}(Q^2,S) = \sum_{i,j} f_{i/h}(x,\mu^2) \otimes f_{j/h'}(x',\mu^2) \otimes d\hat{\sigma}_{ij}(x,x',\mu^2,Q^2,S) + O(\Lambda^2_{\rm QCD}/Q^2)\,, \quad (1)$$

where $i,j = q,\bar{q},g$ represents parton flavor, $f_{i/h}(x,\mu)$ is the PDF as a probability distribution to find an active parton of flavor i inside a colliding hadron h with the parton carrying the hadron's momentum fraction x, probed at a factorization scale $\mu \sim O(Q)$, $d\hat{\sigma}_{ij}$ represents a short-distance partonic scattering, and $\otimes$ indicates an integration over value of x or x', accessible by the scattering cross section. By measuring hadronic cross sections, with perturbatively calculated partonic hard parts $d\hat{\sigma}_{ij}$, PDFs have been extracted from the world data at the state-of-the-art next-to-next-to-leading order (NNLO) accuracy [1].

With the steep falling nature of PDFs as $x \to 1$ and the convolution in Eq. (1), the uncertainty of extracted PDFs at large x is so significant that limits our confidence to push the search for signals of new physics to larger invariant mass. With the nonperturbative nature of PDFs, it is natural to ask if we can calculate PDFs directly in LQCD. A short answer is no since the operators defining PDFs are time-dependent and LQCD is formulated in Euclidean space-time. Recently, stimulated by quasi-PDFs approach proposed by Ji [3], extraction of PDFs from lattice QCD calculation has drawn many new ideas, including the pseudo-PDFs [4], current-current correlators [5] and others approaches [6]. As proposed by two of us in Refs. [5, 7], PDFs can be extracted from any *good* LQCD observables, which was referred to as "Lattice Cross Sections" (LCSs) in position space, that are calculable in LQCD and factorizable into PDFs with perturbatively calculable matching coefficients,

$$\sigma_{n/h}(\omega,\xi^2) \equiv \langle h(p)|T\{\mathcal{O}_n(\xi)\}|h(p)\rangle = \sum_i f_{i/h}(x,\mu) \otimes K_{n/i}(x\omega,\xi^2,\mu^2) + O(\xi^2\Lambda^2_{\rm QCD})\,, \quad (2)$$

where ξ with $\xi^2 \neq 0$ represents the size of nonlocal operator $\mathcal{O}_n(\xi)$ of type n, controlling the short-distance physics of the factorization, and $\omega \equiv p\cdot\xi$ (often referred as Ioffe time). With perturbative matching coefficients $K_{n/i}$ between $\sigma_{n/h}(\omega,\xi^2)$ and $f_{i/h}(x,\mu)$, PDFs can be extracted by QCD global fits of data generated by LQCD calculation of $\sigma_{n/h}(\omega,\xi^2)$ with various operator type n, just like how PDFs have been extracted from the world data on various high energy scattering cross sections [1, 5, 7].

PDFs are universal and should not depend on if they were extracted from high energy scattering data using Eq. (1) or from data on good LQCD observables (or LCSs) using Eq. (2). The universality of PDFs does require the same factorization scheme to be used for calculating the short-distance hard parts, such as $d\hat{\sigma}_{ij}$ in Eq. (1) and $K_{n/i}$ in Eq. (2). Since $\sigma_{n/h}$ in Eq. (2) does not have to be a physical cross section, the operator $\mathcal{O}_n(\xi)$ defining $\sigma_{n/h}$ might require additional ultraviolet (UV) renormalization beyond using renormalized fields. This additional UV renormalization has impacted perturbative calculation and stability of the matching coefficients $K_{n/i}$ for LQCD observables. Although extraction of PDFs from LQCD calculations have made tremendous progresses in recent years [8–44], the state-of-the-art calculation of short-distance matching coefficients is still limited to the next-to-leading order (NLO) in almost all existing approaches [28–31], which is partially

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limited by this additional renormalization and our ability to do perturbative calculation in coordinate space. In this Letter, we derive for the first time the NNLO valence-quark matching coefficients in dimensional regularization, allowing us to extract PDFs from LQCD calculations at the same rigor as those extracted from experimental data. Calculating the matching coefficients at NNLO is not only necessary for being competitive with the effort to extract PDFs from experimental data, but also for addressing concerns that a possible mechanism may break the factorization at NNLO [45].

II. QUARK CORRELATION FUNCTIONS

We focus on the following gauge invariant quark correlation operator

$$\mathcal{O}_q^{\nu,b}(\xi,\mu^2,\delta) = \overline{\psi}_q(\xi)\,\gamma^\nu \Phi^{(f)}(\{\xi,0\})\,\psi_q(0)\big|_{\mu^2,\delta}\,, \quad (3)$$

which is made of renormalized fields with a path ordered gauge link in the fundamental representation, $\Phi^{(f)}(\xi,0) = \mathcal{P}e^{-ig_s\int_0^1 \xi\cdot A^{(f)}(r\xi)\,dr}$. Because the composite quark correlation operator is UV divergent, a UV regulator δ is needed, which may represent lattice spacing a in lattice QCD calculations, or represent $\epsilon \equiv (4-d)/2$ in dimensional regularization (DR) of continuum calculations. μ is a dimensional scale accompanied by the UV regulator. The UV divergence is multiplicatively renormalizable [18, 19], as

$$\mathcal{O}_q^{\nu,\mathrm{RS}}(\xi) = \mathcal{O}_q^{\nu,b}(\xi,\mu^2,\delta)/Z^{\mathrm{RS}}(\xi^2,\mu^2,\delta)\,, \quad (4)$$

where superscript RS indicates a renormalization scheme and $Z^{\mathrm{RS}}(\xi^2,\mu^2,\delta)$ is the multiplicative renormalization constant. We will choose regularization-invariant renormalization conditions so that the renormalized $\mathcal{O}_q^{\nu,\mathrm{RS}}$ are independent of δ and μ^2.

We define quark correlation functions (QCFs) as hadronic matrix elements of $\mathcal{O}_q^{\nu,\mathrm{RS}}(\xi)$

$$F_{q/h}^{\nu,\mathrm{RS}}(\omega,\xi^2) = \langle h(p)|\mathcal{O}_q^{\nu,\mathrm{RS}}(\xi)|h(p)\rangle\,, \quad (5)$$

which is independent of regularization scheme and scale, like physical cross sections. With $\xi^0 = 0$ and $\xi^2\Lambda^2_{\mathrm{QCD}} \ll 1$, $F_{q/h}^{\nu,\mathrm{RS}}(\omega,\xi^2)$ are calculable in LQCD and factorizable into PDFs [5, 7]. In this Letter, we focus on flavor nonsinglet case, factorization formula for which in continuum theory is [5]

$$F_{q_v/h}^{\nu,\mathrm{RS}}(\omega,\xi^2) = \frac{1}{R^{\mathrm{RS}}(\xi^2,\mu^2)}\int_0^1 \frac{dx}{x}\, f_{q_v/h}(x,\mu^2) \times K^\nu(x\omega,\xi^2,\mu^2) + O(\xi^2\Lambda^2_{\mathrm{QCD}})\,, \quad (6)$$

where $R^{\mathrm{RS}}(\xi^2,\mu^2) \equiv Z^{\mathrm{RS}}(\xi^2,\mu^2,\epsilon)/Z^{\overline{\mathrm{MS}}}(\xi^2,\mu^2,\epsilon)$ is a *finite* renormalization factor that transforms any "preferred" regularization-invariant RS scheme to the conventional $\overline{\mathrm{MS}}$ scheme, K^ν are perturbative matching coefficients in $\overline{\mathrm{MS}}$ scheme, and $q_v \equiv q - \bar{q}$ which means

$$f_{q_v/h}(x,\mu^2) \equiv f_{q/h}(x,\mu^2) - f_{\bar{q}/h}(x,\mu^2)\,, \quad (7)$$

$$F_{q_v/h}^{\nu,\mathrm{RS}}(\omega,\xi^2) \equiv F_{q/h}^{\nu,\mathrm{RS}}(\omega,\xi^2) - F_{\bar{q}/h}^{\nu,\mathrm{RS}}(\omega,\xi^2) = F_{q/h}^{\nu,\mathrm{RS}}(\omega,\xi^2) - F_{q/h}^{\nu,\mathrm{RS}}(-\omega,\xi^2)\,. \quad (8)$$

To extract the valence quark distribution $f_{q_v/h}$ from LQCD calculations of $F_{q_v/h}^{\nu,\mathrm{RS}}$ to the NNLO accuracy, we have to perturbatively calculate R^{RS} and K^ν to the power of α_s^2.

III. RENORMALIZATION CONSTANT

The renormalization constant Z^{RS} introduced in Eq. (4) is determined by the short-distance property of the quark correlation operator in Eq. (3) and should not depend on the hadronic state used to define the QCFs of this operator. Because of its multiplicative renormalizability, matrix element of $\mathcal{O}_q^{\nu,b}$ in Eq. (3) inserted into any state could be an allowable renormalization scheme,

$$Z^{\mathrm{RS}}(\xi^2,\mu^2,\delta) = \frac{\langle \mathrm{RS}|\hat{n}\cdot\mathcal{O}_q^b(\xi,\mu^2,\delta)|\mathrm{RS}\rangle}{\langle \mathrm{RS}|\hat{n}\cdot\mathcal{O}_q^b(\xi,\mu^2,\delta)|\mathrm{RS}\rangle^{(0)}}\,, \quad (9)$$

where $\hat{n}$ is any vector keeping the denominator nonvanishing and the superscript "(0)" indicates that the matrix element is evaluated to the lowest order in perturbation theory. Different choice of the state $|\mathrm{RS}\rangle$ corresponds to different renormalization scheme. For example, an off-shell quark state with a specific momentum was used in defining RI′ scheme [14] and RI/MOM scheme [17, 28, 29]; a hadron state with zero momentum was used in calculations of pseudo-PDFs [30] [Matrix element in this case cannot be perturbatively calculated and one should choose the denominator in Eq. (9) as 1]; and the vacuum state was introduced in Ref. [46].

In the following, we define the renormalization constant with the vacuum state and denote RS = vac. By calculating the vacuum expectation value to NNLO, we demonstrate that without an identified external momentum, the renormalization constant Z^{vac} is completely free of IR and CO singularity and its UV divergence is regularized by DR, from which we obtain $Z^{\overline{\mathrm{MS}}}(\xi^2,\mu^2,\epsilon)$ and $R^{\mathrm{vac}}(\xi^2,\mu^2)$ at NNLO level.

In Fig. 1(a,b,c), we show some representative Feynman diagrams, up to NNLO, for the vacuum expectation value of quark correlation operators needed for calculating the renormalization constant defined in Eq. (9). The diagram (a) in Fig. 1 determines the normalization of Z^{vac},

$$\langle\Omega|\hat{n}\cdot\mathcal{O}_{\mathrm{b}}|\Omega\rangle^{(0)} = 2N_c\,\mu^{4-d}\,\pi^{-d/2}\,\Gamma(d/2)\,|\xi|^{-d}\hat{n}\cdot\xi\,, \quad (10)$$

where $|\xi|^2 \equiv -\xi^2$, and the result agrees with Ref. [46].

The Fig. 1(b) is a representative Feynman diagram contributing to NLO Z^{vac},

$$M_b = g_s^2 N_c C_F\,\mu^{8-2d}\int_0^1 dr\int\frac{d^dl_1\,d^dl_2}{(2\pi)^{2d}}\,e^{il_1\cdot\xi+irl_2\cdot\xi} \times \frac{\mathrm{Tr}[(\not{l}_1+\not{l}_2)\not{\xi}\not{l}_1\not{\hat{n}}]}{(l_1^2+i0^+)(l_2^2+i0^+)((l_1+l_2)^2+i0^+)}\,, \quad (11)$$

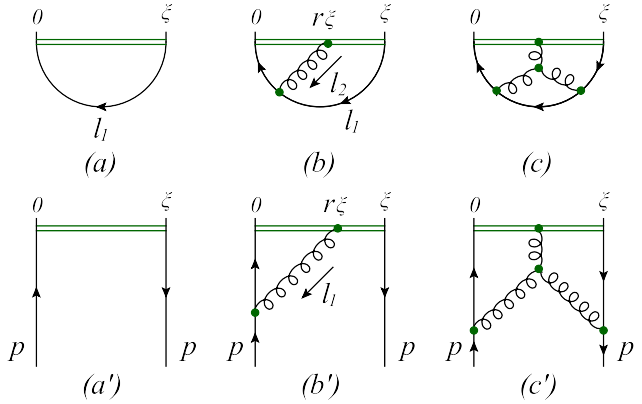

FIG. 1. Representative Feynman diagrams, up to NNLO, for the vacuum expectation value of quark correlation operator (top row), and for the non-singlet quark matrix elements of the same operator (bottom row).

where we assume without loss of generality that z-component ξ_z is only nonzero component of ξ, and $\hat{n}$ satisfies $\hat{n}\cdot l \equiv l_z$ for any vector l. We find that it is convenient to carry out the integration in Eq. (11) by Fourier transforming the ξ_z into q_z in momentum space as $\mathscr{F}[M_b] \equiv \int d\xi_z e^{-i\xi_z q_z} M_b$ to eliminate the exponential factor by using

$$\begin{aligned}&\int d\xi_z e^{-i\xi_z q_z}\xi_z \int_0^1 dr\, e^{-il_{1z}\xi_z - irl_{2z}\xi_z}\,,\\ =&-2i\,\mathrm{Im}\left(\frac{1}{(q_z+l_{1z}+l_{2z}+i0^+)(q_z+l_{1z}+i0^+)}\right),\end{aligned} \tag{12}$$

where $2\pi\delta(x) = -2\,\mathrm{Im}(\frac{1}{x+i0^+})$ is used. The Fourier transformation also ensures that only imaginary part of gauge-link-related propagators are involved, which led to a similar effect of optical theorem. Our matrix element is defined with gauge-link in coordinate space, which is effectively equal to sum over diagrams with cut gauge-link in momentum space. It is the summation of cuts of gauge link that forces the appearance of imaginary part of "forward scattering amplitude". The obtained loop integrals in momentum space can be reduced to linear combination of a small set of integrals, called master integrals (MIs), by using integration-by-parts relations (IBPs) [47, 48]. We use the package `FIRE5` [49] to do this reduction, which results in

$$\begin{aligned}\mathscr{F}[M_b] = ig_s^2 N_c C_F\,\mu^{8-2d}\,\frac{2(d-2)}{d-4}\\ \times\left[\,I_1 - \frac{2(2d-5)(3d-10)}{(d-3)(d-4)}\,q_z^{-1} I_2\right],\end{aligned} \tag{13}$$

with two vacuum MIs defined as

$$\begin{aligned}I_1 =& \int\frac{d^dl_1\,d^dl_2}{(2\pi)^{2d}}\,\frac{1}{(l_1^2+i0^+)(l_2^2+i0^+)}\\ &\times 2\,\mathrm{Im}\left(\frac{1}{(q_z+l_{1z}+i0^+)(q_z+l_{2z}+i0^+)}\right),\\ I_2 =& \int\frac{d^dl_1\,d^dl_2}{(2\pi)^{2d}}\,\frac{1}{(l_1^2+i0^+)(l_2^2+i0^+)}\\ &\times 2\,\mathrm{Im}\left(\frac{1}{q_z+l_{1z}+l_{2z}+i0^+}\right).\end{aligned} \tag{14}$$

To carry out these single-scale vacuum MIs, we use the method presented in Ref. [50] by setting up and solving dimensional recurrence relations and obtain

$$\begin{aligned}I_1 &= \frac{\pi^{-d}}{8}\sin(d\pi)\Gamma(d/2-1)^2\Gamma(3-d)^2\,|q_z|^{2d-9}\,q_z^3\,,\\ I_2 &= \frac{\pi^{-d}}{8}\sin(d\pi)\Gamma(d/2-1)^2\Gamma(5-2d)\,|q_z|^{2d-9}\,q_z^4\,.\end{aligned} \tag{15}$$

We then Fourier transform inversely from q_z dependence into ξ_z dependence to derive the result of M_b in DR. Other two-loop diagrams, including UV counter term diagrams, can be calculated similarly.

All three-loop diagrams like diagram (c) in Fig. 1 can also be calculated similarly as the diagram (b) described above. The only difference is that analytical expression of vacuum MIs cannot be obtained by solving dimensional recurrence relations directly. Instead, we calculate the vacuum MIs to high accuracy by using dimensional recurrence relations and then obtain exact results by using PSLQ algorithm [51] We check the correctness of our exact results numerically with at least 10^3 digits.

By adding all diagrams and UV counter terms together, the remained divergences should be removed by operator renormalization. With a $\overline{\rm MS}$ subtraction scheme, we obtain $Z^{\overline{\rm MS}}(\xi^2,\mu^2,\epsilon)$ and $R^{\rm vac}(\xi^2,\mu^2)$ at NNLO level, with analytical expressions given in Appendix.

IV. MATCHING COEFFICIENTS

By choosing the $\overline{\rm MS}$ scheme for QCFs, we have a similar factorization as Eq. (6), which has the following perturbative expansion if we replace the hadron h by a quark state,

$$\begin{aligned}F^{\nu(n)}_{q_v/q}(\omega,\xi^2,\mu^2) = \sum_{m=0}^{n}\int_0^1\frac{dx}{x}\,f^{(m)}_{q_v/q}(x,\mu^2)\\ \times K^{\nu(n-m)}(x\omega,\xi^2,\mu^2)\,,\end{aligned} \tag{16}$$

with $n,m = 0,1,2$ indicating the power in α_s. While partonic $f^{(n)}_{q_v}$ with $n=0,1,2$ in the $\overline{\rm MS}$ factorization scheme are known [52], we have to calculate partonic version of QCFs in the $\overline{\rm MS}$ scheme perturbatively, denoted as $F^{\nu(n)}_{q_v}$, to derive the NNLO matching coefficient $K^{\nu(n)}$.

Some representative Feynman diagrams for $F^{\nu(n)}_{q_v}$ are shown in Fig. 1 (a′, b′, c′). The diagram 1(a′) gives the tree level result

$$F^{\nu(0)}_{q_v/q} = -4\,i\,p^\nu \cos(\omega)\,. \tag{17}$$

To calculate $F^{\nu}_{q_v/q}(\xi^2\mu^2,\omega)$ at high orders, we again use transformation as Eq. (12) to remove the exponential by going to momentum space, and then reduce the loop integrals to MIs by using IBPs. For example, at NLO we have two MIs:

$$I^{(1)}_1 = \int \frac{d^dl_1}{(2\pi)^d}\,\frac{1}{l_1^2+i0^+}\,2\,\mathrm{Im}\left(\frac{1}{q_z+l_{1z}+i0^+}\right), \tag{18}$$
$$I^{(1)}_2 = \int \frac{d^dl_1}{(2\pi)^d}\,\frac{1}{l_1^2+i0^+}\,2\,\mathrm{Im}\left(\frac{1}{q_z+l_{1z}+p_z+i0^+}\right)$$

and at NNLO we have 21 MIs. The MIs generated from n-loop diagrams for $F^{\nu(n)}_{q_v/q}$ are functions satisfied

$$I^{(n)}_j(y,p_z;d) = |q_z|^{d_n} q_z^{d_{nj}}\,K^{(n)}_j(y;d)\,, \tag{19}$$

where $y \equiv p_z/q_z$, $d_n \equiv -2n\epsilon - 1$, and $d_n + d_{nj}$ are the dimensions of MI $I^{(n)}_j$. These MIs can be solved by the differential equations [53]

$$\partial_y K^{(n)}_j(y;d) = \sum_k A_{jk}(y;d)\,K^{(n)}_k(y;d)\,, \tag{20}$$

with $K^{(n)}_j(0;d)$ serving as boundary conditions. By applying IBPs again, the integrals in boundary conditions can be decomposed into vacuum MIs at n-loop order, which have been calculated in the renormalization procedure. Therefore, $K^{(n)}_j$ can be expanded as a Taylor series of y based on the differential equations in Eq. (20).

After carrying out MIs, we can Fourier transform back to position space and the y dependence is changed to dependence on ω. By adding contributions from all diagrams and then multiplying it by UV renormalization factor $Z^{-1}_{\overline{\rm MS}}$, we obtain perturbative results of $F^{\nu(n)}_{q_v/q}(\omega,\xi^2,\mu^2)$ with $n = 1,2$. We then obtain $\overline{\rm MS}$ matching coefficients $K^{\nu(n)}(x\omega,\xi^2,\mu^2)$ using Eq. (16). As expected, all divergences are canceled and final results of $K^{\nu(n)}$ are finite and given in the Appendix. Using Eq. (6), one can obtain NNLO matching coefficients in other RS by calculating corresponding $R^{\rm RS}$.

V. NUMERICAL RESULTS

Based perturbative results calculated above, we present numerical predictions for the valence coordinate-space QCFs by using Eq. (6) with CT18NNLO PDFs as input [54]. We set $\mu = 2c/|\xi|$ to minimize logarithms encountered in perturbative calculation when $c = 1$, and vary c from 1/2 to 2 to estimate theoretical uncertainties due to ambiguity of scale choice. In Fig. 2, we show $\frac{i}{4\omega}\xi\cdot F^{\rm vac}_{q_v/h}(\omega,\xi^2)$ as a function of ω with fixed $1/|\xi| = 2$ GeV or as a function of $1/|\xi|$ with fixed $\omega = 10$. In either case it is evident that our numerical results have an improved uncertainty when higher order matching coefficients are used. Especially for small $1/|\xi|$, which is the dominant region of lattice data, the NNLO results can reduce theoretical uncertainty by more than a factor of 3 comparing with NLO results.

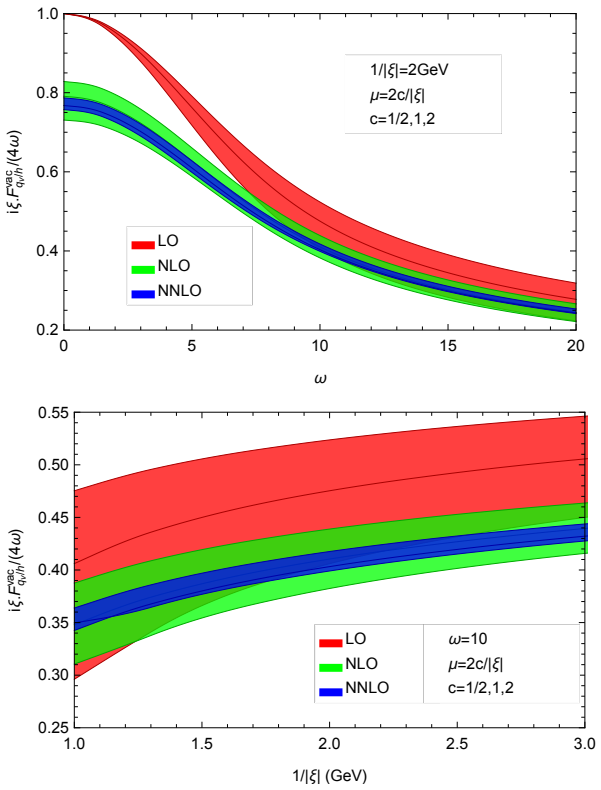

FIG. 2. Numerical predictions for valence quark coordinate-space QCFs with LO, NLO and NNLO matching coefficients and CT18NNLO PDFs.

VI. SUMMARY

We showed that properly renormalized quark correlation functions in position space are good LQCD observables, if $\xi^2\Lambda^2_{\rm QCD}$ is sufficiently small, which are calculable in LQCD and factorizable to PDFs. We discussed the ambiguity and scheme-dependence in defining the multiplicative renormalization constant $Z^{\rm RS}$, and demonstrated that $Z^{\rm RS}$ defined with the vacuum state is advantageous for carrying out the perturbative calculations of the matching coefficients, especially, at high order in α_s. For the first time, we derived a complete NNLO valence-quark coefficient functions for QCFs, and demonstrated that the extraction of PDFs from LQCD calculations in terms of QCD factorization approach are in fact at the

same rigor as the program to extract PDFs from experimental data.

Our definition of QCFs and method of calculations can be easily generalized to evaluate gluon correlation functions and sea-quark coefficient functions, which provide a rigorous program to extract PDFs from lattice QCD calculations. With multiple "good" LQCD observables, including the current-current correlators (better UV behavior) [5], the quark correlation functions defined here, and a generalization to gluon correlation function in position space, the QCD factorization of these observables provide a complementary revenue for extracting PDFs or other partonic structures of hadrons, as well as a tremendous potential to extract partonic structure of hadrons that could be difficult to do scattering experiments with.

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Note added: When this work was being finalized, some related preprints appeared [55–57]. In Ref. [55] the authors obtained NNLO results for $Z^{\overline{\rm MS}}$ and $R^{\rm vac}$, which exactly agree with our results. In Refs. [56, 57] the authors obtained matching coefficients for flavor non-diagonal quark to quark channel that starts from two-loop order.

APPENDIX: PERTURBATIVE RESULTS

Renormalization factor in $\overline{\rm MS}$ subtraction scheme is obtained as

$$Z_{\overline{\rm MS}} = 1 + \frac{\alpha_s S_\epsilon}{\pi\epsilon} C_F + \left(\frac{\alpha_s S_\epsilon}{\pi\epsilon}\right)^2 C_F \left\{ \left[\frac{C_F}{2} - \frac{13C_A}{32} + \frac{n_f T_F}{8}\right] + \left[\left(-\frac{1}{8} + \frac{\pi^2}{12}\right) C_F + \left(\frac{25}{48} - \frac{\pi^2}{48}\right) C_A - \frac{n_f T_F}{6}\right]\epsilon \right\}, \tag{21}$$

where $S_\epsilon \equiv (4\pi)^\epsilon/\Gamma(1-\epsilon)$ is a conventional factor in the $\overline{\rm MS}$ scheme.

The finite renormalization factor $R^{\rm vac}(\xi^2,\mu^2)$ is obtained as

$$\begin{aligned} R^{\rm vac} = 1 &+ \frac{\alpha_s}{\pi} C_F \left(\frac{3}{4}L + 2 + \frac{\pi^2}{3}\right) + \left(\frac{\alpha_s}{\pi}\right)^2 C_F \left\{ \left[\frac{9}{32}C_F + \frac{11}{32}C_A - \frac{1}{8}n_f T_F\right] L^2 \right. \\ &+ \left[\left(\frac{43}{32} + \frac{5\pi^2}{12}\right) C_F + \left(\frac{75}{32} + \frac{19\pi^2}{72}\right) C_A - \left(\frac{7}{8} + \frac{\pi^2}{9}\right) n_f T_F\right] L + \left[\left(\frac{153}{128} + \frac{13\pi^2}{12} - \frac{\zeta(3)}{2} + \frac{\pi^4}{90}\right) C_F \right. \\ &\left. \left. + \left(\frac{6413}{1152} - \frac{5\pi^2}{432} - \frac{13\zeta(3)}{2} - \frac{\pi^4}{90}\right) C_A - \left(\frac{589}{288} - \frac{\pi^2}{27} - 2\zeta(3)\right) n_f T_F\right] \right\}, \end{aligned} \tag{22}$$

where $L \equiv \ln(-\xi^2\mu^2/4) + 2\gamma_E$.

We express $K^\nu(x\omega,\xi^2,\mu^2) \equiv xp^\nu\, A(x\omega,\xi^2,\mu^2) + x\omega\frac{\xi^\nu}{-\xi^2}\, B(x\omega,\xi^2,\mu^2)$, which can be further decomposed as

$$iA(\omega,\xi^2,\mu^2) = 4\cos(\omega) + \frac{\alpha_s}{\pi}\sum_{i=0}^{1} L_f^i C_F A_{i1}^{(1)} + \left(\frac{\alpha_s}{\pi}\right)^2 \sum_{i=0}^{2} L_f^i C_F \left[C_F A_{i1}^{(2)} + C_A A_{i2}^{(2)} + n_f T_F A_{i3}^{(2)}\right], \tag{23}$$

$$iB(\omega,\xi^2,\mu^2) = \frac{\alpha_s}{\pi} C_F B_{01}^{(1)} + \left(\frac{\alpha_s}{\pi}\right)^2 \sum_{i=0}^{1} L_f^i C_F \left[C_F B_{i1}^{(2)} + C_A B_{i2}^{(2)} + n_f T_F B_{i3}^{(2)}\right]. \tag{24}$$

As argued in Ref. [5], $A(\omega,\xi^2,\mu^2)$ and $B(\omega,\xi^2,\mu^2)$ are analytical functions of ω everywhere except infinity. Therefore, expansion of $A(\omega,\xi^2,\mu^2)$ or $B(\omega,\xi^2,\mu^2)$ as Taylor series of ω has infinitely large convergent radius. The first 100-order expansions of $iA(\omega,\xi^2,\mu^2)$ and $iB(\omega,\xi^2,\mu^2)$ are available to download from an ancillary file in the arXiv version, which are far from sufficient for practical use.

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