Extracting Parton Distribution Functions from Lattice QCD Calculations

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(Dated: April 29, 2014)

Parton distribution functions (PDFs) are the most prominent nonperturbative quantities describing the relation between a hadron and the quarks and gluons within it, and play an essential role to connect the dynamics of QCD to the cross sections of colliding hadron(s). Extending Ji’s recent suggestion\textsuperscript{1}, we propose to extract PDFs from QCD global analysis of “data” from lattice QCD calculations of hadronic matrix elements, whose continuum limit can be perturbatively factorized in terms of PDFs. Although the operators defining the quasi-PDFs, introduced by Ji\textsuperscript{1}, could have linear as well as quadratic ultra-violet divergence, we demonstrate to all orders that these quasi-PDFs could be factorized into the normal PDFs. We present the derivation of next-to-leading order factorized coefficient functions.

PACS numbers: 12.38.Bx, 13.88.+e, 12.39.-x, 12.39.St

Introduction—Quantum Chromodynamics (QCD) is believed to be the fundamental theory for strong interactions, and is responsible for holding the quarks and gluons (or in general, partons) together by color force to form nucleons and nuclei, the core of all visible matter in the universe. However, owing to the color confinement which are defined in terms of hadronic matrix elements, no quarks and gluons have ever been directly observed by any detector in high energy scattering experiments. It is the QCD factorization\textsuperscript{2} that enables us to connect the QCD dynamics of quarks and gluons to physically measured hard scattering cross sections of identified hadrons, by systematically separating the physics taking place at different momentum scales. Parton distribution functions (PDFs), $f_{i/h}(x, \mu^2)$, defined as the probability distributions to find a quark or a gluon ($i = q, \bar{q}, g$) in a fast moving hadron carrying the hadron’s momentum fraction between $x$ and $x + dx$, probed at the factorization scale $\mu$, are the most prominent nonperturbative quantities to link the short-distance scattering between quarks and gluons to the confinement-sensitive physics of the colliding hadron(s).

PDFs also carry an invaluable source of information on hadron’s partonic structure - how partons are confined and distributed inside a hadron. Enormous theoretical and experimental efforts have been devoted to the extraction of the PDFs by QCD global analysis of all existing high energy scattering data in the framework of QCD factorization\textsuperscript{3,5}. Although PDFs are not direct physical observables, like cross sections, they are well-defined matrix elements of quark and/or gluon fields in QCD. It is critically important to calculate the PDFs directly from QCD, such as lattice QCD, and compare them with what have been extracted from global fitting of experimental data. However, it is difficult, if not impossible, to calculate PDFs directly in lattice QCD with an Euclidean time since the operators defining PDFs depend on Minkowski time. Recently, Ji\textsuperscript{1} introduced a set of quasi-PDFs, which are defined in terms of hadronic matrix elements of equal time correlators, which could be calculated in lattice QCD\textsuperscript{6}, and suggested that the quasi-PDFs become the normal PDFs when the hadron momentum $P_z$ is boosted to the infinity. However, since the hadron momentum in lattice QCD calculation is effectively bounded by the lattice spacing, the $P_z \rightarrow \infty$ limit is hard to take. The connection between the quasi-PDFs and the normal PDFs is further complicated by the fact that the operator defining the quasi-quark (quasi-gluon) distribution is linearly (quadratically) ultra-violet (UV) divergent, while the operators defining the normal PDFs have only logarithmic UV divergence.

In this Letter, by extending Ji’s suggestion, we propose a program to extract PDFs from QCD global analysis of “data” from lattice “cross sections”, defined as hadronic matrix elements of a finite $P_z$, which are calculable in lattice QCD and whose continuum limit can be perturbatively factorized in terms of PDFs. As an example, we demonstrate to all orders in QCD that at a finite $P_z$, the quasi-PDFs could be factorized into the normal PDFs with calculable coefficient functions, and thus, are good lattice “cross sections”. We derive the coefficient functions at the next-to-leading order (NLO) for all partonic channels to explicitly verify that they are free of UV, infrared (IR) and collinear (CO) divergences\textsuperscript{6}. We also briefly comment the extension of this lattice QCD based approach to the extraction of the generalized PDFs (GPDs)\textsuperscript{9} and transverse momentum dependent PDFs (TMDs)\textsuperscript{10,11} with which we could derive a comprehensive three-dimensional “view” of hadron’s quark and gluon structure.

Lattice “cross section”—We define a lattice “cross section”, $\bar{\sigma}_{E}^{\mu}(\vec{x}, 1/a, P_z)$, as the Fourier transform of a hadronic matrix element, $\langle h(P) \mathcal{O}(\psi, A) | h(P) \rangle$ of hadron momentum $P^\mu = (P^0, 0_\perp, P_z)$ with $P^0 \simeq |P_z|$ and an operator of quark $\psi$ and gluon $A$ field, where $P_z$ mimics the “collision energy”, the transverse lattice spacing $a$ defines the hard scale $\sim 1/a$, and the dimensionless parameter...
\( \tilde{x} \) mimics the “rapidity”. A good \( \tilde{\sigma}^{\text{lat}}_E(\tilde{x}, 1/a, P_z) \) should have the following properties:

- The matrix element must be calculable in lattice QCD with an Euclidean time, indicated by the “E”,
- It has a well-defined continuum limit that is UV and IR safe perturbatively,
- All CO divergences of its continuum limit can be factorized into the normal PDFs with perturbatively calculable hard coefficient functions.

Our strategy to search for good lattice “cross sections” could be summarized by the following schematic plot,

\[
\tilde{\sigma}^{\text{lat}}_E(\tilde{x}, 1/a, P_z) \xrightarrow{\tilde{C}} \tilde{\sigma}_E(\tilde{x}, \mu^2, P_z) \quad (1)
\]

where \( \tilde{\sigma}_E(\tilde{x}, \mu^2, P_z) \) is the Euclidean space continuum limit of \( \tilde{\sigma}^{\text{lat}}_E(\tilde{x}, 1/a, P_z) \), \( \tilde{\sigma}_M(\tilde{x}, \mu^2, P_z) \) is the Minkowski space version of \( \tilde{\sigma}_E(\tilde{x}, \mu^2, P_z) \), as indicated by its subscript “M”, and the \( \mu \) is a hard scale, which could be the UV renormalization scale of the composite operator \( O(\psi, A) \) or a large physical scale \( Q \) other than the \( P_z \) if the operator is made of conserved currents/tensors. Eq. (1) outlines three necessary steps to identify a good lattice “cross section”: (1) demonstrate that \( \tilde{\sigma}_E(\tilde{x}, \mu^2, P_z) \) is UV and IR safe, and the matching coefficients \( \tilde{C}_i \)’s are calculable in lattice QCD perturbation theory, (2) verify that \( \tilde{\sigma}_E(\tilde{x}, \mu^2, P_z) = \tilde{\sigma}_M(\tilde{x}, \mu^2, P_z) \), and (3) show that all perturbative CO divergences of \( \tilde{\sigma}_M(\tilde{x}, \mu^2, P_z) \) can be systematically factorized into the normal PDFs with coefficient functions \( C_i \).

\[
\tilde{\sigma}_M(\tilde{x}, \mu^2, P_z) \approx \sum_i \int_0^1 \frac{dx}{x} f_{i/h}(x, \mu^2) C_i(\tilde{x}, \mu^2, P_z), \quad (2)
\]

with power corrections of \( O(1/\mu^a) \), where \( \mu \) is the factorization scale and the value of \( a \) depends on the nature of \( \tilde{\sigma}_M(\tilde{x}, \mu^2, P_z) \). Equation (2) requires the perturbative CO divergence of good lattice “cross sections” to be process-independent or universal.

Once we identify good lattice “cross sections”, we are able to factorize them in terms of the PDFs directly,

\[
\tilde{\sigma}^{\text{lat}}_E(\tilde{x}, 1/a, P_z) \approx \sum_i \int_0^1 \frac{dx}{x} f_{i/h}(x, \mu^2) \tilde{C}_i(\tilde{x}, 1/a, \mu^2, P_z), \quad (3)
\]

where \( \tilde{C}_i \)’s are perturbative coefficient functions. By applying Eq. (3) to various parton states, \( |h(P)| \to |f(P)| \) with flavor \( f = q, \bar{q}, g \), the \( \tilde{C}_i \)’s can be systematically derived by calculating \( \tilde{\sigma}^{\text{lat}}_E(\tilde{x}, 1/a, P_z) \) on a parton state in lattice QCD perturbation theory and \( f_{i/h}(x, \mu^2) \) of the same parton state in perturbative QCD. Our program to extract the PDFs from lattice calculations is effectively reduced to three separate parts: (1) generate the “data” of \( \tilde{\sigma}^{\text{lat}}_E(\tilde{x}, 1/a, P_z) \) from lattice QCD simulation, (2) derive the matching coefficient functions, \( \tilde{C}_i \)’s, in Eq. (4), and (3) perform QCD global analysis of the lattice “data” to extract the PDFs by using Eq. (5). The last part is effectively the same as the traditional way to extract PDFs except it uses the lattice “data” instead of the data from high energy scattering.

The lattice based approach is less sensitive to the PDFs at small \( x \) because of the limit on lattice size, while it is ideal for extracting PDFs at large \( x \). In the case of extracting GPDs and TMDs, the “cross sections” in Eq. (6) are necessarily to have additional dependence on momentum scales to characterize the physics not collinear to the hadron momentum \( P^\mu \).

**Quasi-PDFs**—The quasi-PDFs, introduced by Ji [1], are defined as

\[
\tilde{f}_{q/p}(\tilde{x}, \mu^2, P_z) = \int \frac{d\xi}{\pi} e^{i\tilde{x}P_z\xi} \langle h(P) | \bar{\psi}(\xi) \frac{\gamma_2 P_z}{2} \psi(0) | h(P) \rangle \quad (4)
\]

for quasi-quark distribution with \( \xi_0 = \xi_\perp = 0 \), and

\[
\tilde{f}_{\bar{q}/p}(\tilde{x}, \mu^2, P_z) = \frac{1}{\tilde{x}P_z} \int \frac{d\xi}{2\pi} e^{-i\tilde{x}P_z\xi} \langle h(P) | F_\nu(\xi_\perp) \rangle \langle F_{\bar{\nu}}(\xi_\perp) | h(0) \rangle \quad (5)
\]

for quasi-gluon distribution with \( \nu \) summing over transverse directions. In Eqs. (4) and (5), \( \tilde{\mu} \) is a renormalization scale, and the gauge links \( \Phi^{(\lambda, a)}_n(\{\xi_\perp, 0\}) = \exp[-ig \int_0^{\xi_\perp} d\eta_\perp A^{(\lambda, a)}_z(\eta_\perp)] \) where the “\( \lambda \)” and “\( a \)” of the superscript represent the fundamental and adjoint representation of QCD’s SU(3) color, respectively, and \( n_\perp = (0, 0, 1) \), \( n_\perp = (0, 0, -1) \), and \( u \cdot n_\perp = -u_3 \) for any vector \( u \). As defined, these quasi-PDFs are gauge invariant and could be calculated in lattice QCD [1]. But, unlike the PDFs, these quasi-PDFs are not boost invariant depending on the hadron momentum \( P_z \), and the “momentum fraction”, \( \tilde{x} = k_z/P_z \in (-\infty, \infty) \) is not bounded by \( P_z \). Furthermore, they do not conserve the total “parton” momentum \( \tilde{M} \).

\[
\tilde{M} = \sum_{i=q,q,g} \int_0^{\infty} d\tilde{x} \tilde{f}_{i}(\tilde{x}, \mu^2, P_z) \neq \text{constant}. \quad (6)
\]

Like the PDFs, the operators defining the quasi-PDFs are singular as \( \xi_\perp \to 0 \) and require UV renormalization. From the UV power counting [10], the operators for quasi-quark and quasi-gluon distribution have linear and quadratic UV divergence, respectively, or \( \tilde{f}_{q} \to \tilde{\mu}/P_z \) and \( \tilde{f}_{\bar{q}} \to (\tilde{\mu}/P_z)^2 \), as \( \tilde{\mu} \to \infty \), which is very different from the logarithmic UV behavior of the normal PDFs [1].

**Factorization of quasi-PDFs**—We show in this subsection with more details in Ref. [1] that quasi-PDFs are IR safe, their CO divergence can be systematically factorized.
into the normal PDFs, and their linear and quadratic UV divergence could be factorized from the logarithmic UV divergence of the PDFs, and renormalized separately.

Like the normal quark distribution, quasi-quark distribution can be represented by the forward scattering Feynman diagram, as shown in the left of Fig. 2 with the active quark of momentum $k$ contracted with the "cut-vertex". The gauge link in Eq. (9) is represented by the "cut" double lines in Fig. 2 with a sum of all possible cuts, because of the identity, $\Phi^{f,a}_n(\{\xi_\ell\}) = \Phi^{f,a}_n(\{\infty, \xi_\ell\}) \Phi^{f,a}_n(\{\infty, 0\})$. Following effectively the same arguments used in Ref. [10], it is straightforward to show that the quasi-PDFs of a parton state are IR safe.

$$\Phi^{f,a}_n(\{\xi_\ell\}) = \Phi^{f,a}_n(\{\infty, \xi_\ell\}) \Phi^{f,a}_n(\{\infty, 0\})$$

FIG. 1: Ladder expansion of the quasi-quark distribution.

We find that the quasi-quark distribution of a parton state of momentum $p$ in a light-cone $n \cdot A = 0$ gauge, with the light-cone vector $n^\mu = (n^+, n^-) = (0, 1, 0, 0)$, can be approximated by a sum of ladder diagrams, as shown in Fig. 3, plus UV counter-terms (UVCT) [10]. In Fig. 3, $C_0$ and $K_0$ are two-particle irreducible (2PI) kernels with all process-dependence included in $C_0$, as shown in Fig. 2, where the gauge link is along the direction $n^\mu$. By definition, $K_0$ includes the two quark propagators connecting to the kernel above. The 2PI kernels with fixed external momenta are finite in a physical gauge [10]. For the leading CO divergence, the spinor trace between two neighboring kernels can be approximated by the decomposition in Fig. 3. The integration of the loop momentum $k_i$ between two neighboring 2PI kernels can be written as $\int d^4k_i = \int dx_i \int d^4k_i \delta(x_i - k_i \cdot n/p \cdot n)$, and be reduced to an one-dimensional integration $\int dx_i$, if we approximate the momentum $k_i$ entering the top kernel as $k_i \approx x_i p \cdot n$. Since the $\gamma \cdot n/2p \cdot n \delta(x_i - k_i \cdot n/p \cdot n)$ is the cut-vertex defining the normal quark distribution, the phase space integration, $\int d^4k_i$ over $K_0$, with its two lower quark lines contracted with $\gamma \cdot p/2$, gives the well-known logarithmic UV and CO divergences of the normal PDFs [10]. A standard UV renormalization of PDFs should remove all logarithmic UV divergences associated with this phase space integration of $K_0$, so that we can introduce a renormalized 2PI as $K \equiv \int d^4k_i \delta(x_i - k_i \cdot n/p \cdot n) \Tr[\gamma \cdot n K_0 \gamma \cdot p] / (4p \cdot n) + \text{UVCT}$, which is UV and IR finite.

To factorize all CO divergences of the quasi-quark distribution of a parton state into PDFs of the same parton state, we introduce a projection operator, $\hat{P}$ to pick up the CO divergence of $K$, and sum up all ladder diagrams in Fig. 3 in the following symbolic form,

$$\hat{f}_{q/p} = \lim_{m \to \infty} C_0 \sum_{i=0}^m K^i + \text{UVCT}$$

$$= \lim_{m \to \infty} C_0 \left[ 1 + \sum_{i=0}^{m-1} K^i (1 - \hat{P}K) \right]_{\text{ren}} + \hat{f}_{q/p} \hat{P} K$$

$$= \lim_{m \to \infty} C_0 \left[ 1 + \sum_{i=1}^m (1 - \hat{P}K)^i \right]_{\text{ren}} + \hat{f}_{q/p} \hat{P} K,$$

where "UVCT" is to remove the UV divergence of quasi-quark distribution that has not been removed by the renormalization of PDFs, and the subscript "ren" indicates the UV renormalization. From Eq. (9), we obtain

$$\hat{f}_{q/p} = \left[ C_0 \frac{1}{1 - (1 - \hat{P}K)} \right]_{\text{ren}} \left[ \frac{1}{1 - \hat{P}K} \right]$$

where all CO divergences of the renormalized quasi-quark distribution are now factorized into the second term, which is equal to the perturbative contribution to the normal quark distribution. Eq. (9) also means that the power UV divergence of quasi-quark is factorized from the logarithmic UV divergence of the normal PDFs, and could be renormalized independently. The same factorization arguments can be applied to the flavor singlet channels, as well as quasi-gluon distribution, because operators defining the normal PDFs have only logarithmic UV divergence [8]. That is, the renormalized quasi-PDFs share the same CO divergence as the normal PDFs, and could be factorized in terms of the PDFs as in Eq. (9), plus the power corrections.

The coefficient functions at NLO—We derive the coefficient functions at the next-to-leading order (NLO) for
all partonic channels in Eq. (2), with $\sigma_M(\tilde{x}, \mu^2, P_z)$ replaced by the quasi-DPFs, to explicitly verify that they are free of UV, IR and CO divergences. We present the derivation of $C_{q/q}^{(1)}$ in this subsection, and all other coefficient functions in Ref. [8].

Letting $\sigma_M(\tilde{x}, \mu^2, P_z) = f^{(0)}_{q/q}(\tilde{x}, \mu^2, P_z) + f^{(1)}_{q/q}(\tilde{x}, \mu^2, P_z)$ in Eq. (2), expanding both sides to order $\alpha_s^0$, and using $\tilde{f}^{(0)}_{q/q}(\tilde{x}) = \delta(1 - \tilde{x})$ and $f^{(0)}_{q/q}(x) = \delta(1 - x)$, we obtain $C_{q/q}^{(0)}(t) = \delta(1 - t)$ with $t = \tilde{x}/x$. By expanding both sides of the equation

$$
\tilde{f}^{(1)}_{q/q}(\tilde{x}) = f^{(0)}_{q/q}(x) \times C^{(1)}_{q/q}(\tilde{x}/x) + f^{(1)}_{q/q}(x) \times C^{(0)}_{q/q}(\tilde{x}/x) + \ldots,
$$

where $\times$ represents the convolution over $x$ in Eq. (3). Using the LO results above, we obtain

$$
C_{q/q}^{(1)}(t, \mu^2, \mu^2, P_z) = \tilde{f}^{(1)}_{q/q}(t, \mu^2, P_z) - f^{(1)}_{q/q}(t, \mu^2).
$$

Both $\tilde{f}^{(1)}_{q/q}$ and $f^{(1)}_{q/q}$ can be calculated by using the Feynman diagrams in Fig. 3 but with $n_z \cdot A = 0$ and $n \cdot A = 0$ gauge, and $\gamma_z/2P_z$ and $\gamma^+ / 2P^+$ "cut-vertex", respectively. The $f^{(1)}_{q/q}$ and its derivation are well known [10].

![FIG. 4: Next-to-leading order diagrams contribute to the quasi-particle distribution of a quark.](image)

to order $\alpha_s$, and keeping only the flavor nonsinglet contribution, we obtain [8]

$$
f^{(1)}_{q/q}(\tilde{x}) = f^{(0)}_{q/q}(x) \times C^{(1)}_{q/q}(\tilde{x}/x) + f^{(1)}_{q/q}(x) \times C^{(0)}_{q/q}(\tilde{x}/x),
$$

where $f^{(0)}_{q/q}$ and $f^{(1)}_{q/q}$ are any well-behaved function. When $P_z \to \infty$, $\Lambda_t = C(O(\mu^2/P_z^2)$, and terms within "..." vanish, which is consistent with the large $P_z$ limit found in Ref. [8]. Our result for $C_{q/q}^{(1)}(\tilde{x}/x)$ is consistent with the results obtained in Ref. [10].

As expected, the $C_{q/q}^{(1)}$ in Eq. (12), so as the NLO coefficient functions for other partonic channels [8], are free of any UV, IR, and CO divergences, while the results of coefficient functions could depend on the choice of renormalization scheme. More discussion on the scheme and its consequences is given in Ref. [8].

Summary—In summary, we proposed a program to extract PDFs from lattice QCD calculations based on QCD factorization of lattice “cross sections”. We demonstrated to all orders in perturbative QCD that the renormalized quasi-DPFs could be systematically factorized into the normal PDFs with perturbative coefficient functions, to serve as good lattice “cross sections” with a finite $P_z$ as “collision energy”, $\mu$ as the hard scale, and $\tilde{x} \in (-\infty, \infty)$ as the “rapidity. We verified this explicitly by calculating the NLO coefficient functions $C^{(1)}$’s for all partonic channels [8].

By calculating the quasi-DPFs in lattice QCD for finite $\tilde{x}$ and $P_z$, and the NLO matching coefficients $C$ in Eq. (3), we could extract the PDFs from the lattice QCD calculation at the NLO accuracy. However, due to the size limit of the lattice, this lattice based program is more suited for extracting PDFs at a relatively larger $x$, complementary to the global fitting program based on data from high energy scattering. The precision of extracted PDFs from lattice calculations could be greatly improved if we identify more “good” lattice cross sections” [8]. This new lattice global fitting program could be naturally extended to the calculations of TMDs and GPDs, by identifying corresponding lattice observables [11] [8] [13].
Acknowledgments—We thank T. Ishikawa, X.D. Ji, G. Sterman, S. Yoshida and H. Zhang for helpful discussions. This work was supported in part by the U. S. Department of Energy under contract No. DE-AC02-98CH10886, and the National Science Foundation under grant No. PHY-0969739 and -1316617.

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