Next-to-Next-to-Leading-Order QCD Corrections to Pion Electromagnetic Form Factors

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(Received 9 February 2024; revised 27 March 2024; accepted 12 April 2024; published 13 May 2024)

We calculate the next-to-next-to-leading-order (NNLO) QCD radiative correction to the pion electromagnetic form factor with large momentum transfer. We explicitly verify the validity of the collinear factorization to two-loop order for this observable and obtain the respective IR-finite two-loop hard-scattering kernel in the closed form. The NNLO QCD correction turns out to be positive and significant. Incorporating this new ingredient of correction, we then make a comprehensive comparison between the finest theoretical predictions and numerous data for both space- and timelike pion form factors. Our phenomenological analysis provides a strong constraint on the second Gegenbauer moment of the pion light-cone distribution amplitude obtained from recent lattice QCD studies.

DOI: 10.1103/PhysRevLett.132.201901

Introduction.—Originally proposed by Yukawa as the strong nuclear force carrier in 1935 [1], subsequently discovered in the cosmic rays in 1947 [2], the π mesons have always occupied central stage throughout the historic advancement of the strong interaction. As the lightest particles in the hadronic world (hence the highly relativistic bound systems composed of light quarks and gluons), π mesons entail extremely rich QCD dynamics, exemplified by the color confinement and chiral symmetry breaking. Notwithstanding extensive explorations during the past decades, there still remain some great myths about the internal structure of the π mesons.

A classic example of probing the internal structure of the charged π is the pion electromagnetic (EM) form factor,

$$\langle \pi^+(P')|J^{\mu}_{\rm EM}|\pi^+(P)\rangle = F_{\pi}(Q^2)(P^{\mu}+P'^{\mu}),$$
 (1)

with $Q^2 \equiv -(P - P')^2$. The electromagnetic current is defined by $J^{\mu}_{\rm EM} = \sum_f e_f \bar{f} \gamma^{\mu} f$, with $e_u = 2/3$ and $e_d = -1/3$ indicating the electric charges of the *u* and *d* quarks.

During the past half century, the pion EM form factor has been intensively studied experimentally [3–29]. From the theoretical perspective, the pion EM form factor at small Q^2 can be investigated in chiral perturbation theory [30] and lattice QCD [31–35]. On the other hand, at large momentum transfer, the $F_{\pi}(Q^2)$ is expected to be adequately described by perturbative QCD. Within the collinear factorization framework tailored for hard exclusive reactions [36–42] (for a review, see Ref. [43]), at the lowest order in 1/Q, the pion EM form factor can be expressed in the following form:

$$F_{\pi}(Q^{2}) = \int \int dx \, dy \Phi_{\pi}^{*}(x,\mu_{F}) T\left(x,y,\frac{\mu_{R}^{2}}{Q^{2}},\frac{\mu_{F}^{2}}{Q^{2}}\right) \Phi_{\pi}(y,\mu_{F}),$$
(2)

where T(x, y) signifies the perturbatively calculable hard-scattering kernel, and $\Phi_{\pi}(x, \mu_F)$ represents the nonperturbative yet universal leading-twist pion light-cone distribution amplitude (LCDA), i.e., the probability amplitude of finding the valence *u* and \bar{d} quark inside π^+ carrying the fractional momenta *x* and $\bar{x} \equiv 1 - x$, respectively. The leading-twist pion LCDA assumes the following operator definition:

$$\Phi_{\pi}(x,\mu_F) = \int \frac{dz^-}{2\pi i} e^{iz^- xP^+} \langle 0|\bar{d}(0)\gamma^+\gamma_5 \\ \times \mathcal{W}(0,z^-)u(z^-)|\pi^+(P)\rangle,$$
(3)

where W signifies the lightlike gauge link to ensure the gauge invariance. Conducting the UV renormalization for (3), one is led to the celebrated Efremov-Radyushkin-Brodsky-Lepage (ERBL) evolution equation [38,40],

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$$\frac{d\Phi_{\pi}(x,\mu_F)}{d\ln\mu_F^2} = \int_0^1 dy \, V(x,y) \Phi_{\pi}(y,\mu_F), \tag{4}$$

with V(x, y) referring to the perturbatively calculable ERBL kernel.

Equation (2) is expected to hold to all orders in perturbative expansion. The hard-scattering kernel can thus be expanded in the power series

$$T = \frac{16C_F \pi \alpha_s}{Q^2} \left\{ T^{(0)} + \frac{\alpha_s}{\pi} T^{(1)} + \left(\frac{\alpha_s}{\pi}\right)^2 T^{(2)} + \cdots \right\}, \quad (5)$$

where $C_F = [(N_c^2 - 1)/2N_c]$, and $N_c = 3$ is the number of colors.

The leading-order (LO) result was known shortly after the advent of QCD [37,38,40,42,44–46]. The next-toleading-order (NLO) correction was originally computed by three groups in early 1980s [47–49]. Scrutinizing the previous calculations, in 1987 Braaten and Tse traced the origin of the discrepancies among the earlier work and presented the correct expression of the NLO hard-scattering kernel [50]. In 1999, Melić *et al.* conducted a comprehensive phenomenological study by incorporating the NLO correction as well as the evolution effect of pion LCDA [51]. The central goal of this Letter is to compute the next-to-next-to-leading-order (NNLO) perturbative correction to the pion EM form factor and critically examine its phenomenological impact [52].

Setup of perturbative matching.—The strategy of deducing the short-distance coefficients is through the standard matching procedure. Since the hard-scattering kernel is insensitive to the long-distance physics, it is legitimate to replace the physical π^+ by a free quark-antiquark pair $u\bar{d}$ and compute both sides of (2) in perturbation theory, order by order in α_s . To make things simpler, we neglect the transverse motion and assign the momenta of the *u* and \bar{d} in the incoming "pion" to be *uP* and $\bar{u}P$ and assign the momenta of the *u* and \bar{d} in the outgoing pion to be vP' and $\bar{v}P'$, with *u*, *v* ranging from 0 to 1.

On the left-hand side of (2), we extract the scalar form factor F(u, v) through the partonic reaction $\gamma^* + u(uP)\overline{d}(\overline{u}P) \rightarrow u(vP')\overline{d}(\overline{v}P')$. Some typical Feynman diagrams through two-loop order are depicted in Fig. 1. It is subject to a perturbative expansion,



FIG. 1. Sample parton-level Feynman diagrams for the reaction $\gamma^* \pi(P) \to \pi(P')$ at (a) LO, (b) NLO, (c) NNLO.

$$F(u, v) = \frac{16C_F \pi \alpha_s}{Q^2} \left[F^{(0)}(u, v) + \frac{\alpha_s}{\pi} F^{(1)}(u, v) + \left(\frac{\alpha_s}{\pi}\right)^2 F^{(2)}(u, v) + \cdots \right].$$
(6)

On the right-hand side of (2), one can expand the renormalized pion LCDA as

$$\Phi(x|u) = \Phi^{(0)}(x|u) + \frac{\alpha_s}{\pi} \Phi^{(1)}(x|u) + \left(\frac{\alpha_s}{\pi}\right)^2 \Phi^{(2)}(x|u) + \cdots$$
(7)

At tree level, the fictitious pion LCDA in (3) simply reduces to $\Phi^{(0)}(x|u) = \delta(x-u)$ [up to a normalization factor that also appears in F(u, v)]. By equating both sides of (2), one reproduces the well-known tree-level expression $T^{(0)}(x, y)$ [36–42],

$$T^{(0)}(x,y) = \frac{e_u}{\bar{x}\,\bar{y}}(1-\epsilon) - \begin{bmatrix} e_u \to e_d\\ \bar{x} \to x, \bar{y} \to y \end{bmatrix}, \qquad (8)$$

which holds true in $d = 4 - 2\epsilon$ spacetime dimensions.

Once beyond the tree level, the UV and IR divergences inevitably arise and we use the dimensional regularization (DR) to regularize both types of divergences. Nevertheless, the bare pion LCDA remains intact since the scaleless integrals vanish in DR. The renormalized pion LCDA is related to the bare one via

$$\Phi(x|u) = \int dy Z(x, y) \Phi_{\text{bare}}(y|u) = Z(x, u), \quad (9)$$

which is solely composed of various IR poles.

Z(x, y) in (9) signifies the renormalization function in the $\overline{\text{MS}}$ scheme, which can be cast into the following Laurent-expanded form in ϵ :

$$Z(x, y) = \delta(x - y) + \sum_{k=1}^{\infty} \frac{1}{\epsilon^k} Z_k(x, y).$$
 (10)

Note that the prefactor of the single pole in (10) is related to the ERBL kernel V(x, y) in (4) via $V(x, y) = -\alpha_s \partial Z_1 / \partial \alpha_s$ [57]. Note that the two-loop [49,58–61] and three-loop corrections [62] to V(x, y) have been available.

The two-loop renormalized pion LCDA $\Phi^{(2)}$ also contains a double IR pole. The Z_2 can be obtained through the recursive relation [63]

$$\alpha_s \frac{\partial Z_2}{\partial \alpha_s} = \alpha_s \frac{\partial Z_1}{\partial \alpha_s} \otimes Z_1 + \beta(\alpha_s) \frac{\partial Z_1}{\partial \alpha_s}, \qquad (11)$$

where $d\alpha_s/d\ln\mu^2 = -\epsilon\alpha_s + \beta(\alpha_s)$.

With the aid of (9) and (10), we then determine the $\mathcal{O}(\alpha_s)$ and $\mathcal{O}(\alpha_s^2)$ corrections to the renormalized pion LCDA in (7).

At one-loop order, the matching equation for a fictitious pion state becomes

$$Q^{2}F^{(1)}(u,v) = T^{(1)}(u,v) + \Phi^{(1)}(x|u) \bigotimes_{x} T^{(0)}(x,v) + \Phi^{(1)}(y|v) \bigotimes_{y} T^{(0)}(u,y),$$
(12)

where \bigotimes_x signifies the convolution over *x*. Note that the renormalized scalar form factor $F^{(1)}(u, v)$ still contains a single collinear pole. However, the renormalized $\Phi^{(1)}(x|u)$ and $\Phi^{(1)}(y|v)$ also contain the same IR poles. Upon solving this matching equation, one ends up with both UV- and IR-finite $T^{(1)}(x, y)$. Our expressions agree with the known NLO result [51].

To the desired two-loop order, the following matching equation descends from (2):

$$Q^{2}F^{(2)}(u,v) = T^{(2)}(u,v) + \Phi^{(2)}(x|u) \bigotimes_{x} T^{(0)}(x,v) + \Phi^{(2)}(y|v) \bigotimes_{y} T^{(0)}(u,y) + \Phi^{(1)}(x|u) \bigotimes_{x} T^{(1)}(x,v) + \Phi^{(1)}(y|v) \bigotimes_{y} T^{(1)}(u,y) + \Phi^{(1)}(x|u) \bigotimes_{x} T^{(0)}(x,y) \bigotimes_{y} \Phi^{(1)}(y|v).$$
(13)

More severe IR divergences are expected to arise in both $F^{(2)}(u, v)$ and $\Phi^{(2)}(x|u)$. Clearly one also needs to compute $T^{(1)}(x, y)$ to $\mathcal{O}(\epsilon)$.

Description of the calculation.—We use HepLib [64] and FeynArts [65] to generate Feynman diagrams and the corresponding amplitudes for the reaction $\gamma^* + u(uP)d(\bar{u}P) \rightarrow$ $u(vP')\overline{d}(\overline{v}P')$. We employ the covariant projector technique to enforce each $u\bar{d}$ pair to bear zero helicity. For our purpose, it suffices to adopt the naive anticommutation relation to handle γ_5 in DR. There are about 1600 two-loop diagrams, one of which is depicted in Fig. 1(c). We employ the packages APART [66], to conduct partial fraction, and FIRE [67] for integration-by-part reduction. We end up with 116 independent master integrals (MIs). The MIs are calculated by utilizing the differential equation method [68–70]. Note that these MIs are considerably more involved than what are encountered in the two-loop corrections for the $\pi - \gamma$ transition form factor [71,72]. We have attempted two independent ways to construct and solve the differential equation systems, one of which is based on the method developed in [73–76]. The analytic results are expressed in terms of the Goncharov polylogarithms (GPLs) [77]. Two independent calculations yield the identical answer. We also numerically check our results against the package AMFLOW [78] and found perfect agreement. Technical details will be included in the future long write-up.

Upon renormalizing the QCD coupling in the $\overline{\text{MS}}$ scheme, we end up with a rather lengthy expression for $F^{(2)}(u, v)$. Being UV finite, it still contains severe IR divergences that start at order $1/\epsilon_{\text{IR}}^2$. Inspecting the matching equation (13), piecing all the known ingredients together, we are able to solve for the intended two-loop hard-scattering kernel. Hearteningly, $T^{(2)}(x, y)$ is indeed IR finite. Therefore, our explicit calculation verifies that the collinear factorization does hold at two-loop level for the pion EM form factor. The analytical expression of $T^{(2)}(x, y)$ is too lengthy to be reproduced here. For the sake of clarity, in the Supplemental Material [79] we provide the asymptotic expressions of $T^{(1,2)}(x, y)$ near the end point regions.

Master formula for pion EM form factor at NNLO.— Given a certain parametrized form of pion LCDA, the twofold integration in (2) turns out to be difficult to conduct numerically, mainly due to numerical instability caused by the spurious singularity as $x \rightarrow y/x \rightarrow \bar{y}$ in $T^{(2)}(x, y)$. Our recipe to circumvent this technical challenge is to present the two-loop results in an analytical manner, which enables us to achieve exquisite precision.

The leading-twist pion LCDA is conveniently expanded in the Gegenbauer polynomial basis,

$$\Phi_{\pi}(x,\mu_F) = \frac{f_{\pi}}{2\sqrt{2N_c}} \sum_{n=0}' a_n(\mu_F) \psi_n(x), \qquad (14a)$$

$$\psi_n(x) = 6x\bar{x}C_n^{3/2}(2x-1),$$
(14b)

where the pion decay constant $f_{\pi} = 0.131$ GeV, and \sum' signifies the sum over even integers. Note all the nonperturbative dynamics are encoded in the Gegenbauer moments $a_n(\mu_F)$.

Substituting (14) into (2), we reexpress the pion EM form factor as

$$Q^{2}F_{\pi}(Q^{2}) = \frac{2C_{F}\pi^{2}(e_{u} - e_{d})f_{\pi}^{2}}{3} \times \sum_{k=0}^{\infty} \left(\frac{\alpha_{s}}{\pi}\right)^{k+1} \sum_{m,n'} a_{n}(\mu_{F})a_{m}(\mu_{F})\mathcal{T}_{mn}^{(k)},$$
(15)

with ${\cal T}_{mn}^{(k)}$ defined by

$$\mathcal{T}_{mn}^{(k)} = \frac{1}{e_u - e_d} \psi_m(x) \bigotimes_x T^{(k)} \left(x, y, \frac{\mu_R^2}{Q^2}, \frac{\mu_F^2}{Q^2} \right) \bigotimes_y \psi_n(y).$$
(16)

For simplicity, we will set $\mu_R = \mu_F = \mu$ and $n_L = 3$ from now on. The twofold integrations in (16) can be

readily worked out at tree and one-loop levels. For instance, we have

$$\mathcal{T}_{mn}^{(0)} = 9, \qquad \mathcal{T}_{00}^{(1)} = \frac{1}{4}(81L_{\mu} + 237), \qquad (17)$$

with $L_{\mu} \equiv \ln(\mu^2/Q^2)$.

Remarkably, the two-loop coefficients $\mathcal{T}_{mn}^{(2)}$ can also be computed analytically, thanks to the fact that $T^{(2)}$ can be expressed in terms of the GPLs. Although the integrand in (16) contains about $\mathcal{O}(10^5)$ individual terms, the final result after twofold integration becomes exceedingly compact, which can be expressed in terms of the rational numbers and Riemann ζ function. For instance, the expression of $\mathcal{T}_{00}^{(2)}$ reads

$$\mathcal{T}_{00}^{(2)} = \frac{729L_{\mu}^{2}}{8} - \left(8\zeta_{3} + \frac{35\pi^{2}}{6} - \frac{4365}{8}\right)L_{\mu} + 205\zeta_{5} - \frac{3\pi^{4}}{20} - \frac{759\zeta_{3}}{2} - \frac{1829\pi^{2}}{96} + \frac{36559}{32}.$$
 (18)

Because of the length restriction, we refrain from providing the analytical expressions for other $\mathcal{T}_{mn}^{(1,2)}$. For the reader's convenience, in Table I we tabulate the numerical values of $\mathcal{T}_{mn}^{(1,2)}$ for $0 \le m$, $n \le 6$, which is sufficient for most phenomenological analyses.

With the input from Table I, Eq. (15) constitutes our master formula for yielding phenomenological predictions through the two-loop accuracy. Compared with the original factorization formula (2), we have simplified an integration task into an algebraic one.

It is straightforward to adapt our master formula from the spacelike region to the timelike one, provided that one makes the replacement $L_{\mu} \rightarrow L_{\mu} + i\pi$ in Table I, with Q^2 now indicating the squared invariant mass of the $\pi^+\pi^-$ pair.

Input parameters.—As the key nonperturbative input, our knowledge on the pion LCDA is still not confirmative enough. In the early days, it was popular to assume asymptotic form, Chernyak-Zhitnitsky parametrization

TABLE I. The numerical values for $\mathcal{T}_{mn}^{(1)} = c_1 L_{\mu} + c_2$ and $\mathcal{T}_{mn}^{(2)} = d_1 L_{\mu}^2 + d_2 L_{\mu} + d_3$, with $0 \le m, n \le 6$.

(m, n)	c_1	<i>c</i> ₂	d_1	d_2	d_3
(0,0)	20.25	59.25	91.1250	478.436	696.210
(0,2)	32.75	112.473	170.118	1094.39	2025.84
(0,4)	38.45	147.638	211.902	1541.23	3206.98
(0,6)	42.2571	174.359	241.822	1901.22	4265.06
(2,2)	45.25	192.871	266.472	2178.25	4953.36
(2,4)	50.95	240.181	316.173	2875.57	7237.52
(2,6)	54.7571	274.974	351.380	3415.43	9172.70
(4,4)	56.65	292.970	369.484	3704.29	10222.5
(4,6)	60.4571	331.411	407.102	4337.65	12698.8
(6,6)	64.2643	372.282	446.331	5037.27	15588.4

[43], and the Bakulev-Mikhailov-Stefanis parametrizations [80,81]. In recent years there have emerged extensive investigations of the profile of the pion distribution amplitude from different methodologies, including QCD lightcone sum rule [82] with nonlocal condensate [80,83] or fitted from dispersion relation [84] or platykurtic [85], Dyson-Schwinger equation [86,87], basis light-front quantization [88], light-front quark model [89], holographic QCD [90], and very recently, from the lattice simulation [91,92]. The predicted values of various Gegenbauer moments are scattered in a wide range.

Since lattice QCD provides the first-principle predictions, in this Letter we will take the most recent lattice results as inputs. In 2019, the RQCD Collaboration presented a precise prediction for the second Gegenbauer moment of pion LCDA in the $\overline{\text{MS}}$ scheme, with $a_2(2 \text{ GeV}) = 0.116^{+0.019}_{-0.020}$ [91].

An important progress in lattice QCD is expedited by the advent of the large-momentum effective theory (LaMET) a decade ago [93,94], which allows one to access the lightcone distributions in Euclidean lattice directly in the xspace. Very recently, the LPC Collaboration presented the whole profile of the pion LCDA [92], from which various Gegenbauer moments can be inferred: $a_2(2 \text{ GeV}) =$ 0.258 ± 0.087 , $a_4(2 \text{ GeV}) = 0.122 \pm 0.056$, $a_6(2 \text{ GeV}) = 0.122 \pm 0.056$ 0.068 ± 0.038 . It is curious that the value of a_2 reported by the LPC Collaboration is about 2 times greater than that reported by the RQCD Collaboration. This discrepancy might be attributed to the fact that the LaMET approach receives a large power correction in the end point region. On the other hand, it is very challenging for the local operator matrix element approach [91] to compute the higher Gegenbauer moments, thus making it difficult to reconstruct the whole profile of the LCDA.

Phenomenological exploration.—We use the three-loop evolution equation [62,95] to evolve each a_n evaluated at 2 GeV by lattice simulation to any intended scale μ . We only retain those Gegenbauer moments with n up to 6. We also use the package FAPT [96] to evaluate the running QCD coupling constant to three-loop accuracy.



FIG. 2. Theoretical predictions vs data for $Q^2 F_{\pi}(Q^2)$ in the spacelike (left) and timelike (right) regions. We take the central values of a_2 , a_4 , and a_6 determined by LPC. The red, green, and blue curves correspond to the LO, NLO, and NNLO results, and the respective bands are obtained by sliding μ from Q/2 to Q. Experimental data points are taken from NA7 [11], Bebek *et al.* [5], Huber *et al.* [16], and *BABAR* [27].



FIG. 3. Same as Fig. 2, except the predictions are made by taking the central value of a_2 determined by RQCD, with a_4 and a_6 set to zero.

For the sake of comparison, we take the pion EM form factor data in the spacetime region from the NA7 Collaboration [11], Cornell data compiled by Bebek *et al.* [5], and the reanalyzed Jefferson Lab data [16] and take the timelike pion EM form factor data entirely from the *BABAR* experiment [27]. We discard many irrelevant small- Q^2 data.

In Figs. 2 and 3, we confront our predictions at various perturbative accuracy with the available data, including both space- and timelike regimes. One clearly visualizes that the NNLO correction is positive and substantial. In Fig. 2, we set the various Gegenbauer moments of pion LCDA to the central values given by the LPC Collaboration [92]. It appears that the NNLO predictions significantly overshoot the experimental data at large Q^2 (> 5 GeV²), especially for the timelike regime with high-statistics data. This symptom is mainly due to the large value of a_2 .

In Fig. 3 we present our predictions with a_2 taken from RQCD while setting the values of a_4 and a_6 to zero. We find satisfactory agreement between our NNLO predictions and the data, both in space- and timelike regimes. This may indicate that the value of a_2 given by RQCD might be more trustworthy. It is of utmost importance for RQCD and LPC Collaborations to settle the discrepancy in the value of a_2 in the future.

The prospective Electron-Ion Collider (EIC) program plans to measure the spacelike pion EM form factor with Q^2 as large as 30 GeV² [97], where perturbative QCD should be definitely reliable. We are eagerly awaiting to confront our NNLO predictions with the future EIC data.

Summary.—In this Letter, we report the first calculation of the NNLO QCD corrections to the pion electromagnetic form factor. We have explicitly verified the validity of the collinear factorization to two-loop order for this observable and obtain the UV- and IR-finite two-loop hard-scattering kernel in closed form. The NNLO QCD correction turns to be positive and important. We then confront our finest theoretical predictions with various space- and timelike pion form factor data. Our phenomenological study reveals that adopting the second Gegenbauer moment computed by RQCD can yield a decent agreement with large- Q^2 data (above the resonance region in the timelike case). Nevertheless, to make a definite conclusion, it seems imperative to resolve the discrepancy between LPC and RQCD Collaborations on the value of a_2 in future study. Furthermore, we look forward to the future high-statistics larger- Q^2 pion EM form factor data for critically testing our NNLO predictions. It will also be very interesting to confront our NNLO predictions with the available highquality kaon EM form factor data.

We are indebted to Jun Hua for providing the value of the Gegenbauer moment a_6 based on the recent LPC study [92]. The work of L.-B.C. is supported by the NNSFC Grant No. 12175048. The work of W.C. is supported by National Natural Science Foundation of China under Contract No. 11975200. The work of F. F. is supported by the NNSFC Grant No. 12275353. The work of Y.J. is supported in part by the NNSFC Grants No. 11925506 and No. 12070131001 (CRC110 by DFG and NSFC).

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