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Transition form factors $\gamma^*\gamma \to \eta$ and $\gamma^*\gamma \to \eta'$ in QCD

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We update the theoretical framework for the QCD calculation of transition form factors $\gamma^*\gamma \to \eta$ and $\gamma^*\gamma \to \eta'$ at large photon virtualities including full next-to-leading order analysis of perturbative corrections, the charm quark contribution, and taking into account $SU(3)$-flavor breaking effects and the axial anomaly contributions to the power-suppressed twist-four distribution amplitudes. The numerical analysis of the existing experimental data is performed with these improvements.

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I. INTRODUCTION

During the last years, properties of the light pseudoscalar η and η' mesons, their quark-gluon structure and hard processes involving these particles, e.g. electromagnetic transition form factors (FFs) and weak decays $B \to \eta(\eta')$, were the subject of numerous experimental and theoretical studies. Especially the recent measurements of the electromagnetic transition FFs $\gamma^*\gamma \to \eta$ and $\gamma^*\gamma \to \eta'$ at spacelike momentum transfers in the interval 4–40 GeV^2 [1] and at the very large timelike momentum transfer 112 GeV^2 [2] by the *BABAR* Collaboration caused much excitement. These measurements and their comparison to the spacelike data for $\gamma^*\gamma \to \pi^0$ FF in the similar range by *BABAR* and Belle collaborations [3,4] stimulated a flurry of theoretical activity; see e.g. [5–8]. This debate focuses on the question of whether hard exclusive hadronic reactions are under theoretical control, which is highly relevant for all future high-intensity, medium-energy experiments like, e.g., Belle II and PANDA.

In the exact flavor $SU(3)$ limit the η meson is part of the flavor octet whereas η' is a pure flavor singlet whose properties are intimately related to the celebrated axial anomaly [9,10]. However, it is known empirically that the $SU(3)$ breaking effects are large and have a nontrivial structure. These effects are usually described in terms of a certain mixing scheme that considers the physical η, η' mesons as a superposition of fundamental (e.g. flavor singlet and octet) fields in the low-energy effective theory; see e.g. [11] and references therein. It is not obvious whether and to what extent the approach based on state mixing is adequate for the description of hard processes that are dominated by meson wave functions at small transverse separations, dubbed distribution amplitudes (DAs); however, it can be taken as a working hypothesis to avoid proliferation of parameters.

One particularly important issue is that eta mesons, in difference to the pion, can contain a significant admixture of the two-gluon state at low scales, hence a comparably large two-gluon DA. Several different reactions were considered in an effort to extract or at least constrain these contributions. Nonleptonic exclusive isosinglet decays [12] and central exclusive production [13] act as prominent probes for the gluonic Fock state since the gluon production diagram enters already at leading order (LO). Exclusive semileptonic decays of heavy mesons were calculated in the framework of light-cone sum rules (LCSRs) [14,15] and k_T factorization [16]. From a calculational point of view these decays are simpler but the interesting gluon contribution enters only at next-to-leading order (NLO). Numerically it was shown that the gluonic contributions to η production are negligible while they can reach a few percent in the η' channel. Up to now experimental data are not conclusive in all these decays, with a vanishing gluonic DA being possible at a low scale. On the other hand, a large gluon contribution was advocated in [17] from the analysis of $B_d \to J/\Psi\eta^{(\prime)}$ transitions (see also [18]).

In this paper we consider electromagnetic transition form factors $\gamma^*\gamma \to \eta, \eta'$ that are the simplest relevant processes and are best understood from the theory side. Also in this case we will find that the present experimental data are insufficient to draw definite conclusions. However, the forthcoming upgrade of the Belle experiment and the KEKB accelerator [19], which aims to increase the experimental data set by the factor of 50, will allow one to measure transition form factors and related observables with unprecedented precision.

The special role of the transition FFs as the "gold plated" observables for the study of meson DAs is widely recognized. To leading power accuracy in the photon virtuality these FFs can be calculated rigorously in QCD in the framework of collinear factorization (pQCD) [20–23]. The main advantage of transition FFs in comparison to other hard reactions with the same property is that the leading hard contribution starts already at tree level and is not suppressed by the usual perturbative penalty factor $\alpha_s/\pi \sim 1/10$. For the leading-twist collinear factorization to hold, the pQCD contribution has to win against the power-suppressed (end-point or higher-twist) corrections, and this is expected to happen for transition FFs already at

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moderate photon virtualities that are accessible in present experiments. One more advantage is that soft contributions are simpler and can be modeled to a reasonable accuracy using, e.g., LCSRs.

The theory of $\gamma^*\gamma \to \eta^{(\prime)}$ decays is, on the one hand, similar to the QCD description of the $\gamma^*\gamma \to \pi^0$ transition FF, but contains specific new issues due to the two-gluon state admixture, contributions of heavy quarks, and also potentially large meson mass corrections. Our goal is to present a state-of-the-art treatment of these special issues using a combination of perturbative QCD for the calculation of the leading terms and LCSRs for the estimate of power corrections, complementing our study [24,25] of $\gamma^*\gamma \to \pi^0$. For earlier work related to this program, see [6,26–29].

An alternative approach to the calculation of transition form factors makes use of transverse momentum-dependent (TMD) meson wave functions (TMD or k_T factorization [30]). This is a viable technique that has been advanced recently to NLO, see e.g. [31,32] for the electromagnetic pion form factor and $\gamma^*\gamma \to \pi^0$, and which can be applied to the $\gamma^*\gamma \to \eta^{(\prime)}$ transitions as well. Because of a more complicated nonperturbative input, interpretation of the corresponding results in terms of DAs is, however, not straightforward so that we prefer to stay within the collinear factorization framework in what follows.

The theoretical updates implemented in this work are the following:

(i) the c-quark contribution to the coefficient function of the two-gluon DA;

(ii) complete NLO treatment of the scale dependence of DAs including quark-gluon mixing;

(iii) consistent treatment of the corrections due to the strange quark mass to $\mathcal{O}(m_s)$ accuracy including an update of the $SU(3)$-breaking corrections in twist-four DAs;

(iv) partial account of the anomalous contributions and implementation of $\eta - \eta'$ mixing schemes in the twist-four DAs.

We further use these improvements for a numerical analysis of the existing spacelike and timelike data, including a careful analysis of the uncertainties, and the prospects to constrain the two-gluon $\eta^{(\prime)}$ DAs if more precise data on transition FFs become available.

The presentation is organized as follows. Section II is introductory. We collect here the definitions for twist-two and twist-three DAs and introduce necessary notation in both the quark-flavor and singlet-octet bases. Different mixing schemes are introduced and discussed. Section III is devoted to the calculation of the $\gamma^*\gamma \to \eta, \eta'$ electromagnetic transition FFs in the collinear factorization framework. Complete NLO expressions for the leading-twist contributions are given. We also demonstrate the cancellation of the end-point divergences in twist-four contributions at the tree (LO) level. The necessity to distinguish between the notion of "power-suppressed" and "higher-twist" contributions is emphasized. A separate subsection contains the discussion of the difference of timelike and spacelike FFs in pQCD; the results are compared to data [2]. In Sec. IV we start by explaining why the twist expansion of the product of electromagnetic currents does not provide the complete result for the FFs if one of the photons is real, and present the calculation of the remaining soft contributions within the LCSR framework that is based on dispersion relations and quark-hadron duality. A detailed numerical analysis of the spacelike experimental data in this framework is presented in Sec. V. The final Sec. VI is reserved for a summary and outlook.

The paper contains two appendixes where more technical material and/or long expressions are collected. Appendix A is devoted to the two- and three-particle twist-four DAs of the η, η' mesons. It contains an update of the existing expressions [33–35] taking into account $SU(3)$-breaking effects, and also a partial calculation of anomalous contributions to the higher-twist DAs that arise from the axial anomaly. In Appendix B complete NLO expressions for the scale dependence of the leading-twist DAs are presented.

II. η, η' MIXING AND DISTRIBUTION AMPLITUDES

The description of the transition FFs $\gamma^*\gamma \to \eta, \eta'$ requires knowledge of the momentum fraction distributions of valence quarks in the mesons at small transverse separations, the meson distribution amplitudes. We define the leading-twist DA for a given quark flavor at a given scale μ as

$$\begin{aligned}
&\langle 0|\bar{q}(z_2 n)\not{n}\gamma_5 q(z_1 n)|M(p)\rangle \\
&\quad = iF_M^{(q)}(pn)\int_0^1 du e^{-iz_{21}^u(pn)}\phi_M^{(q)}(u,\mu), \\
&\langle 0|\bar{s}(z_2 n)\not{n}\gamma_5 s(z_1 n)|M(p)\rangle \\
&\quad = iF_M^{(s)}(pn)\int_0^1 du e^{-iz_{21}^u(pn)}\phi_M^{(s)}(u,\mu),
\end{aligned} \tag{1}$$

where $q = u$ or d, n_μ is an auxiliary lightlike vector, $n^2 = 0$, and we use a notation

$$z_{21}^u = \bar{u}z_2 + uz_1, \qquad \bar{u} = 1 - u. \tag{2}$$

In the following we also abbreviate

$$z_{21} = z_2 - z_1. \tag{3}$$

The gauge links between the quark fields are implied. In all equations $M = \eta, \eta'$ denotes the physical pseudoscalar meson state. We assume exact isospin symmetry and identify

$$m_q = \frac{1}{2}(m_u + m_d). \tag{4}$$

The normalization is chosen such that

$$\int_0^1 du \phi_M^{(q,s)}(u,\mu) = 1 \tag{5}$$

and the couplings $F_M^{(u)} = F_M^{(d)}$, $F_M^{(s)}$ are the matrix elements of flavor-diagonal axial vector currents that we also write in the form

$$F_M^{(u)} = F_M^{(d)} = \frac{f_M^{(q)}}{\sqrt{2}}, \qquad F_M^{(s)} = f_M^{(s)}, \tag{6}$$

where

$$\langle 0|J_{\mu 5}^{(r)}|M(p)\rangle = i f_M^{(r)} p_\mu, \qquad r = q, s, \tag{7}$$

with the currents

$$J_{\mu 5}^{(q)} = \frac{1}{\sqrt{2}}[\bar{u}\gamma_\mu\gamma_5 u + \bar{d}\gamma_\mu\gamma_5 d], \qquad J_{\mu 5}^{(s)} = \bar{s}\gamma_\mu\gamma_5 s. \tag{8}$$

The scale dependence of the DAs can be simplified by introducing flavor-singlet and flavor-octet combinations

$$\begin{aligned} f_M^{(8)}\phi_M^{(8)} &= \sqrt{\frac{1}{3}} f_M^{(q)}\phi_M^{(q)} - \sqrt{\frac{2}{3}} f_M^{(s)}\phi_M^{(s)}, \\ f_M^{(1)}\phi_M^{(1)} &= \sqrt{\frac{2}{3}} f_M^{(q)}\phi_M^{(q)} + \sqrt{\frac{1}{3}} f_M^{(s)}\phi_M^{(s)}. \end{aligned} \tag{9}$$

Here

$$\langle 0|J_{\mu 5}^{(i)}|M(p)\rangle = i f_M^{(i)} p_\mu, \qquad i = 1, 8, \tag{10}$$

where $J_{\mu 5}^{(1)}$ and $J_{\mu 5}^{(8)}$ denote the $SU(3)$ flavor-singlet and octet currents

$$\begin{aligned} J_{\mu 5}^{(1)} &= \frac{1}{\sqrt{3}}[\bar{u}\gamma_\mu\gamma_5 u + \bar{d}\gamma_\mu\gamma_5 d + \bar{s}\gamma_\mu\gamma_5 s], \\ J_{\mu 5}^{(8)} &= \frac{1}{\sqrt{6}}[\bar{u}\gamma_\mu\gamma_5 u + \bar{d}\gamma_\mu\gamma_5 d - 2\bar{s}\gamma_\mu\gamma_5 s]. \end{aligned} \tag{11}$$

Equation (9) can be viewed as an orthogonal transformation from the quark-flavor (QF) to the singlet-octet (SO) basis

$$\begin{pmatrix} f_M^{(8)}\phi_M^{(8)}(u,\mu) \\ f_M^{(1)}\phi_M^{(1)}(u,\mu) \end{pmatrix} = U(\varphi_0)\begin{pmatrix} f_M^{(q)}\phi_M^{(q)}(u,\mu) \\ f_M^{(s)}\phi_M^{(s)}(u,\mu) \end{pmatrix} \tag{12}$$

where

$$U(\varphi_0) = \begin{pmatrix} \sqrt{\frac{1}{3}} & -\sqrt{\frac{2}{3}} \\ \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} \end{pmatrix} = \begin{pmatrix} \cos\varphi_0 & -\sin\varphi_0 \\ \sin\varphi_0 & \cos\varphi_0 \end{pmatrix} \tag{13}$$

with $\varphi_0 = \arctan(\sqrt{2})$.

The main advantage of this representation is that the SO couplings and DAs do not mix with each other via renormalization. In particular the octet coupling $f_M^{(8)}$ is scale independent whereas the singlet coupling $f_M^{(1)}$ evolves due to the $U(1)$ anomaly [36]:

$$\mu\frac{d}{d\mu} f_M^{(1)}(\mu) = -4n_f\left(\frac{\alpha_s}{2\pi}\right)^2 f_M^{(1)} + \mathcal{O}(\alpha_s^3), \tag{14}$$

or

$$f_M^{(1)}(\mu) = f_M^{(1)}(\mu_0)\left\{1 + \frac{2n_f}{\pi\beta_0}[\alpha_s(\mu) - \alpha_s(\mu_0)]\right\}, \tag{15}$$

where n_f is the number of light quark flavors.

The DAs can be expanded in terms of orthogonal polynomials $C_n^{3/2}(2u-1)$ that are eigenfunctions of the one-loop flavor-nonsinglet evolution equation:

$$\phi_M^{(1,8)}(u,\mu) = 6u\bar{u}\left[1 + \sum_{n=2,4,\ldots} c_{n,M}^{(1,8)}(\mu) C_n^{3/2}(2u-1)\right]. \tag{16}$$

The sum in Eq. (16) goes over polynomials of even dimension $n = 2, 4, \ldots$. This restriction is a consequence of C-parity that implies that quark-antiquark DAs are symmetric functions under the interchange of the quark momenta

$$\phi_M^{(1,8)}(u,\mu) = \phi_M^{(1,8)}(\bar{u},\mu). \tag{17}$$

In addition we introduce a two-gluon leading-twist DA $\phi_M^{(g)}(u,\mu)$,

$$\begin{aligned} &\langle 0|G_{n\xi}(z_2 n)\tilde{G}^{n\xi}(z_1 n)|M(p)\rangle \\ &\quad = \frac{C_F}{2\sqrt{3}} f_M^{(1)}(pn)^2 \int_0^1 du e^{-iz_{21}^u(pn)} \phi_M^{(g)}(u,\mu), \end{aligned} \tag{18}$$

where $C_F = 4/3$, $\tilde{G}_{\mu\nu}$ is the dual gluon field strength tensor $\tilde{G}_{\mu\nu} = (1/2)\epsilon_{\mu\nu\alpha\beta}G^{\alpha\beta}$ and $G_{n\xi} = G_{\mu\xi}n^\mu$. We use the conventions $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ and $\epsilon_{0123} = 1$, following [37]. The gluon DA is antisymmetric

$$\phi_M^{(g)}(u,\mu) = -\phi_M^{(g)}(\bar{u},\mu) \tag{19}$$

and can be expanded in a series of Gegenbauer polynomials $C_{n-1}^{5/2}(2u-1)$ of odd dimension

$$\phi_M^{(g)}(u,\mu) = 30u^2\bar{u}^2 \sum_{n=2,4,\ldots} c_{n,M}^{(g)}(\mu) C_{n-1}^{5/2}(2u-1). \quad (20)$$

The flavor-octet Gegenbauer coefficients $c_{n,M}^{(8)}(\mu)$ are renormalized multiplicatively at LO, and get mixed with the coefficients $c_{k,M}^{(8)}(\mu)$ with $k < n$ starting at NLO. The flavor-singlet coefficients $c_{n,M}^{(1)}(\mu)$ get mixed with the gluon coefficients $c_{n,M}^{(g)}(\mu)$ already at LO, and also with the coefficients of the polynomials with lower dimension starting at NLO; see Appendix B for details. In what follows we refer to these coefficients as shape parameters. The values of shape parameters at a certain scale μ_0 encode all nonperturbative information on the DAs.

In the exact $SU(3)$ flavor symmetry limit the η meson is part of a flavor octet, $\eta = \eta_8$, and η' is a flavor singlet, $\eta' = \eta_1$. In this limit $f_\eta^{(s)} = -\sqrt{2} f_\eta^{(q)}$, $f_{\eta'}^{(s)} = 1/\sqrt{2} f_{\eta'}^{(q)}$ and $f_\eta^{(q)} = f_\pi$ where f_π is the pion decay constant; in our normalization $f_\pi = 131$ MeV. However, it is known empirically that the $SU(3)$-breaking corrections are large and have a rather nontrivial structure. In chiral effective theory the η' meson can be included in the framework of the $1/N_c$ expansion [38]. In this approach the leading effect is due to the axial anomaly that introduces an effective mass term for the η, η' states that is not diagonal in the SO basis if $SU(3)$ flavor symmetry is broken. In addition, there is also an off-diagonal contribution to the kinetic term $\partial_\mu \eta_8 \partial^\mu \eta_1$ at loop level [39]. As a result, the relation of physical η, η' states to the basic octet and singlet fields in the chiral Lagrangian, η_8 and η_1, becomes complicated and involves two different mixing angles, see, e.g., a discussion in Ref. [11]. There is no reason to expect that these mixing angles are the same for the matrix elements of all operators of higher dimension that determine moments of DAs. Thus the classification based on the SO mixing scheme without additional assumptions does not seem to be particularly useful in this context as the number of parameters is not reduced.

In the last years a specific approximation has become popular that we will refer to as the Feldmann-Kroll-Stech (FKS) scheme [11]. This construction is motivated by the observation that the vector mesons ω and ϕ are to a very good approximation pure $\bar{u}u + \bar{d}d$ and $\bar{s}s$ states and the same pattern is observed in tensor mesons. The smallness of mixing is a manifestation of the celebrated Okubo-Zweig-Iizuka (OZI) rule that is phenomenologically very successful. If the axial $U(1)$ anomaly is the *only* effect that makes the situation in pseudoscalar channels different, it is natural to assume that physical states are related to the flavor states by an orthogonal transformation

$$\begin{pmatrix} |\eta\rangle \\ |\eta'\rangle \end{pmatrix} = U(\varphi) \begin{pmatrix} |\eta_q\rangle \\ |\eta_s\rangle \end{pmatrix}, \qquad U(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}. \quad (21)$$

This *state* mixing is a very strong assumption that implies that the same mixing pattern applies to the decay constants and, more generally, to the wave functions so that

$$\begin{pmatrix} f_\eta^{(q)} & f_\eta^{(s)} \\ f_{\eta'}^{(q)} & f_{\eta'}^{(s)} \end{pmatrix} = U(\varphi) \begin{pmatrix} f_q & 0 \\ 0 & f_s \end{pmatrix}, \quad (22)$$

and

$$\begin{pmatrix} f_\eta^{(q)}\phi_\eta^{(q)} & f_\eta^{(s)}\phi_\eta^{(s)} \\ f_{\eta'}^{(q)}\phi_{\eta'}^{(q)} & f_{\eta'}^{(s)}\phi_{\eta'}^{(q)} \end{pmatrix} = U(\varphi) \begin{pmatrix} f_q\phi_q & 0 \\ 0 & f_s\phi_s \end{pmatrix}, \quad (23)$$

with the same mixing angle φ.

This is a far reaching conjecture that allows one to reduce the four DAs of the physical states η, η' to the two DAs $\phi_q(u,\mu)$, $\phi_s(u,\mu)$ of the flavor states:

$$\phi_\eta^{(q)}(u) = \phi_{\eta'}^{(q)}(u) = \phi_q(u),$$
$$\phi_\eta^{(s)}(u) = \phi_{\eta'}^{(s)}(u) = \phi_s(u). \quad (24)$$

The singlet and octet DAs in this scheme are given by

$$\begin{pmatrix} f_\eta^{(8)}\phi_\eta^{(8)} & f_\eta^{(1)}\phi_\eta^{(1)} \\ f_{\eta'}^{(8)}\phi_{\eta'}^{(8)} & f_{\eta'}^{(1)}\phi_{\eta'}^{(1)} \end{pmatrix} = U(\varphi) \begin{pmatrix} f_q\phi_q & 0 \\ 0 & f_s\phi_s \end{pmatrix} U^T(\varphi_0) \quad (25)$$

and the same relation is valid separately for the couplings $f_M^{(r)}$ and the couplings multiplied by the shape parameters $f_M^{(r)} c_{n,M}^{(r)}$ (16). The couplings f_q, f_s and the mixing angle ϕ in the FKS scheme have been determined in Ref. [11] from a fit to experimental data:

$$f_q = (1.07 \pm 0.02) f_\pi,$$
$$f_s = (1.34 \pm 0.06) f_\pi,$$
$$\varphi = 39.3^\circ \pm 1.0^\circ. \quad (26)$$

A newer analysis [40] exploiting more recent data but only a subset of the processes investigated in [11] yields

$$f_q = (1.09 \pm 0.03) f_\pi,$$
$$f_s = (1.66 \pm 0.06) f_\pi,$$
$$\varphi = 40.7^\circ \pm 1.4^\circ, \quad (27)$$

where the mixing angle is the average of φ_q and φ_s from [40]. The difference between the two sets can be viewed as an intrinsic uncertainty of the FKS approximation. For consistency with earlier work, e.g. [6], we will accept by default the original set of parameters from Ref. [11], Eq. (26), for numerical calculations in this work. A recent discussion of the ongoing investigations of $\eta - \eta'$ mixing from a more general perspective can be found in [41].

Since the flavor-singlet and flavor-octet couplings have different scale dependence, Eq. (25) cannot hold at all scales. It is natural to assume that the FKS scheme refers to a low renormalization scale $\mu_0 \sim 1$ GeV and the DAs at higher scales are obtained by QCD evolution (that also generates nonvanishing OZI-violating contributions). Figure 1 shows a comparison of the $\gamma^*\gamma \to \pi^0$ experimental data with the nonstrange $\gamma^*\gamma \to |\eta_q\rangle$ FF extracted from the combination of *BABAR* and CLEO measurements of $\gamma^*\gamma \to \eta$ and $\gamma^*\gamma \to \eta'$ assuming the FKS mixing scheme. Were this scheme exact, the two FFs would coincide in the whole Q^2 range, up to tiny isospin breaking corrections. It is seen that the existing measurements do not contradict the FKS approximation at low-to-moderate $Q^2 \lesssim 10\ \mathrm{GeV}^2$, whereas at larger virtualities the comparison is inconclusive because of significant discrepancies between the *BABAR* and Belle pion data. The *BABAR* data taken alone show a dramatic difference between the $\gamma^*\gamma \to \pi^0$ and $\gamma^*\gamma \to |\eta_q\rangle$ FFs at large virtualities that cannot be explained by perturbative evolution effects. If this difference were confirmed, it would be a stark indication that the concept of state mixing is not applicable to the η and η' DAs so that the corresponding relations between higher-order Gegenbauer coefficients are strongly broken already at a low scale.

Staying with the state mixing picture, for the gluon DA we have to assume that

$$\langle 0|G_{n\xi}(z_2 n)\tilde{G}^{n\xi}(z_1 n)|\eta_q\rangle = \langle 0|G_{n\xi}(z_2 n)\tilde{G}^{n\xi}(z_1 n)|\eta_s\rangle$$

and as a consequence

$$\phi_\eta^{(g)}(u) = \phi_{\eta'}^{(g)}(u), \tag{28}$$

that is similar to Eq. (24).

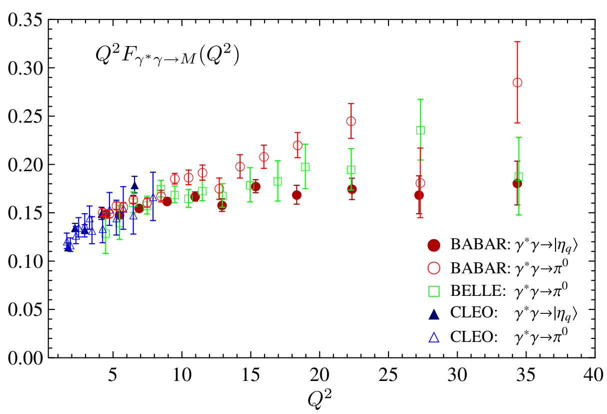

FIG. 1 (color online). The experimental data on $\gamma^*\gamma \to \pi^0$ [3,4,42] (open symbols) compared with the nonstrange component of the eta meson transition FF, $\gamma^*\gamma \to |\eta_q\rangle$ (filled symbols), from the combination of *BABAR* and CLEO measurements [1,42] on η and η' production in the FKS mixing scheme, Eqs. (22) and (23).

Two-particle twist-three DAs for the strange quarks can be defined as

$$2m_s\langle 0|\bar{s}(z_2 n)i\gamma_5 s(z_1 n)|M(p)\rangle = \int_0^1 du e^{-iz_{21}^u(pn)}\phi_{3M}^{(s)p}(u), \tag{29}$$

and

$$2m_s\langle 0|\bar{s}(z_2 n)\sigma_{\mu\nu}\gamma_5 s(z_1 n)|M(p)\rangle = \frac{iz_{12}}{6}(p_\mu n_\nu - p_\nu n_\mu)\int_0^1 du e^{-iz_{21}^u(pn)}\phi_{3M}^{(s)\sigma}(u) \tag{30}$$

with the normalization condition

$$\int_0^1 du\phi_{3M}^{(s)p}(u) = \int_0^1 du\phi_{3M}^{(s)\sigma}(u) = H_M^{(s)}, \tag{31}$$

where

$$H_M^{(s)} = m_M^2 F_M^{(s)} - a_M, \quad a_M = \langle 0|\frac{\alpha_s}{4\pi}G_{\mu\nu}^A\tilde{G}^{A,\mu\nu}|M(p)\rangle, \tag{32}$$

that follows from the anomaly relation

$$\partial^\mu J_{\mu 5}^{(s)} = 2m_s\bar{s}i\gamma_5 s + \frac{\alpha_s}{4\pi}G_{\mu\nu}^A\tilde{G}^{A,\mu\nu}. \tag{33}$$

Twist-three DAs for the light $q = u, d$ quarks can be defined by similar expressions with obvious substitutions $s \to q$, e.g. $H_M^{(q)} = m_M^2 F_M^{(q)} - a_M$. In what follows we also use the notation, cf. (6),

$$H_M^{(u)} = H_M^{(d)} = \frac{h_M^{(q)}}{\sqrt{2}}, \qquad H_M^{(s)} = h_M^{(s)}. \tag{34}$$

We do not present here the definitions of three-particle quark-antiquark-gluon twist-three DAs as it turns out that they do not contribute to the FFs of interest at LO in perturbation theory.

Assuming the FKS mixing scheme at low scales one can rewrite the four DAs $\phi_{3M}^{(q,s)p}$ in terms of two functions as in Eq. (23), and similar for $\phi_{3M}^{(q,s)\sigma}$, introducing two new parameters h_q and h_s [43]

$$h_q = 0.0015 \pm 0.004, \qquad h_s = 0.087 \pm 0.006. \tag{35}$$

Note that h_q is small and consistent with zero. It is easy to convince oneself that matrix elements of operators with an even number of γ matrices enter the calculation of the $\gamma^*\gamma \to \eta$ and $\gamma^*\gamma \to \eta'$ transition FFs always multiplied by quark masses, as on the left-hand-side of Eqs. (29) and (30).

In this situation the contribution of light $q = u, d$ quarks is tiny and can safely be neglected. To this accuracy

$$\phi^{(s)p}_{3\eta'}(u) = \cos\varphi\phi^{p}_{3s}(u), \qquad \phi^{(s)p}_{3\eta}(u) = -\sin\varphi\phi^{p}_{3s}(u),$$
$$\phi^{(s)\sigma}_{3\eta'}(u) = \cos\varphi\phi^{\sigma}_{3s}(u), \qquad \phi^{(s)\sigma}_{3\eta}(u) = -\sin\varphi\phi^{\sigma}_{3s}(u), \tag{36}$$

where

$$\phi^{p}_{3s}(u) = h_s + 60 m_s f_{3s} C_2^{1/2}(2u-1) + \ldots,$$
$$\phi^{\sigma}_{3s}(u) = 6\bar{u}u[h_s + 10 m_s f_{3s} C_2^{3/2}(2u-1) + \ldots]. \tag{37}$$

The ellipses stand for the contributions of higher conformal spin and corrections $\mathcal{O}(m_s^2)$ which we neglect for consistency with the calculation of twist-four corrections (see the next section). The coupling f_{3s} is defined as

$$\langle 0|\bar{s}\sigma_{n\xi}\gamma_5 g G^{n\xi} s|\eta_s(p)\rangle = 2i(pn)^2 f_{3s} \tag{38}$$

and we assume that $f^{(s)}_{3\eta'} = \cos\varphi f_{3s}$, $f^{(s)}_{3\eta} = -\sin\varphi f_{3s}$. The corresponding coupling for the charged π meson is estimated to be (at the scale 1 GeV) [35]

$$f_{3\pi} \sim 0.0045\ \mathrm{GeV}^2. \tag{39}$$

Lacking any information about the flavor-singlet contribution, we adopt this number as a (possibly crude) estimate for f_{3s}. With this choice

$$\frac{2 m_s f_{3s}}{h_s} \sim 0.01 \tag{40}$$

and one may hope that the corresponding ambiguity in FF predictions is not very large. We will return to this question in the next section. The scale dependence of f_{3s} is given by [35]

$$f_{3s}(\mu) = L^{55/(9\beta_0)} f_{3s}(\mu_0) + \mathcal{O}(m_s f_s) \tag{41}$$

where $L = \alpha_s(\mu)/\alpha_s(\mu_0)$.

Finally, we will need the DAs of twist four that are rather numerous. The corresponding expressions, including some new results, are collected in Appendix A.

III. $\gamma^*\gamma \to \eta, \eta'$ FORM FACTORS IN QCD FACTORIZATION

A. Leading twist

The FFs $F_{\gamma^*\gamma^*\to M}(q_1^2, q_2^2)$, $M = \eta, \eta'$ describing the meson transition in two (in general virtual) photons are defined by the following matrix element of the product of two electromagnetic currents

$$\int d^4x e^{iq_1x}\langle M(p)|T\{j^{\mathrm{em}}_\mu(x) j^{\mathrm{em}}_\nu(0)\}|0\rangle$$
$$= ie^2\varepsilon_{\mu\nu\alpha\beta} q_1^\alpha q_2^\beta F_{\gamma^*\gamma^*\to M}(q_1^2, q_2^2), \tag{42}$$

where

$$j^{\mathrm{em}}_\mu(x) = e_u\bar{u}(x)\gamma_\mu u(x) + e_d\bar{d}(x)\gamma_\mu d(x) + \ldots,$$

p is the meson momentum and $q_2 = q_1 + p$. We will mainly consider the spacelike FF, in which case photon virtualities are negative. In the experimentally relevant situation one virtuality is large and the second one small (or zero). For definiteness we take

$$q_1^2 = -Q^2, \qquad q_2^2 = -q^2, \tag{43}$$

assuming that $q^2 \ll Q^2$. Most of the following equations are written for $q^2 = 0$, and we use a shorthand notation

$$F_{\gamma^*\gamma\to M}(Q^2) \equiv F_{\gamma^*\gamma^*\to M}(q_1^2 = -Q^2, q^2 = 0).$$

The leading contribution $\mathcal{O}(1/Q^2)$ to the FFs can be written in factorized form as a convolution of leading-twist DAs with coefficient functions that can be calculated in QCD perturbation theory.

The contribution of heavy (charm) quarks requires some attention. There are two basic possibilities to take into account heavy quarks in the QCD factorization formalism [44–47] which correspond, essentially, to the two choices of the (physical) factorization scale. It can be smaller, $\mu \ll m_h$, or larger, $\mu \gg m_h$ than the heavy quark mass. If $\Lambda_{\mathrm{QCD}} \ll \mu \ll m_h, Q$, i.e. if the (heavy) quark mass m_h is very large, of the order of the photon virtuality $m_h \sim Q$, it is natural to write the structure function as a convolution of coefficient functions and parton densities that involve only light quark flavors u, d, s and gluons. This approach is usually referred to as the decoupling scheme, or fixed flavor number scheme (FFNS). Another possibility is to assume the hierarchy $\Lambda_{\mathrm{QCD}}, m_h \ll \mu \ll Q$ (which implies $m_h \ll Q$) and write the FFs as a sum involving heavy flavors. This is usually dubbed variable flavor number scheme (VFNS), with $\overline{\mathrm{MS}}$ subtraction for all flavors.

In this work we adopt the first scheme which has the advantage that the complete heavy quark dependence is retained in the coefficient functions. A potential problem in this case is that for $m_h \ll Q$ the coefficient functions involve large logarithms $\sim \ln Q^2/m_h^2$ which one would like to resum to all orders. This resummation is naturally done in the VFNS schemes where it corresponds to the resummation of collinear logarithms using the Efremov-Radyushkin-Brodsky-Lepage (ERBL) equation, but the price to pay is that this can only be done to leading power accuracy in the m_h^2/Q^2 expansion. There exists vast literature devoted to heavy quark contributions to deep inelastic lepton hadron scattering (DIS), discussing how the advantages of both approaches can be combined by matching at the scale $\mu \simeq m_h$; see e.g. [46]. We leave such improvements for future work, as the numerical impact of resummation on the transition FFs is not likely to be large. For the same reason we do not take into account terms $\sim\alpha_s^2 \ln Q/m_h$ in the coefficient functions of light quark DAs.

Thus we write

$$\begin{aligned}F_{\gamma^*\gamma\to M}(Q^2) = &\frac{f_M^{(8)}}{3\sqrt{6}}\int_0^1 du T_H^{(8)}(u,Q^2,\mu,\alpha_s(\mu))\phi_M^{(8)}(u,\mu)\\ &+\frac{2f_M^{(1)}}{3\sqrt{3}}\int_0^1 du T_H^{(1)}(u,Q^2,\mu,\alpha_s(\mu))\phi_M^{(1)}(u,\mu)\\ &+\frac{2f_M^{(1)}}{3\sqrt{3}}\int_0^1 du T_H^{(g)}(u,Q^2,\mu,\alpha_s(\mu))\phi_M^{(g)}(u,\mu),\end{aligned} \tag{44}$$

where $\phi_M^{(8,1,g)}(u,\mu)$ are the light quark octet (singlet), and gluon DAs defined in the previous section.

The coefficient function for the quark DA is known in the $\overline{\text{MS}}$ scheme to NLO in the strong coupling [48–50] and is the same for flavor-octet and flavor-singlet contributions. Taking into account the symmetry of the quark DAs (17) it can be written as

$$\begin{aligned}T_H^{\rm NLO} = \frac{2}{uQ^2}\bigg\{1 + C_F\frac{\alpha_s(\mu)}{2\pi}\bigg[&\frac{1}{2}\ln^2 u - \frac{1}{2}\frac{u}{\bar u}\ln u\\ &-\frac{9}{2}+\left(\frac{3}{2}+\ln u\right)\ln\frac{Q^2}{\mu^2}\bigg]\bigg\}.\end{aligned} \tag{45}$$

The leading-order gluon coefficient function is calculated from the diagrams in Fig. 2. The contribution of light u, d, s quarks reads [6,27]

$$T_H^g|_{\rm light} = -C_F\frac{\alpha_s(\mu)}{2\pi}\frac{2\ln u}{\bar u^2 Q^2}\left\{\frac{1}{u}-3+\frac{1}{2}\ln u + \ln\frac{Q^2}{\mu^2}\right\} \tag{46}$$

and the c-quark contribution is equal to

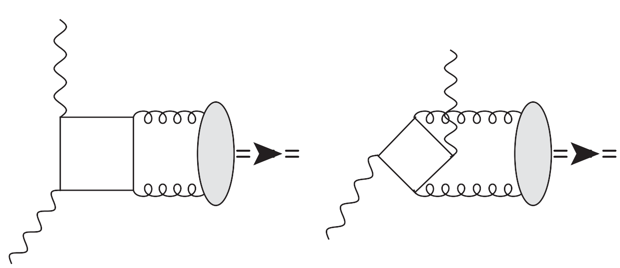

FIG. 2. Box diagrams contributing to the gluon coefficient function.

$$\begin{aligned}T_H^g|_{\rm charm} = C_F\frac{\alpha_s(\mu)}{2\pi}\frac{2}{3}\frac{1}{u\bar u^2 Q^2}\bigg\{&\ln^2\left[\frac{\beta(Q^2)+1}{\beta(Q^2)-1}\right]\\ &- u\ln^2\left[\frac{\beta(uQ^2)+1}{\beta(uQ^2)-1}\right] - 4\beta(Q^2)\ln\left[\frac{\beta(Q^2)+1}{\beta(Q^2)-1}\right]\\ &+2(3u-1)\beta(uQ^2)\ln\left[\frac{\beta(uQ^2)+1}{\beta(uQ^2)-1}\right]\bigg\},\end{aligned} \tag{47}$$

where

$$\beta(Q^2) = \sqrt{1+\frac{4m_c^2}{Q^2}}. \tag{48}$$

In numerical calculations we use the value $m_c = 1.42$ GeV for the c-quark pole mass. The b-quark contribution is given by the same expression with an obvious replacement of the quark mass $m_c \to m_b$ and extra factor $1/4$ from the electric charge $e_c^2 \to e_b^2$. It is very small for the whole experimentally accessible region $Q^2 \lesssim 100$ GeV^2 and can safely be neglected.

In the formal $Q^2 \to \infty$ limit the transition form factors have to approach their asymptotic values [51]

$$\begin{aligned}&\lim_{Q^2\to\infty} Q^2 F_{\gamma^*\gamma\to M}(Q^2)\\ &\quad = \sqrt{\frac{2}{3}}\left[f_M^{(8)} + 2\sqrt{2}f_M^{(1)}(\mu_0)\left(1-\frac{2n_f}{\pi\beta_0}\alpha_s(\mu_0)\right)\right].\end{aligned} \tag{49}$$

Note that the scale dependence of the flavor-singlet axial coupling (15) gives rise to a finite renormalization factor ~ 0.85 which is not negligible. Using $n_f = 4$, $\mu_0 = 1$ GeV, $\alpha_s(1\text{ GeV}) = 0.5$ and the FKS parameters in (26) we obtain

$$\begin{aligned}Q^2 F^{\rm asy}_{\gamma^*\gamma\to\eta}(Q^2) &\to 0.173(0.158)\ \text{GeV},\\ Q^2 F^{\rm asy}_{\gamma^*\gamma\to\eta'}(Q^2) &\to 0.247(0.270)\ \text{GeV}.\end{aligned} \tag{50}$$

The asymptotic FF values corresponding to the parameter set in (27) are shown in parenthesis for comparison. The finite renormalization correction to the flavor-singlet contribution is not taken into account in [1,6,27]. It is only a $\lesssim 5\%$ effect for the η meson but leads to a 20% reduction of the asymptotic value of the FF for the η', in which case the effect is amplified by the cancellation between the flavor-singlet and flavor-octet contributions, $f_{\eta'}^{(1)} = 0.15(0.17)$, $f_{\eta'}^{(8)} = -0.06(-0.08)$. In this way the discrepancy between the data [1] and the expected asymptotic behavior of the $\gamma^*\gamma \to \eta'$ FF is removed, see Sec. V.

B. Higher twist corrections

One source of power corrections $\sim 1/Q^2$ to the transition FFs $F_{\gamma^*\gamma^*\to M}$ corresponds to contributions of less singular terms $\sim 1/x^2$, $\ln x^2$, etc., as compared to the leading contribution $\sim 1/x^4$ in the operator product expansion of the two electromagnetic currents in Eq. (42). They can be calculated in terms of meson DAs of higher twist and will be referred to as higher-twist corrections in what follows. To LO in perturbation theory one obtains including the twist-four contribution

$$Q^2 F_{\gamma^*\gamma\to M}(Q^2) = 2\sum_{\psi=u,d,s} e_\psi^2 F_M^{(\psi)} \int_0^1 \frac{du}{u}\left\{\phi_M^{(\psi)}(u) - \frac{\bar{u} m_M^2}{Q^2}\phi_M^{(\psi)}(u) + \frac{1}{6uQ^2}\phi_{3M}^{(\psi)\sigma}(u) - \frac{1}{uQ^2}\mathbb{A}_{4;M}^{(\psi)}(u)\right\}, \quad (51)$$

where the function $\mathbb{A}_{4;M}(u)$ is written in terms of two-particle and three-particle DAs of twist-four defined in Appendix A:

$$\mathbb{A}_{4;M}(u) = \frac{1}{4}\phi_{4M}(u) - \int_0^u d\alpha_1 \int_0^{\bar{u}} d\alpha_2 \left[\frac{1}{\alpha_3}\tilde{\Phi}_{4M}(\underline{\alpha}) + \frac{2u-1-\alpha_1+\alpha_2}{\alpha_3^2}\Phi_{4M}(\underline{\alpha})\right]\Bigg|_{\alpha_3=1-\alpha_1-\alpha_2}. \quad (52)$$

Using explicit expressions for the twist-four DAs (see Appendix A), we obtain

$$Q^2 F_{\gamma^*\gamma\to M}(Q^2) = 2\sum_{\psi=u,d,s} e_\psi^2 F_M^{(\psi)}\left\{3(1+c_{2,M}^{(\psi)}) - \frac{1}{Q^2}\left[\frac{h_M^{(\psi)}}{f_M^{(\psi)}}(2+3c_{2,M}^{(\psi)}) + \frac{80}{9}\delta_M^{2(\psi)} - \frac{h_M^{(\psi)}}{f_M^{(\psi)}}\left(\frac{67}{360}-\frac{5}{4}c_{2,M}^{(\psi)}\right) - \frac{3}{2}\frac{m_\psi f_{3M}^{(\psi)}}{f_M^{(\psi)}}\right]\right\}, \quad (53)$$

where we included, for comparison, the leading-order leading-twist contribution and ignored the scale dependence. Note the following:

(i) The end-point divergence at $u \to 0$ in the contribution of the twist-three DA $\phi_M^{(\psi)}(u)$ exactly cancels the similar divergence in the twist-four contributions that are related to twist-three operators by equations of motion; this cancellation is general and does not depend on the shape of the twist-three DAs.

(ii) Assuming the FKS mixing scheme the expression for the $1/Q^2$ correction (in square brackets) does not depend on the meson states, η or η'. Using the numbers quoted in Eqs. (26) and (35) we obtain for the ratio

$$h_M^{(s)}/f_M^{(s)} = 0.50 \pm 0.04\ \mathrm{GeV}^2, \quad (54)$$

whereas the similar ratio for the light u, d quarks is compatible with zero.

(iii) The higher-twist correction is dominated by the contribution of $\delta_M^{2(\psi)} \simeq 0.2\ \mathrm{GeV}^2$ (see Appendix A) whereas the contribution of the twist-three quark-antiquark-gluon matrix element $\sim m_s f_{3M}^{(s)}/f_M^{(s)}$ is completely negligible.

Plugging in the numbers we obtain a rough estimate of the twist-four contribution

$$F_{\gamma^*\gamma\to M}(Q^2) = \left[1 - \frac{0.9\ \mathrm{GeV}^2}{Q^2}\right] F_{\gamma^*\gamma\to M}^{\text{twist-two}}(Q^2). \quad (55)$$

This is a small correction. However, one can show that contributions of *arbitrary* twist produce a $1/Q^2$ correction as well (see a detailed discussion in [24]), indicating that the light-cone dominance of the transition form factor with one virtual and one real photon does not hold beyond leading power accuracy. An estimate of the twist-six contribution [24] results in a small positive $1/Q^2$ correction, enhanced by an additional $\ln Q^2$ factor. The mismatch of twist- and power-counting is due to the fact that to power accuracy one must consider the contributions of large light-cone distances between the currents, that are not "seen" in the twist expansion. To leading order in the QCD coupling such terms can simply be added and there is no double counting. An example of such a correction is the contribution of real photon emission at large distances calculated in Ref. [24]:

$$F_{\gamma^*\gamma\to\pi^0}(Q^2) = \frac{\sqrt{2}f_\pi}{3}\frac{16\pi\alpha_s\chi\langle\bar{q}q\rangle^2}{9f_\pi^2 Q^4} \times \int_0^1 dx\,\frac{\phi_{3;\pi}^p(x)}{x}\int_0^1 dy\,\frac{\phi_\gamma(y)}{\bar{y}^2}, \quad (56)$$

where $\phi_\gamma(y) \simeq 6y(1-y)$ is the leading-twist photon DA [52,53] and $\chi \simeq 3.5\ \mathrm{GeV}^{-2}$ (at the scale $\mu = 1$ GeV) is the magnetic susceptibility of the quark condensate [53–57]. The integrals over the quark momentum fractions in (56) are both logarithmically divergent at the end-points $x \to 0$, $y \to 1$, which signals that there is an overlap with the soft region. Such soft contributions are related to the overlap between the light-cone wave functions of the pseudoscalar meson and the real photon and can be taken into account in the framework of LCSRs described in the next section.

C. Timelike form factors

In Ref. [2] the processes $e^+e^- \to \gamma^* \to (\eta,\eta')\gamma$ were studied at a center-of-mass energy of $\sqrt{s} = 10.58$ GeV. The measurements can be interpreted in terms of the $\gamma^*\gamma \to \eta,\eta'$ FFs at remarkably high timelike photon virtuality $Q^2 = -s = -112\ \mathrm{GeV}^2$:

$$|Q^2 F_{\gamma^*\gamma\to\eta}(Q^2)|_{Q^2=-112\,\mathrm{GeV}^2} = (0.229 \pm 0.031)\,\mathrm{GeV},$$
$$|Q^2 F_{\gamma^*\gamma\to\eta'}(Q^2)|_{Q^2=-112\,\mathrm{GeV}^2} = (0.251 \pm 0.021)\,\mathrm{GeV}, \quad (57)$$

where we added the statistical and systematic uncertainties in quadrature. Note that the timelike FFs are complex numbers, whereas only the absolute value is measured.

To leading-twist accuracy, the timelike FFs can be obtained from their Euclidean (spacelike) expressions by the analytic continuation

$$Q^2 \mapsto -s - i\epsilon. \quad (58)$$

The imaginary parts arise both from the analytic continuation of the hard coefficient functions and the DAs which become complex at timelike scales $\mu^2 \sim Q^2 = -s$; see e.g. [58].

Since transition form factors are linear functions of the meson DAs, the results of the QCD calculation can be written as a sum of contributions of different Gegenbauer polynomials at the low reference scale

$$Q^2 F^{\text{twist-two}}_{\gamma^*\gamma\to\eta}(Q^2)|_{Q^2=-112\ \mathrm{GeV}^2} = 0.161\ \mathrm{GeV} + \sum_{p=q,s,g}\sum_{n=2,4,\ldots} f^{(p)}_{\eta;n} c^{(p)}_n(\mu_0^2),$$
$$Q^2 F^{\text{twist-two}}_{\gamma^*\gamma\to\eta'}(Q^2)|_{Q^2=-112\ \mathrm{GeV}^2} = 0.241\ \mathrm{GeV} + \sum_{p=q,s,g}\sum_{n=2,4,\ldots} f^{(p)}_{\eta';n} c^{(p)}_n(\mu_0^2), \quad (59)$$

where the asymptotic DA contributions are almost the same in the timelike and spacelike regions, and the coefficients $f^{(p)}_{M;n} \equiv f^{(p)}_{M;n}(Q^2/\mu^2, \alpha_s(\mu^2); \mu_0^2)$ absorb all dependence on Q^2. Numerical values of these coefficients with the choice of factorization scale $\mu^2 = Q^2$, continued analytically to the timelike values $Q^2 = -s$, are presented for η and η' mesons in comparison with the corresponding spacelike coefficients for $n = 2, 4$ in Table I. Note that the Gegenbauer coefficients at the low scale $c^{(p)}_n(\mu_0)$ do not depend on the type of the meson—η or η'—by assumption of the FKS state mixing. For this calculation we have taken the set of parameters in Eq. (26). The given numbers correspond to the choice of the scale $\mu^2 = Q^2$; they change by at most 10% if the scale is varied in the interval $Q^2/2 < \mu^2 < 2Q^2$.

We see that the coefficients of higher Gegenbauer polynomials are in general rather small, which is due to suppression by the anomalous dimensions. These coefficients acquire rather large phases; however, for realistic values of the Gegenbauer coefficients $c^{(q)}_{2,4} \sim c^{(s)}_{2,4} \approx 0.1-0.2$ the corresponding contributions to the FF appear to be marginal as compared to the leading terms in (59). Thus the overall phase is small and the absolute values of the FF in the spacelike and timelike regions remain close to each other. This result is in agreement with the conclusion in [58] that perturbative corrections cannot generate a significant difference between the spacelike and timelike transition FFs.

Beyond the leading power accuracy the situation is less clear. Note that the overall $1/Q^2$ correction to the spacelike transition form factors is negative (this can be shown in many ways; see, e.g. [24,25]) and by virtue of the sign change in Q^2 one expects a positive correction to the timelike form factors if the analytic continuation is justified to power accuracy which is, however, not obvious. The higher-twist contributions corresponding to less singular terms in the light-cone expansion of the product of the two electromagnetic currents are small and tend to have alternating signs; cf. the discussion in the previous section. They are unlikely to play any role at $|Q^2| \sim 100\ \mathrm{GeV}^2$. The soft contributions can, however, be significant.

Within the LCSR approach to soft contributions discussed in the next section, their magnitude is correlated with the shape of the leading-twist DA: broader DAs generally lead to larger soft corrections and vice verse. A rough estimate (69) gives

$$Q^2 F_{\gamma^*\gamma\to\eta}(Q^2) \simeq Q^2 F^{\mathrm{QCD}}_{\gamma^*\gamma\to\eta}(Q^2)\left[1 - \frac{(3\text{–}7)\ \mathrm{GeV}^2}{Q^2}\right], \quad (60)$$

where the larger number corresponds to a broad DA of the type [24] required to describe the *BABAR* data [3] on $\gamma^*\gamma \to \pi^0$, and the smaller one is obtained for the asymptotic DA. Assuming that the soft correction changes sign in the timelike region, we conclude that the difference between the timelike and spacelike form factors at $|Q^2| = 112\ \mathrm{GeV}^2$ can be of the order of ~5%–13% for

TABLE I. Coefficients (59) of the contributions of different Gegenbauer polynomials in the expansion of DAs to the transition form factors at the timelike $Q^2 = -s = -112\ \mathrm{GeV}^2$, assuming validity of the FKS mixing scheme (26) at the low scale $\mu_0 = 1$ GeV. The corresponding spacelike coefficients for $Q^2 = 112\ \mathrm{GeV}^2$ are also given for comparison. All numbers in units of GeV.

Meson	Scale	$f_2^{(q)}$	$f_2^{(s)}$	$f_2^{(g)}$	$f_4^{(q)}$	$f_4^{(s)}$	$f_4^{(g)}$
η	spacelike	0.126	−0.037	0.010	0.105	−0.030	0.006
	timelike	0.113 + 0.032i	−0.033 − 0.009i	0.011 − 0.001i	0.086 + 0.039i	−0.025 − 0.011i	0.006 + 0.001i
η'	spacelike	0.103	0.045	0.061	0.086	0.037	0.037
	timelike	0.093 + 0.026i	0.040 + 0.011i	0.069 − 0.005i	0.070 + 0.032i	0.030 + 0.014i	0.040 + 0.005i

the "narrow" and "broad" meson DA, respectively. This difference can further be enhanced by Sudakov-type corrections; see the discussion in [58] and references therein.

It is interesting that the experimental result for $\gamma^*\gamma \to \eta'$ at $Q^2 = -112\ \mathrm{GeV}^2$ [2] is very close to the contribution of the asymptotic η' meson DA in Eq. (59), whereas the asymptotic contribution to $\gamma^*\gamma \to \eta$ is almost 50% below the data; cf. (57). This result urgently needs verification. If correct, it can probably only be explained by much larger soft contributions such as a much broader DA of the η meson as compared to η', which would be in conflict with the state mixing approximation for DAs.

IV. LIGHT-CONE SUM RULES

The LCSR approach was proposed in [52,59–61] and adapted for the present situation in [62]. This technique is well known and has been used repeatedly for $\gamma^*\gamma \to \pi^0$ [24,25,63–70] so that in what follows we will only give a short introduction and present the necessary NLO expressions, generalized and/or adapted for the case of $\eta^{(\prime)}$ mesons.

The idea is to consider a more general transition FF for two nonvanishing photon virtualities, $q_1^2 = -Q^2$ and $q_2^2 = -q^2$, and perform the analytic continuation to the real photon limit $q^2 = 0$ employing dispersion relations.

On the one hand, $F_{\gamma^*\gamma^*\to M}(Q^2, q^2)$ satisfies an unsubtracted dispersion relation in the variable q^2 for fixed Q^2. Separating the contribution of the lowest-lying vector mesons ρ, ω we can write

$$F_{\gamma^*\gamma^*\to M}(Q^2, q^2) = \frac{\sqrt{2} f_\rho F_{\gamma^*\rho\to M}(Q^2)}{m_\rho^2 + q^2} + \frac{1}{\pi}\int_{s_0}^{\infty} ds \frac{\mathrm{Im} F_{\gamma^*\gamma^*\to M}(Q^2, -s)}{s + q^2}, \quad (61)$$

where s_0 is some effective threshold. Here, the ρ and ω contributions are combined in one resonance term assuming $m_\rho \simeq m_\omega$ and the zero-width approximation is used; $f_\rho \sim 200$ MeV is the usual vector meson decay constant. Note that since there are no massless states, the real photon limit is recovered by the simple substitution $q^2 \to 0$ in (61).

On the other hand, the same FF can be calculated using QCD perturbation theory and the operator product expansion (OPE). The QCD result obeys a similar dispersion relation

$$F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, q^2) = \frac{1}{\pi}\int_0^{\infty} ds \frac{\mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s)}{s + q^2}. \quad (62)$$

The basic assumption, usually referred to as quark-hadron duality, is that the physical spectral density above the threshold $s > s_0$ coincides with the QCD spectral density as given by the OPE:

$$\mathrm{Im} F_{\gamma^*\gamma^*\to M}(Q^2, -s) = \mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s). \quad (63)$$

This equality has to be understood in the sense of distributions, with both sides integrated with a smooth test function.

Equating the two representations in (61) and (62) at $q^2 \to -\infty$ and subtracting the contributions of $s > s_0$ from both sides one obtains

$$\sqrt{2} f_\rho F_{\gamma^*\rho\to M}(Q^2) = \frac{1}{\pi}\int_0^{s_0} ds \mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s). \quad (64)$$

This relation explains why s_0 is usually referred to as the interval of duality. The perturbative QCD spectral density $\mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s)$ is a smooth function and does not vanish at small $s \to 0$. It is very different from the physical spectral density $\mathrm{Im} F_{\gamma^*\gamma^*\to M}(Q^2, -s) \sim \delta(s - m_\rho^2)$. However, the integral of the QCD spectral density over a certain region of energies coincides with the integral of the physical spectral density over the same region; in this sense the QCD description of correlation functions in terms of quark and gluons is dual to the description in terms of hadronic states.

In practical applications of this method one uses a trick borrowed from QCD sum rules [71], to reduce the sensitivity to the duality assumption in Eq. (63) and also to suppress contributions arising from higher order terms in the OPE. To this end one attempts to match the "true" and calculated FF at a finite value $q^2 \sim 1$–$2\ \mathrm{GeV}^2$ instead of the $q^2 \to \infty$ limit. This is done by going over to the Borel representation $1/(s + q^2) \to \exp[-s/M^2]$, the final effect being the appearance of an additional weight factor under the integral

$$\sqrt{2} f_\rho F_{\gamma^*\rho\to M}(Q^2) = \frac{1}{\pi}\int_0^{s_0} ds e^{-(s - m_\rho^2)/M^2} \times \mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s). \quad (65)$$

Varying the Borel parameter within a certain window one may test the sensitivity of the results to a chosen model for the spectral density.

With this refinement, substituting Eq. (65) in (61) and using Eq. (63) we obtain for $q^2 \to 0$

$$F^{\mathrm{LCSR}}_{\gamma^*\gamma\to M}(Q^2) = \frac{1}{\pi}\int_0^{s_0} \frac{ds}{m_\rho^2} \mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s) e^{(m_\rho^2 - s)/M^2} + \frac{1}{\pi}\int_{s_0}^{\infty} \frac{ds}{s} \mathrm{Im} F^{\mathrm{QCD}}_{\gamma^*\gamma^*\to M}(Q^2, -s). \quad (66)$$

This expression contains two nonperturbative parameters, the vector meson mass m_ρ^2, and the effective threshold $s_0 \simeq 1.5\ \mathrm{GeV}^2$, as compared to the "pure" QCD calculations.

Taking into account Eq. (62) one can rewrite the same result as

$$F^{\rm LCSR}_{\gamma^*\gamma\to M}(Q^2) = F^{\rm QCD}_{\gamma^*\gamma\to M}(Q^2) + \frac{1}{\pi}\int_0^{s_0}\frac{ds}{m_\rho^2}\left[e^{(m_\rho^2-s)/M^2} - \frac{m_\rho^2}{s}\right] \times {\rm Im}F^{\rm QCD}_{\gamma^*\gamma^*\to M}(Q^2,-s), \quad (67)$$

separating the result of a "pure" QCD calculation and the correction.

To get an impression of how this modification affects the QCD result, we insert the leading-order and leading-twist expression for ${\rm Im}F^{\rm QCD}_{\gamma^*\gamma^*\to M}(Q^2,-s)$ and rewrite the dispersion integral in terms of a variable $x = Q^2/(s+Q^2)$ that corresponds to the fraction of the meson momentum carried by the interacting quark:

$$F^{\rm LCSR}_{\gamma^*\gamma\to M}(Q^2) = \sum_{i=1,8} C^i f_M^{(i)}\frac{1}{Q^2}\left[\int_0^1\frac{dx}{\bar x}\phi_M^{(i)}(x) + \int_{x_0}^1\frac{dx}{\bar x}\left(\frac{\bar x Q^2}{x m_\rho^2}e^{\frac{x m_\rho^2-\bar x Q^2}{x M^2}} - 1\right)\phi_M^{(i)}(x)\right], \quad (68)$$

where $C^1 = \frac{4}{3\sqrt{3}}$, $C^8 = \frac{2}{3\sqrt{6}}$, $\bar x = 1-x$ and $x_0 = \frac{Q^2}{s_0+Q^2}$. The first contribution is the LO perturbative result while the second part represents the soft end-point correction from the region $x > x_0 = 1 - \mathcal{O}(s_0/Q^2)$, due to the modification of the spectral density in the LCSR framework.

For a rough estimate of the soft correction we expand the integrand for small $1-x_0$

$$F^{\rm LCSR}_{\gamma^*\gamma\to M}(Q^2) \approx \sum_{i=1,8} C^i f_M^{(i)}\frac{1}{Q^2}\left[\int_0^1\frac{dx}{\bar x}\phi_M^{(i)}(x) + \bar x_0\left(\frac{s_0}{2m_\rho^2}e^{\frac{m_\rho^2-s_0}{M^2}} - 1\right)\phi_M^{\prime(i)}(0)\right], \quad (69)$$

where $\phi_M^{\prime(i)}(0) \equiv (d/dx)\phi_M^{(i)}(x)|_{x=0}$ and we assumed that the DA vanishes linearly at the end points. Using

$$\phi_M^{\prime(i)}(0) = 3\left[2 + \sum_{n=2,4,\ldots}(n+1)(n+2)c_n^{(i)}\right],$$

$$\int_0^1\frac{dx}{\bar x}\phi_M^{(i)}(x) = 3\left[1 + \sum_{n=2,4,\ldots}c_n^{(i)}\right],$$

and assuming that the numerical values of the Gegenbauer moments for the singlet and octet DAs are the same, we arrive at the estimate in Eq. (60).

A. Twist-two contribution

For our purposes it is convenient to write the required imaginary part of $F^{\rm QCD}_{\gamma^*\gamma^*\to M}(Q^2,q^2)$ as a sum of terms corresponding to the expansion of the meson DAs $\phi_M(x,\mu)$ in Gegenbauer polynomials. The twist-two quark components of the spectral densities with NLO accuracy can be obtained from relevant expressions presented in our work [24]. Thus we write, for the flavor-octet contribution,

$$\frac{1}{\pi}{\rm Im}F^{\rm QCD(8)}_{\gamma^*\gamma^*\to M}(Q^2,-s) = \frac{f_M^{(8)}}{3\sqrt{6}}\sum_{n=0}^{\infty}c_{n,M}^{(8)}(\mu)\left[\rho_n^{(0)}(Q^2,s) + \frac{C_F\alpha_s}{2\pi}\rho_n^{(1)}(Q^2,s;\mu)\right]. \quad (70)$$

The LO partial spectral density is proportional to the meson DA

$$\rho_n^{(0)}(Q^2,s) = \frac{2\varphi_n(x)}{Q^2+s}, \qquad \varphi_n(x) = 6x\bar x C_n^{3/2}(2x-1), \quad (71)$$

where $x = Q^2/(Q^2+s)$.

The NLO spectral density can be written in the following form:

$$\rho_n^{(1)}(Q^2,s;\mu) = \frac{1}{Q^2+s}\left\{\left\{-3[1+2(\psi(2)-\psi(2+n))] + \frac{\pi^2}{3} - \ln^2\left(\frac{\bar x}{x}\right) - \frac{\gamma_n^{(0)}}{C_F}\ln\left(\frac{s}{\mu^2}\right)\right\}\varphi_n(x) + \frac{\gamma_n^{(0)}}{C_F}\int_0^{\bar x}du\frac{\varphi_n(u)-\varphi_n(\bar x)}{u-\bar x} - \left[\int_x^1 du\frac{\varphi_n(u)-\varphi_n(x)}{u-x}\ln\left(1-\frac{x}{u}\right) + (x\to\bar x)\right]\right\}, \quad (72)$$

where $\gamma_n^{(0)}$ is the flavor-nonsinglet LO anomalous dimension (B6).

The flavor-singlet quark contribution can be written similarly as

$$\frac{1}{\pi}{\rm Im}F^{\rm QCD(1)}_{\gamma^*\gamma^*\to M}(Q^2,-s) = \frac{2f_M^{(1)}}{3\sqrt{3}}\sum_{n=0}^{\infty}c_{n,M}^{(1)}(\mu)\left[\rho_n^{(0)}(Q^2,s) + \frac{C_F\alpha_s}{2\pi}\rho_n^{(1)}(Q^2,s;\mu)\right] \quad (73)$$

with the same functions $\rho_n^{(0)}(Q^2,s)$ and $\rho_n^{(1)}(Q^2,s;\mu)$, the difference being encoded in the decay constants $f_M^{(i)}$, the expansion coefficients $c_{n,M}^{(i)}$ and numerical factors.

In order to find the contribution of the gluon DA one has to calculate the relevant Feynman diagrams (Fig. 1) for light quarks in the loop and two nonzero photon virtualities, Q^2 and q^2. One obtains, omitting the factor $C_F\alpha_s/4\pi$,

$$T_H^g|_{\rm light}(u,Q^2,q^2) = -\frac{1}{u^2\bar u^2(Q^2-q^2)^2}\left\{Q^2u^2\ln\left(\frac{uQ^2+\bar uq^2}{Q^2}\right)\left[\ln\left(\frac{uQ^2+\bar uq^2}{\mu^2}\right)+\ln\left(\frac{Q^2}{\mu^2}\right)\right]\right.$$
$$-q^2\bar u^2\ln\left(\frac{uQ^2+\bar uq^2}{q^2}\right)\left[\ln\left(\frac{uQ^2+\bar uq^2}{\mu^2}\right)+\ln\left(\frac{q^2}{\mu^2}\right)\right]$$
$$\left.+2\left[Q^2u(3\bar u-2)\ln\left(\frac{uQ^2+\bar uq^2}{Q^2}\right)+q^2\bar u(2-3u)\ln\left(\frac{uQ^2+\bar uq^2}{q^2}\right)\right]\right\}. \tag{74}$$

It is not difficult to verify that the result in (74) reproduces the known expression (46) in the limit $q^2\to 0$. The corresponding contribution to the spectral density reads, replacing $q^2\to -s$,

$$\frac{1}{\pi}{\rm Im}T_H^g|_{\rm light}(u,Q^2,-s) = -\frac{2x}{Q^2}\left\{\frac{1}{u^2\bar u^2}\left[\Theta(u-x)\left[(x\bar u^2+\bar xu^2)\ln\left(1-\frac{\bar u}{\bar x}\right)+u\bar u\right]\right]\right.$$
$$\left.+\left[\Theta(u-x)\frac{x}{u^2}-\Theta(x-u)\frac{\bar x}{\bar u^2}\right]\left[\ln\frac{Q^2}{\mu^2}+\ln\frac{\bar x}{x}-2\right]\right\}. \tag{75}$$

A recalculation of the heavy c-quark contribution is not needed since the corresponding spectral density is not affected by the LCSR modification. Thus the result in Eq. (47) obtained for $q^2=0$ can be used as it stands.

The contributions of different Gegenbauer polynomials in the expansion of the two-gluon DA

$$\omega_n(u) = 30u^2\bar u^2C_{n-1}^{5/2}(2u-1) \tag{76}$$

defined as

$$\rho_n^g(Q^2,s;\mu) = \frac{1}{\pi}\int_0^1 du{\rm Im}T_H^g|_{\rm light}(u,Q^2,-s)\omega_n(u), \tag{77}$$

can readily be computed from the above expressions. We obtain for $n=2$ and $n=4$:

$$\rho_2^g(Q^2,s,\mu) = \frac{5x}{Q^2}\left[-\frac{{}^{gq}\gamma_2^{(0)}}{C_F}\left(\ln\frac{\bar xQ^2}{x\mu^2}-2\right)\varphi_2(x)+\frac{5}{6}\bar x^2(65x^2-30x+1)\right],$$
$$\rho_4^g(Q^2,s,\mu) = \frac{5x}{Q^2}\left[-\frac{{}^{gq}\gamma_4^{(0)}}{C_F}\left(\ln\frac{\bar xQ^2}{x\mu^2}-2\right)\varphi_4(x)+\frac{14}{15}\bar x^2(1827x^4-2457x^3+959x^2-105x+1)\right], \tag{78}$$

where $\varphi_n(x)$ are defined in (71) and the respective quark-gluon mixing anomalous dimension appears, because the coefficient of $\ln Q^2/\mu^2$ in (75) is just the evolution kernel $V^{qg}(x,u)$.

Collecting all factors, the final expression for the contribution of the light quark box diagrams to the spectral density takes the following form:

$$\frac{1}{\pi}{\rm Im}F^{\rm QCD(g)}_{\gamma^*\gamma^*\to M}(Q^2,-s) = \frac{2f_M^{(1)}}{3\sqrt{3}}\sum_{n=2}^{\infty}c_{n,M}^{(g)}(\mu)\frac{C_F\alpha_s}{2\pi}\rho_n^g(Q^2,s;\mu). \tag{79}$$

As mentioned above, the contribution of charm quarks does not need to be written in this form as it is not affected by the LCSR subtraction.

B. Higher-twist and meson mass corrections

The bulk of the higher-twist corrections corresponding to the contributions of two-particle and three-particle twist-four DAs can be taken into account using the expressions given in Ref. [24] with the substitution of pion DAs by their η,η' counterparts. The latter have been studied previously in [34,35] but, as we found, the results given there are not complete. The corresponding update is presented in Appendix A. We take into account quark mass corrections in the relations between different matrix elements imposed by QCD equations of motion (EOM) and also consider, for the first time, anomalous contributions to the flavor-singlet twist-four DAs.

In addition, one has to take into account the contribution of the twist-three DA, which appears due to the non-vanishing strange quark mass, and an extra meson mass correction $\sim m_M^2$ coming from the expansion of the leading-order amplitude.

In the expressions given below we collect the results for the spectral densities for the higher-twist contributions defined as

$$\rho_M^{(i)} = \frac{1}{\pi}{\rm Im}F^{{\rm QCD}(i)}_{\gamma^*\gamma^*\to M}(Q^2,-s). \tag{80}$$

The superscript $i=m,3,4$ corresponds to the meson mass, twist-three DA, and twist-four DA contributions, respectively. All higher-twist contributions can most conveniently be written as a sum of contributions of different quark flavors

$$\rho_M^{(i)}(Q^2,s) = 2e_s^2\rho_M^{(i),s}(Q^2,s) + \sqrt{2}(e_u^2+e_d^2)\rho_M^{(i),q}(Q^2,s). \tag{81}$$

The rewriting in terms of the parameters in the FKS scheme is then done using Eqs. (23) and (36) for the leading twist and the same transformation rules for the higher-twist matrix elements $f_{3M}^{(a)}$ and $f_M^{(a)}\delta_M^{2(a)}$ where $a = q, s$.

The meson mass correction to the contribution of the nth Gegenbauer term in the expansion of the leading-twist DA, cf. (70), takes the form

$$\rho_{M,n}^{(m),a}(Q^2,s) = \frac{x^2}{Q^4}h_M^a\left(\xi_x\varphi_n(x) - x\bar{x}\frac{d}{dx}\varphi_n(x)\right). \tag{82}$$

Here we used a shorthand notation

$$\xi_x = 2x - 1$$

and made a substitution $m_M^2 f_M^{(a)} \to h_M^{(a)}$ motivated in Appendix A, Eq. (A35), for consistency with the calculation of twist-four contributions.

The contribution of the twist-three DA to NLO accuracy in the conformal expansion reads

$$\rho_M^{(3),a}(Q^2,s) = -\frac{x^2}{Q^4}(h_M^a\xi_x + 60m_a f_{3M}^a C_3^{1/2}(2x-1)), \tag{83}$$

and the twist-four contribution, to the same accuracy, can be brought into the form

$$\begin{aligned}\rho_M^{(4),a}(Q^2,s) = -\frac{x^2\xi_x}{Q^4}\Bigg\{&\frac{160}{3}f_M^a(\delta_M^a)^2 x\bar{x}\\ &+ m_a f_{3M}^a[60 - 210x\bar{x}(3 - x\bar{x})]\\ &+ h_M^a\left[1 - x\bar{x}\left(\frac{13}{6} - \frac{21}{2}x\bar{x}\right)\right.\\ &\left.+ c_{2M}^{(a)}x\bar{x}(21 - 135x\bar{x})\right]\Bigg\}.\end{aligned} \tag{84}$$

In all expressions $a = q, s$ and $x = Q^2/(s + Q^2)$.

The twist-six contributions to the $\gamma^*\gamma \to \pi^0$ transition FF have been calculated in the factorization approximation in Ref. [24]. The extension of these results to $\gamma^*\gamma \to \eta, \eta'$ is not immediate as in order to include $SU(3)$ flavor violation effects we would have to recalculate all the diagrams keeping terms linear in the quark masses. These would lead in the factorization approximation to contributions proportional to the twist-two distribution amplitude times quark condensate. We postpone this calculation to a forthcoming publication and prefer to neglect the twist-six contributions altogether since at this level we would only be able to include them consistently for the octet but not the singlet. Neglecting them amounts to an additional uncertainty at the level of 2%–3% and we will see that neither theoretical nor experimental precision are up to now sufficient to make these terms relevant.

V. NUMERICAL ANALYSIS

A. Sum rule parameters

All numerical results in this work are obtained using the two-loop running QCD coupling with $\Lambda_{\rm QCD}^{(4)} = 326$ MeV and $n_f = 4$ active flavors. Validity of the FKS mixing scheme for the DAs is assumed at the renormalization scale $\mu_0 = 1$ GeV, $\alpha_s(\mu_0) = 0.494$. Unless stated otherwise, we use the set of FKS parameters specified in Eq. (26). All given values of nonperturbative parameters refer to the same scale $\mu_0 = 1$ GeV.

A natural factorization and renormalization scale μ in the calculation of the meson transition FFs with two large photon virtualities is given by the virtuality of the quark propagator $\mu^2 \sim \bar{x}Q^2 + xq^2$. If $q^2 \to 0$, in the LCSR framework the relevant factorization scale becomes $\mu^2 \sim \bar{x}Q^2 + xM^2$ or $\mu^2 \sim \bar{x}Q^2 + xs_0$ if $M^2 \gg s_0$; see e.g. [72]. Note that the restriction $s < s_0$ in the first integral in (66) translates to $\bar{x} < s_0/(s_0 + Q^2)$ and hence the quark virtuality remains finite $\mu^2 \simeq 2s_0$ as $Q^2 \to \infty$, in agreement with the interpretation of this term as the "soft" contribution. Using the x-dependent factorization scale is inconvenient so that we replace x by the average $\langle x\rangle$ which is varied within a certain range:

$$\mu^2 = \langle\bar{x}\rangle Q^2 + \langle x\rangle s_0, \qquad 1/4 < \langle x\rangle < 3/4. \tag{85}$$

The choice of the Borel parameter in LCSRs is discussed in [73,74]. The difference to the classical QCD sum rules is that the twist expansion in LCSRs goes in powers of $1/(xM^2)$ rather than $1/M^2$. Hence one has to use somewhat larger values of M^2 compared to the QCD sum rules for two-point correlation functions in order to ensure the same hierarchy of contributions. We choose as the "working window"

$$1 < M^2 < 2\ \text{GeV}^2 \tag{86}$$

and $M^2 = 1.5\ \text{GeV}^2$ as the default value in our calculations.

We use the standard value $s_0 = 1.5\ \text{GeV}^2$ for the continuum threshold, and the range

$$1.3 < s_0 < 1.7\ \text{GeV}^2 \tag{87}$$

in the error estimates. We did not attempt to consider corrections due to the finite width of the ρ, ω resonances.

The estimates in Ref. [68] suggest that such corrections may result in an enhancement of the form factor by 2%–4% in the small-to-medium Q^2 region where the resonance part dominates. We believe that such uncertainties are effectively covered by our (conservative) choice of the continuum threshold.

Finally, we use the values of the twist-three parameters h_q and h_s [43] specified in Eq. (35), and also use $\delta_M^{2(q)} = \delta_M^{2(s)} = 0.2 \pm 0.04\ \text{GeV}^2$ [65,75] (at the scale 1 GeV) for the normalization parameter for twist-four DAs (A7).

B. Models of DAs and comparison with the data

The LCSR calculation of the FFs is compared with the experimental data [1,42] in Fig. 3. The dependence of the results on the Borel parameter, continuum threshold, normalization of the higher-twist contributions and, to a lesser extent, the factorization scale, can be viewed as an intrinsic irreducible uncertainty of the LCSR method. This uncertainty is shown in the figures by the dark blue bands.

In this work we use the FKS mixing scheme [11] as the simplest working hypothesis that allows one to reduce the

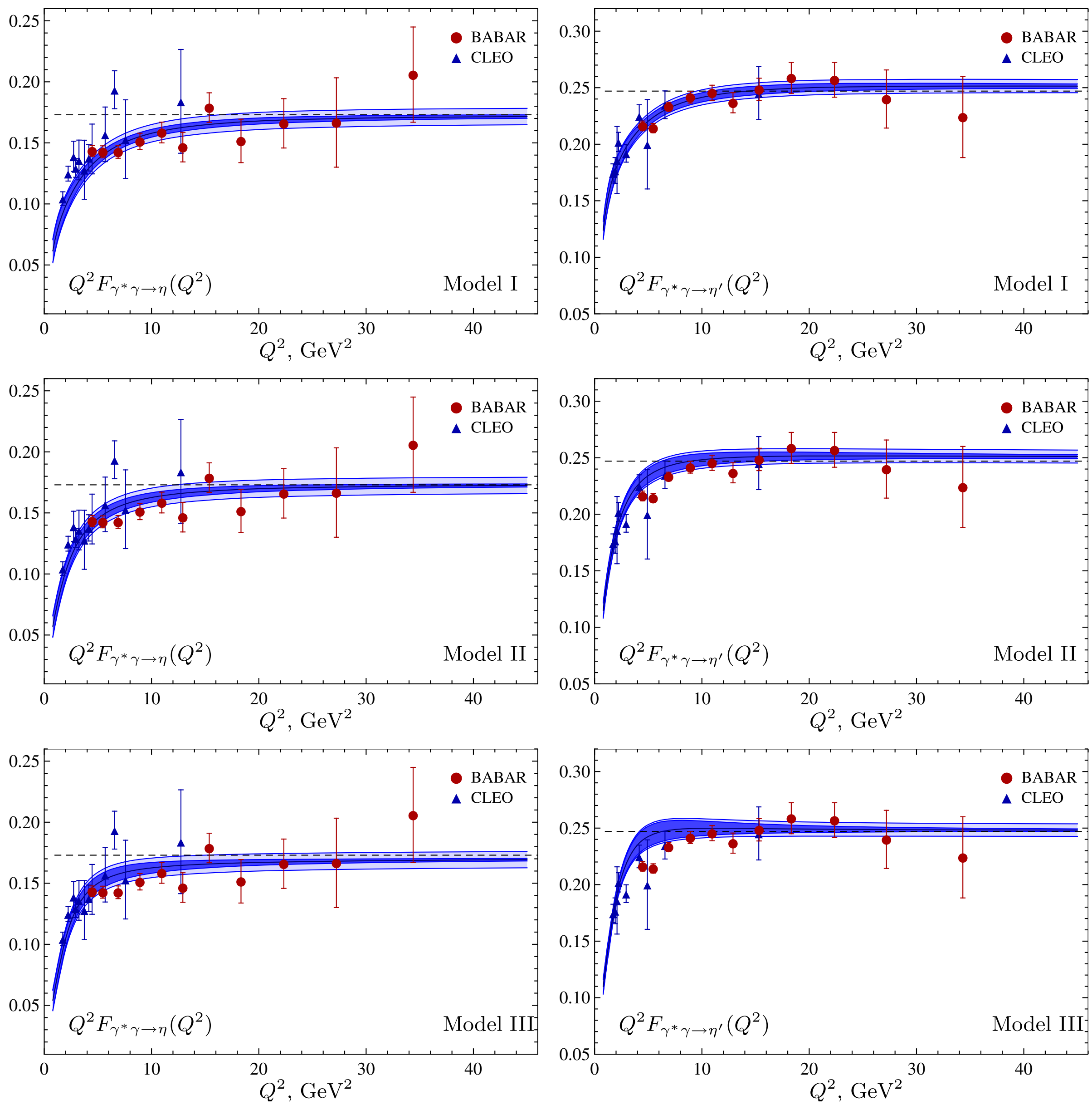

FIG. 3 (color online). Transition form factors $\gamma^*\gamma \to \eta$ (left panels) and $\gamma^*\gamma \to \eta'$ (right panels) [1,42] compared to the LCSR calculation with three models of the leading-twist DAs specified in Table II. Asymptotic values at large photon virtualities (50) corresponding to the central values of the FKS parameters in Eq. (26) are shown by the horizontal dashed lines. The dark blue shaded areas correspond to uncertainties of the calculation due to the choice of the LCSR parameters M^2 and s_0, factorization scale μ, and the higher-twist parameters $h^{(q,s)}, \delta^{2(q,s)}$; see text. The light blue areas are obtained by adding the uncertainties in the FKS parameters, Eq. (26).

number of parameters, assuming that it holds for complete wave functions, and therefore also for the DAs, at an *ad hoc* low scale $\mu_0 = 1$ GeV. The error bands corresponding to adding the uncertainties of the FKS parameters as given in Eq. (26) to the LCSR uncertainties specified above is shown by light blue bands. We assume that all errors are statistically independent and add them in quadrature. We expect that the bulk of these uncertainties will be eliminated in the future by using first-principle lattice calculations of the couplings f_η, $f_{\eta'}$ that are not bound to any mixing scheme.

Asymptotic values of the form factors for large photon virtuality for the central values of the FKS parameters in Eq. (26) are shown by the horizontal dashed lines; cf. Eq. (50). The asymptotic value for $\gamma^*\gamma \to \eta'$ differs considerably from the one assumed in [1,6,27], which is an effect of the finite renormalization correction to the flavor-singlet contribution; see Eq. (49). Note that experimental measurements for both η and η' FFs at large virtualities are consistent with the expected asymptotic behavior.

The remaining nonperturbative input in the calculations is provided by the shape parameters of the DAs. We do not view this dependence as "uncertainty." Indeed, on the one hand, extraction of the information about DAs is the primary motivation behind the studies of transition form factors. On the other hand, lowest nontrivial moments of DAs can also be studied in lattice QCD [76,77]. Such calculations are ongoing and the corresponding parameters will eventually be known to a sufficient precision.

In the FKS approximation the remaining information about the DAs is encoded in three constants, $c_n^{(q)}(\mu_0)$, $c_n^{(s)}(\mu_0)$, and $c_n^{(g)}(\mu_0)$, for each Gegenbauer moment $n = 2, 4$, etc. The nonstrange coefficients, $c_n^{(q)}(\mu_0)$, should be similar to the corresponding coefficients for the pion DA. Unfortunately the situation with the pion DA is far from being settled. Direct calculations using QCD sum rules and lattice simulations do not have sufficient accuracy so far, whereas the constraints from the experimental data on the $\gamma^*\gamma \to \pi^0$ FF are inconclusive because of the discrepancy between the *BABAR* and Belle measurements [3,4]. A detailed discussion can be found in [24,25].

Because of this uncertainty, we present the results for three different models of the DAs specified in Table II where the coefficients $c_n^{(q)}(\mu_0)$ are chosen in the range that corresponds to popular models for the pion DA, the $SU(3)$ breaking in these parameters is neglected (see below), and the gluon coefficients are fitted to describe the data. The first model corresponds to the pion DA used in Ref. [25] to describe the Belle data [4] (truncated to $n = 2, 4$), the second (simplest) model corresponds to a typical ansatz used in vast literature on the weak $B \to \pi$ decays, and the third model with a negative $n = 4$ coefficient is advocated by the Bochum-Dubna group; see e.g. [69] and references therein.

TABLE II. Gegenbauer coefficients of three sample models of the leading-twist DAs [u, d quarks (q), s quarks (s), and gluons (g)] at the scale $\mu_0 = 1$ GeV; cf. Fig. 3.

Model	$c_2^{(q)}$	$c_2^{(s)}$	$c_4^{(q)}$	$c_4^{(s)}$	$c_2^{(g)}$
I	0.10	0.10	0.10	0.10	−0.26
II	0.20	0.20	0.0	0.0	−0.31
III	0.25	0.25	−0.10	−0.10	−0.25

On general grounds one expects [78] that the DAs of hadrons containing strange quarks are more narrow than those built of u, d quarks, i.e.

$$c_n^{(s)}(\mu_0) < c_n^{(q)}(\mu_0); \tag{88}$$

however, existing numerical estimates of this effect are rather uncertain. QCD sum rule calculations (see e.g. [34,35]) and lattice calculations [76,77] do not seem to indicate any large difference so that we have assumed $c_n^{(s)}(\mu_0) = c_n^{(q)}(\mu_0)$ for the present study. Setting instead $c_n^{(s)}(\mu_0) = 0$, which is probably extreme, the FF $\gamma^*\gamma \to \eta$ gets increased by 5%–6% and the FF $\gamma^*\gamma \to \eta'$ decreases by 4%–5% for $Q^2 > 5$ GeV^2 as compared to the results shown in Fig. 3.

The gluon DA mainly contributes to the η' FF, whereas its effect on the η is small. To illustrate this dependence we show in Fig. 4 the results of the calculation with $c_2^{(q)} = c_4^{(q)} = 0.1$ and $c_2^{(g)} = 0$ corresponding to model I with gluon contribution put to zero (blue curve), and the shaded area in light green obtained by varying $c_2^{(g)}$ in the range $-0.5 < c_2^{(g)} < 0.5$. Note that the gluon DA contribution is significantly enhanced (by a factor 5/3 for large Q^2) by including the c-quark contribution, which is one of the new elements of our analysis.

The three models in Table II lead to an equally good description of the experimental data at large $Q^2 >$ 10–15 GeV^2 but differ at smaller Q^2 where model I seems to be preferred. Unfortunately, the uncertainties of the calculation also increase in this region, especially for model III which suffers from a stronger dependence on the Borel parameter. For this reason we think that none of the considered models can be excluded and, also in the future, the experimental data on transition FFs alone will not be sufficient to pin down the shape of DAs. One needs a combined effort of theory and experiment, supplementing FF data with lattice calculations of at least a few key parameters.

Finally, in Fig. 5 we show the same results on a logarithmic scale in Q^2, where we have also included the timelike momentum transfer data point [2] at $|Q^2| =$ 112 GeV^2 (red stars) for comparison.

One sees that the measurement of $e^+e^- \to \gamma^* \to \eta'\gamma$ appears to be in good agreement with the expected

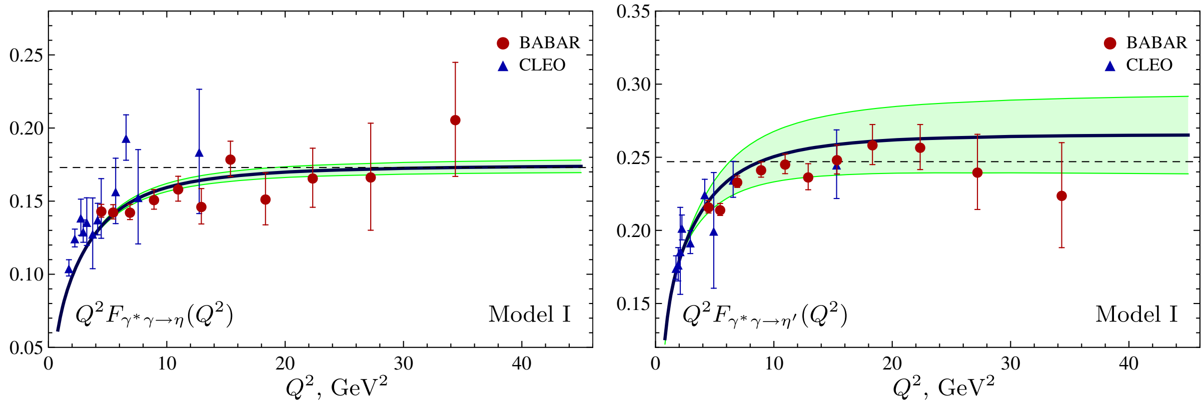

FIG. 4 (color online). Same as in Fig. 3 for the first model of the leading-twist DAs specified in Table II except for the normalization parameter of the gluon DA $c_2^{(g)}$ which is set to zero. The shaded area in light green shows the effect of the variation of this parameter in the range $c_2^{(g)} = \pm 0.5$.

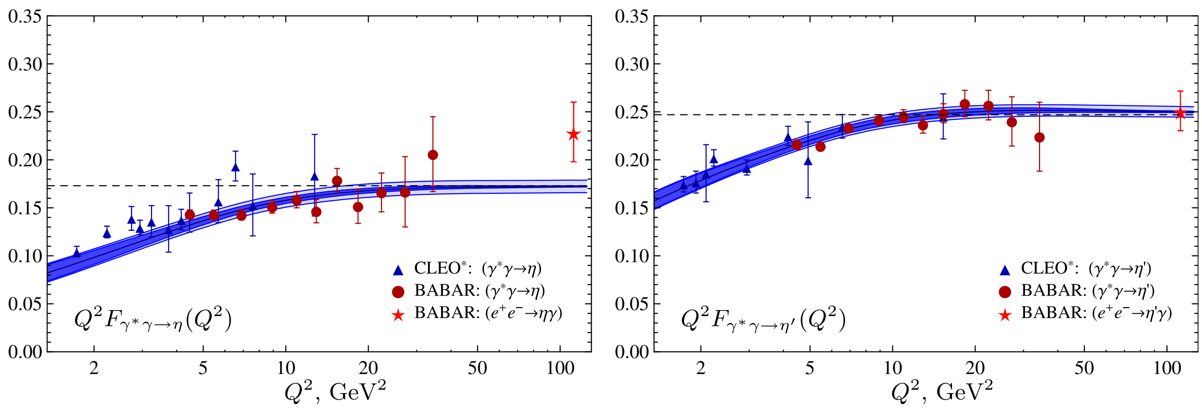

FIG. 5 (color online). Same as in Fig. 3 using a logarithmic scale in Q^2. The calculation uses the first model of the leading-twist DAs specified in Table II. The timelike data point [2] at $|Q^2| = 112$ GeV^2 is shown by red stars for comparison.

asymptotic behavior in the spacelike region, whereas the result for $e^+e^- \to \gamma^* \to \eta\gamma$ is considerably higher. This difference is interesting and surprising. The Sudakov enhancement of the timelike FFs as compared to their spacelike conterparts, usually quoted in this context, is universal and should affect both η and η' production equally strongly. As already discussed in Sec. III. C, the large difference can only be attributed to nonperturbative corrections corresponding to the soft (end-point) integration regions. Although a rigorous connection of such contributions to the DAs does not exist, one can plausibly argue that large soft corrections are correlated with the end-point enhancements in the DAs, of the type that have been discussed in connection with the large scaling violation in the $\gamma^*\gamma \to \pi^0$ form factor reported in [3]. For this reason we expect that, if the large value of the timelike form factor for the η meson is confirmed, the corresponding spacelike form factor should exhibit the similar scaling violating behavior as observed by *BABAR* for the pion. In fact the existing data may support such a trend, see Fig. 5, although it is not statistically significant.

VI. SUMMARY AND CONCLUSIONS

In anticipation for the possibility of high-precision measurements of the transition form factors $\gamma^*\gamma \to \eta$ and $\gamma^*\gamma \to \eta'$ at the upgraded KEKB facility, in this work we update the corresponding theoretical framework. The presented formalism incorporates several new elements in comparison to the existing calculations, in particular a full NLO analysis of perturbative corrections, the charm quark contribution, and revisited twist-four contributions taking into account $SU(3)$-flavor breaking and the axial anomaly. A numerical analysis of the existing experimental data is performed with these improvements.

For the numerical analysis we have used the FKS state mixing assumption for the η, η' DAs at a low scale of 1 GeV as a working hypothesis to avoid proliferation of parameters. This assumption does not contradict the data on the FFs at small-to-moderate photon virtualities and can be relaxed in the future, if necessary.

The most important effect of the NLO improvement is due to the finite renormalization of the flavor-singlet axial current which results in a 20% reduction of the expected asymptotic value of the $\gamma^*\gamma \to \eta'$ form factor at large photon virtualities. Taking into account this correction brings the result in agreement with *BABAR* measurements [1].

We also want to emphasize the importance of taking into account the charm quark contribution. This effect is negligible at small Q^2, but increases the contribution of the most interesting two-gluon DA by a factor 5/3 at large scales, so that a consistent implementation of the c-quark mass threshold effects is mandatory.

The update of the higher-twist corrections does not have a large numerical impact, but is necessary for theoretical consistency with taking into account the meson mass corrections to the leading-twist diagrams. Identifying the hadron mass corrections in hard exclusive reactions is in general a nontrivial problem [79], and it is made even more difficult by the axial anomaly. We have calculated the anomalous contribution to the twist-four DA for one particular case and found a specific mechanism how this contribution can restore the relations between η, η' masses implied by the state-mixing assumption for higher twist.

Our results for the FFs at Euclidean virtualities are, in general, in good agreement with the experimental data [1], although the present statistical accuracy of the measurements is insufficient to distinguish between different models of the DAs specified in Table. II. We expect that experimental errors will become smaller in the future, and also that some of the parameters, most importantly the decay constants f_η, $f_{\eta'}$, will be calculated with high precision on the lattice. In this way the comparison of the QCD calculation with experiment will allow one to study the structure of η, η' mesons at short interquark separations, encoded in the DAs, on a quantitative level.

We have given a short discussion of the transition form factors in the timelike region $q^2 = -Q^2 > 0$. The result by *BABAR* [2] suggesting a large enhancement of the η form factor in the timelike as compared to the spacelike region, and at the same time no such enhancement for η', is rather puzzling. If confirmed, this difference would imply a significant difference in the end-point behavior of η and η' DAs.

ACKNOWLEDGMENTS

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APPENDIX A: DISTRIBUTION AMPLITUDES OF TWIST FOUR

This Appendix contains a detailed discussion and an update of the twist-four DAs of pseudoscalar mesons. To this end we follow the classification and notations in Ref. [35] adapted for our present case. The presentation is divided into two parts. In the first subsection we ignore anomalous contributions. This part contains the necessary definitions and an update of the results in [34] and [35] taking into account quark mass corrections in the relations between different matrix elements. The given expressions can be used as written for the flavor-octet contributions but have to be modified for flavor-singlet ones. Anomalous contributions to the flavor-singlet twist-four DAs are considered in the second subsection. This is an entirely new subject; we are not aware of any related studies beyond twist-two accuracy. The complete solution requires a full NLO evaluation of twist-four contributions and goes beyond the scope of this work. Instead, we formulate a simple substitution rule that is based on a sample calculation of the anomaly for one particularly important case, and is likely to take into account the bulk of the effect.

1. General classification and quark mass corrections

There exist four different three-particle twist-four DAs that can be defined as, e.g. for the strange quarks

$$
\begin{aligned}
&\langle 0|\bar{s}(z_2 n)\gamma_\mu\gamma_5 g G_{\alpha\beta}(z_3 n) s(z_1 n)|M(p)\rangle \\
&\quad = p_\mu(p_\alpha n_\beta - p_\beta n_\alpha)\frac{1}{pn} F_M^{(s)}\Phi_{4;M}^{(s)}(\underline{z}, pn) \\
&\qquad + (p_\beta g^\perp_{\alpha\mu} - p_\alpha g^\perp_{\beta\mu}) F_M^{(s)}\Psi_{4;M}^{(s)}(\underline{z}, pn) + \dots, \\
&\langle 0|\bar{s}(z_2 n)\gamma_\mu i g \tilde{G}_{\alpha\beta}(z_3 n) s(z_1 n)|M(p)\rangle \\
&\quad = p_\mu(p_\alpha n_\beta - p_\beta n_\alpha)\frac{1}{pn} F_M^{(s)}\tilde{\Phi}_{4;M}^{(s)}(\underline{z}, pn) \\
&\qquad + (p_\beta g^\perp_{\alpha\mu} - p_\alpha g^\perp_{\beta\mu}) F_M^{(s)}\tilde{\Psi}_{4;M}^{(s)}(\underline{z}, pn) + \dots, \qquad \text{(A1)}
\end{aligned}
$$

with the shorthand notation

$$
\begin{aligned}
\mathcal{F}(\underline{z}, pn) &= \int \mathcal{D}\underline{\alpha}\, e^{-ipn(\alpha_1 z_1 + \alpha_2 z_2 + \alpha_3 z_3)}\mathcal{F}(\underline{\alpha}), \\
\int \mathcal{D}\underline{\alpha} &= \int_0^1 d\alpha_1 d\alpha_2 d\alpha_3\, \delta\Big(1 - \sum \alpha_i\Big) \qquad \text{(A2)}
\end{aligned}
$$

and $g^\perp_{\alpha\mu} = g_{\alpha\mu} - (p_\alpha n_\mu + p_\mu n_\alpha)/(pn)$, etc. The ellipses stand for contributions of twist higher than four. C-parity implies that the DAs Φ and Ψ are antisymmetric under the interchange of the quark momenta, $\alpha_1 \leftrightarrow \alpha_2$, whereas $\tilde{\Phi}$ and $\tilde{\Psi}$ are symmetric. The three-particle twist-four DAs for $q = (u, d)$ quarks are defined by the same expressions with obvious substitution of the quark fields and the superscripts $(s) \to (q)$; cf. Eq. (1).

Three-particle DAs can be expanded in orthogonal polynomials that correspond to contributions of increasing spin in the conformal expansion. Taking into account contributions of the lowest and the next-to-lowest spin, one obtains [33–35]

$$\Phi^{(s)}_{4;M}(\underline{\alpha}) = 120\alpha_1\alpha_2\alpha_3[\phi^{(s)}_{1,M}(\alpha_1-\alpha_2)],$$
$$\tilde{\Phi}^{(s)}_{4;M}(\underline{\alpha}) = 120\alpha_1\alpha_2\alpha_3[\tilde{\phi}^{(s)}_{0,M}+\tilde{\phi}^{(s)}_{2,M}(3\alpha_3-1)],$$
$$\tilde{\Psi}^{(s)}_{4;M}(\underline{\alpha}) = -30\alpha_3^2\Big\{\psi^{(s)}_{0,M}(1-\alpha_3)+\psi^{(s)}_{1,M}[\alpha_3(1-\alpha_3)-6\alpha_1\alpha_2] + \psi^{(s)}_{2,M}\Big[\alpha_3(1-\alpha_3)-\frac{3}{2}(\alpha_1^2+\alpha_2^2)\Big]\Big\},$$
$$\Psi^{(s)}_{4;M}(\underline{\alpha}) = -30\alpha_3^2(\alpha_1-\alpha_2)\Big\{\psi^{(s)}_{0,M}+\psi^{(s)}_{1,M}\alpha_3 + \frac{1}{2}\psi^{(s)}_{2,M}(5\alpha_3-3)\Big\}. \qquad \text{(A3)}$$

The coefficients $\phi^{(s)}_{k,M}$, $\psi^{(s)}_{k,M}$ are related by QCD equations of motion [33]. One such relation is rather nontrivial and involves the divergence (in the mathematical sense) of the spin-three conformal operator

$$\mathbb{O}^{(\bar{s}s)}_{\mu\alpha\beta} = \bar{s}\overset{\leftrightarrow}{D}_\alpha\overset{\leftrightarrow}{D}_\beta\gamma_\mu\gamma_5 s - \frac{1}{5}\partial_\alpha\partial_\beta\bar{s}\gamma_\mu\gamma_5 s, \qquad \text{(A4)}$$

where the symmetrization in all Lorentz indices and subtraction of traces are implied. Ignoring possible anomalous contributions to be discussed later, we obtain

$$\begin{aligned} 6\partial^\mu\mathbb{O}^{(\bar{s}s)}_{\mu\alpha\beta} = {}& -24i\bar{s}\gamma^\rho(G_{\rho\beta}\overrightarrow{D}_\alpha - \overleftarrow{D}_\alpha G_{\rho\beta})\gamma_5 s \\ & + 4im_s\bar{s}\overset{\leftrightarrow}{D}_\alpha\overset{\leftrightarrow}{D}_\beta\gamma_5 s - 16im_s\bar{s}\sigma^{\alpha\rho}G_{\rho\beta}\gamma_5 s \\ & - \frac{16}{3}\partial_\beta\bar{s}\gamma^\rho\tilde{G}_{\rho\alpha}s - 8\partial^\rho\bar{s}\gamma_\beta\tilde{G}_{\alpha\rho}s \\ & - \frac{4}{15}im_s\partial_\alpha\partial_\beta\bar{s}\gamma_5 s - \text{traces}. \end{aligned} \qquad \text{(A5)}$$

The quark mass corrections in this expression $\sim\mathcal{O}(m_s)$ are a new result; they have not been taken into account in [34] and [35].

After some algebra we obtain

$$\tilde{\phi}^{(s)}_{0,M} = \psi^{(s)}_{0,M} = -\frac{1}{3}\delta^{2(s)}_M, \qquad \text{(A6)}$$

where the parameter $\delta^{2(s)}_M$ is defined as

$$\langle 0|\bar{s}\gamma^\rho ig\tilde{G}_{\rho\mu}s|M(p)\rangle = p_\mu f^{(s)}_M\delta^{2(s)}_M, \qquad \text{(A7)}$$

and

$$\begin{aligned} \tilde{\phi}^{(s)}_{2M} &= \frac{21}{8}\delta^{2(s)}_M\omega^{(s)}_{4M}, \\ \phi^{(s)}_{1M} &= \frac{21}{8}\Big[\delta^{2(s)}_M\omega^{(s)}_{4M} + \frac{2}{45}m_M^2\Big(1-\frac{18}{7}c^{(s)}_{2M}\Big)\Big], \\ \psi^{(s)}_{1M} &= \frac{7}{4}\Big[\delta^{2(s)}_M\omega^{(s)}_{4M} + \frac{1}{45}m_M^2\Big(1-\frac{18}{7}c^{(s)}_{2M}\Big) + 4m_s\frac{f^{(s)}_{3M}}{f^{(s)}_M}\Big], \\ \psi^{(s)}_{2M} &= \frac{7}{4}\Big[2\delta^{2(s)}_M\omega^{(s)}_{4M} - \frac{1}{45}m_M^2\Big(1-\frac{18}{7}c^{(s)}_{2M}\Big) - 4m_s\frac{f^{(s)}_{3M}}{f^{(s)}_M}\Big], \end{aligned} \qquad \text{(A8)}$$

where

$$\begin{aligned} &\langle 0|\bar{s}[iD_\mu, ig\tilde{G}_{\nu\xi}]\gamma_\xi s - \frac{4}{9}i\partial_\mu\bar{s}ig\tilde{G}_{\nu\xi}\gamma_\xi s|M(p)\rangle \\ &\quad = f^{(s)}_M\delta^{2(s)}_M\omega^{(s)}_{4M}\Big(p_\mu p_\nu - \frac{1}{4}m_M^2 g_{\mu\nu}\Big) + \mathcal{O}(\text{twist}\,5). \end{aligned} \qquad \text{(A9)}$$

The expressions in (A8) differ from those in [34] and [35] in terms $\sim m_M^2$ that arise from the quark mass corrections in the divergence of the conformal operator (A5) and, surprisingly, also in terms $\sim m_M^2 c^{(s)}_{2M}$: The result for such terms obtained in [34] (and used in [35]) is recovered if in our expressions $m_M^2 c^{(s)}_{2M} \to (3/2)m_M^2 c^{(s)}_{2M}$.

In addition one defines the two-particle twist-four DAs as corrections $\sim\mathcal{O}(x^2)$ in the light-cone expansions $x^2\to 0$ of the nonlocal matrix element

$$\begin{aligned} &\langle 0|\bar{s}(z_2x)\gamma_\mu\gamma_5 s(z_1x)|M(p)\rangle \\ &\quad = ip_\mu F^{(s)}_M\int_0^1 du e^{-iz^u_{21}(px)}\Big[\phi^{(s)}_M(u) + \frac{z_{12}^2x^2}{16}\phi^{(s)}_{4M}(u)\Big] \\ &\qquad + \frac{i}{2}\frac{x_\mu}{(px)}F^{(s)}_M\int_0^1 du e^{-iz^u_{21}(px)}\psi^{(s)}_{4M}(u). \end{aligned} \qquad \text{(A10)}$$

The DAs $\phi^{(s)}_{4M}(u)$, $\psi^{(s)}_{4M}(u)$ can be calculated in terms of the three-particle DAs of twist four and the DAs of lower twist defined in the main text, making use of the operator identities (see e.g. [35])

$$\begin{aligned} &\frac{\partial}{\partial x^\mu}\bar{s}(x)[x,-x]\gamma_\mu\gamma_5 s(-x) \\ &\quad = -i\int_{-1}^1 dv\, v\bar{s}(x)[x,vx]x^\alpha gG_{\alpha\mu}(vx)\gamma^\mu\gamma_5[vx,-x]s(-x), \end{aligned} \qquad \text{(A11)}$$

and

$$\begin{aligned} &\partial_\mu\{\bar{s}(x)[x,-x]\gamma^\mu\gamma_5 s(-x)\} \\ &\quad = -i\int_{-1}^1 dv\bar{s}(x)[x,vx]x^\alpha gG_{\alpha\mu}(vx)\gamma^\mu\gamma_5[vx,-x]s(-x) \\ &\qquad + 2m_s\bar{s}(x)[x,-x]i\gamma_5 s(-x), \end{aligned} \qquad \text{(A12)}$$

where $[x, y]$ is the straight-line-ordered Wilson line connecting the points x, y and ∂_μ is the total derivative defined as

$$\partial_\mu\{\bar{u}(x)\Gamma d(-x)\} \equiv \frac{\partial}{\partial y_\mu}\{\bar{u}(x+y)[x+y,-x+y]\Gamma d(-x+y)\}\Big|_{y\to 0}. \tag{A13}$$

Taking the matrix elements of these identities and putting $x^2 \to 0$ afterwards, one obtains the expressions for two-particle DAs $\psi_{4M}^{(s)}(u)$ and $\phi_{4M}^{(s)}$ that can conveniently be separated in "genuine" twist-four contributions and meson mass corrections as

$$\psi_{4M}^{(s)}(u) = \psi_{4M}^{(s)\mathrm{twist}}(u) + m_M^2\psi_{4M}^{(s)\mathrm{mass}}(u) \tag{A14}$$

with

$$\begin{aligned}\psi_{4M}^{(s)\mathrm{twist}}(u) &= \frac{20}{3}\delta_M^{2(s)}C_2^{1/2}(2u-1) + 30m_s\frac{f_{3M}^{(s)}}{f_M^{(s)}}\\ &\quad\times\left(\frac{1}{2} - 10u\bar{u} + 35u^2\bar{u}^2\right),\\ \psi_{4M}^{(s)\mathrm{mass}}(u) &= \frac{17}{12} - 19u\bar{u} + \frac{105}{2}u^2\bar{u}^2\\ &\quad + c_{2,M}^{(s)}\left(\frac{3}{2} - 54u\bar{u} + 225u^2\bar{u}^2\right)\end{aligned} \tag{A15}$$

and similarly

$$\phi_{4M}^{(s)}(u) = \phi_{4M}^{(s)\mathrm{twist}}(u) + m_M^2\phi_{4M}^{(s)\mathrm{mass}}(u), \tag{A16}$$

where

$$\begin{aligned}\phi_{4M}^{(s)\mathrm{twist}}(u) &= \frac{200}{3}\delta_M^{2(s)}u^2\bar{u}^2 + 21\delta_M^{2(s)}\omega_{4M}^{(s)}\{u\bar{u}(2+13u\bar{u})\\ &\quad + 2[u^3(10-15u+6u^2)\ln u + (u\leftrightarrow\bar{u})]\}\\ &\quad + 20m_s\frac{f_{3M}^{(s)}}{f_M^{(s)}}u\bar{u}[12 - 63u\bar{u} + 14u^2\bar{u}^2],\\ \phi_{4M}^{(s)\mathrm{mass}}(u) &= u\bar{u}\left[\frac{88}{15} + \frac{39}{5}u\bar{u} + 14u^2\bar{u}^2\right]\\ &\quad - c_{2,M}^{(s)}u\bar{u}\left[\frac{24}{5} - \frac{54}{5}u\bar{u} + 180u^2\bar{u}^2\right]\\ &\quad + \left(\frac{28}{15} - \frac{24}{5}c_{2,M}^{(s)}\right)[u^3(10-15u+6u^2)\ln u\\ &\quad + (u\leftrightarrow\bar{u})].\end{aligned} \tag{A17}$$

These results supersede the corresponding expressions in Refs. [35] and [80].

2. Anomalous contributions

The general reason why the results in the previous subsection are incomplete is that the operator identities (A5), (A11), (A12) are valid in this form only for bare (unrenormalized) operators. The renormalization Z factor for the light-ray operator on the left-hand side of, e.g., Eq. (A12) can be written as an integral operator acting on the field coordinates; see [81]. The derivative ∂_μ can be brought inside the integral so that the algebra leading to the expression on the right-hand side of this equation remains unchanged. However, the result is not yet written in terms of renormalized operators. Since the overall expression is finite (as a derivative of a finite operator) it can further be reexpanded in contributions of renormalized operators. In this way the coefficient functions of the operators that are already present will be modified by α_s corrections and *all other* operators with proper quantum numbers can appear, with coefficient functions starting at order $\mathcal{O}(\alpha_s)$. Whereas this complication is, generally speaking, only relevant if the calculation of twist-four corrections is done to NLO accuracy (in which case the α_s corrections to the coefficient functions of the OPE of the product of two electromagnetic currents have to be taken into account as well), the contribution of gluon operators related to the axial anomaly deserves special attention because of its role in the pattern of chiral symmetry breaking for pseudoscalar mesons.

To begin with, we recall the derivation of the celebrated anomaly relation (33) for the axial current:

$$\partial_\mu\bar{s}\gamma^\mu\gamma_5 s = 2m_s\bar{s}i\gamma_5 s + \bar{s}[(\overleftarrow{\not{D}} - im_s)\gamma_5 - \gamma_5(\overrightarrow{\not{D}} + im_s)]s. \tag{A18}$$

The EOM terms (Dirac operator applied to a quark field) can be substituted inside the QCD path integral by a functional derivative with respect to the corresponding antiquark field,

$$(\overrightarrow{\not{D}} + im_s)s(y)e^{iS_\psi} = -\frac{\delta}{\delta\bar{s}(y)}e^{iS_\psi}, \tag{A19}$$

where S_ψ is the fermion part of the action. Such contributions can usually be dispensed of by partial integration inside the path integral, producing contact terms. Anomalous contributions arise when the derivative $\delta/\delta\bar{s}(y)$ acts on the antiquark field in the same composite operator, in our case the axial current, producing ill-defined contributions $\sim\delta^4(0)$ that have to be regularized.

A well-known method to avoid this problem is to use Schwinger's split-point regularization

$$\bar{s}(0)\gamma_\mu\gamma_5 s(0) \mapsto \bar{s}(x)[x,-x]\gamma_\mu\gamma_5 s(-x), \tag{A20}$$

where x^μ should be sent to zero at the end of the calculation. In this case the EOM terms in the divergence can be dropped, but an extra contribution appears due to the Wilson line:

$$\partial_\mu \bar{s}(x)\gamma^\mu\gamma_5 s(-x) = 2m_s\bar{s}(x)i\gamma_5 s(-x) - 2i\bar{s}(x)x^\alpha gG_{\alpha\mu}(0)\gamma^\mu\gamma_5 s(-x); \quad \text{(A21)}$$

cf. Eq. (A12). Using the standard expression for the short-distance expansion of the quark propagator in a background field [82]

$$\overline{s(-x)\bar{s}}(x) = -\frac{i\not{x}}{16\pi^2x^4} + \frac{ix^\rho g\widetilde{G}_{\rho\sigma}}{16\pi^2x^2}\gamma^\sigma\gamma_5 + \ldots \quad \text{(A22)}$$

and the symmetric limit $x^\mu \to 0$ such that

$$x_\rho x_\sigma \longrightarrow \frac{1}{4}g_{\rho\sigma}x^2, \quad \text{(A23)}$$

one arrives after a little algebra at the expression in (33).

The light-ray operators that enter the definitions of DAs are *defined* as generating functions of renormalized local operators so that the same problem with EOM contributions occurs and can be treated in a similar manner. We start with a regularized version of the light-ray operator by shifting it slightly off the light cone

$$\bar{s}(z_2n)[z_2n, z_1n]\gamma_\mu\gamma_5 s(z_1n) \mapsto \bar{s}(x_2)[x_2, x_1]\gamma_\mu\gamma_5 s(x_1) \quad \text{(A24)}$$

where

$$x_1 = z_1n - x, \qquad x_2 = z_2n + x, \qquad (x\cdot n) = 0. \quad \text{(A25)}$$

and

$$\Delta^2 = (x_1 - x_2)^2 = x^2. \quad \text{(A26)}$$

Then

$$\partial_\mu\{\bar{q}(x_2)\gamma^\mu[x_2, x_1]\gamma_5 q(x_1)\} = +i\int_0^1 dv\bar{q}(x_2)\Delta^\alpha gG_{\alpha\mu}(\bar{v}x_1 + vx_2)\gamma^\mu\gamma_5 q(x_1) + 2m_q\bar{q}(x_2)i\gamma_5 q(x_1). \quad \text{(A27)}$$

The light-cone expansion of the quark propagator reads [81]

$$\overline{q(x_1)\bar{q}}(x_2) = \frac{i\not{\Delta}}{2\pi^2\Delta^4}[x_1, x_2] - \frac{\Delta^\rho\gamma^\sigma}{8\pi^2\Delta^2}\int_0^1 du \times \left\{ig\widetilde{G}_{\rho\sigma}\gamma_5 + \bar{\alpha}\alpha(\Delta D)gG_{\rho\sigma}\right\}(ux_1 + \bar{u}x_2) + \ldots \quad \text{(A28)}$$

where the terms shown by ellipses have at most a logarithmic singularity $\ln\Delta^2 = \ln x^2$ and do not contribute in the limit $x \to 0$.

The propagator (A28) is traced in (A27) with $\gamma^\mu\gamma_5$, so that only the term in $ig\tilde{G}_{\rho\sigma}\gamma_5$ is relevant. It has a $1/x^2$ singularity, hence we need to collect all contributions with two powers of x in the numerator. They can come either from factors of Δ, that give rise, in the symmetric limit (A23), to the term

$$\frac{\alpha_s}{4\pi}\int_0^1 dv\int_0^1 du G^A_{\alpha\mu}(z^v_{21}n)\tilde{G}^A_{\alpha\mu}(z^u_{12}n)$$

or from the expansion of the gluon fields in powers of the deviation from the light-cone direction, producing contributions of the type

$$\frac{\alpha_s}{8\pi}z_{12}\int_0^1 dv\int_0^1 du(2v-1)D^\alpha G_{\alpha\mu}(z^v_{21}n)\tilde{G}^A_{n\mu}(z^u_{12}n).$$

Using the EOM $D^\alpha G^A_{\alpha\mu} = -g\sum_q \bar{q}\,t^A\gamma_\mu q$ these contributions can be rewritten in terms of the same quark-antiquark-gluon operators that enter Eqs. (A11) and (A12), i.e. they are of the same order as the NLO $\mathcal{O}(\alpha_s)$ corrections to the coefficient functions of twist-four operators. Hence they can (should) be neglected if the calculation is done to LO accuracy. We obtain

$$\partial_\mu\{\bar{q}(z_1n)\gamma^\mu[z_1n, z_2n]\gamma_5 q(z_2n)\} = -iz_{12}\int_0^1 dv\bar{q}(z_1n)n^\alpha gG_{\alpha\mu}(z^v_{21}n)\gamma^\mu\gamma_5 q(z_2n) + 2m_q\bar{q}(z_1n)i\gamma_5 q(z_2n) + \frac{\alpha_s}{4\pi}\int_0^1 dv\int_0^1 du G^A_{\alpha\mu}(z^v_{21}n)\tilde{G}^{A;\alpha\mu}(z^u_{12}n). \quad \text{(A29)}$$

Taking the matrix element of this relation one obtains an equation for the DA $\psi^{(s)}_{4M}(u)$ which can be solved as in [33] and [34]

$$f^{(s)}_M\psi^{(s)}_{4M}(u) = 2\phi^{(s)p}_{3M}(u) - 2m^2_M f^{(s)}_M\phi^{(s)}_M(u) + f^{(s)}_M\frac{d}{du} \times \int_0^u d\alpha_1\int_0^{\bar{u}} d\alpha_2\frac{2[\Phi^{(s)}_{4M}(\underline{\alpha}) - 2\Psi^{(s)}_{4M}(\underline{\alpha})]}{1-\alpha_1-\alpha_2} + 2a_M\delta\psi^{(s)}_{4M}(u), \quad \text{(A30)}$$

where the last term $\delta\psi^{(s)}_{4M}(u)$ is new—it stems from the anomalous contribution in Eq. (A30); a_M is defined in Eq. (32).

This extra term can be expressed in terms of the twist-four gluon DA

$$\langle 0|\frac{\alpha_s}{4\pi}G(z_2n)\tilde{G}(z_1n)|M(p)\rangle = a_M\int_0^1 due^{-iz^u_{21}pn}\phi^{(g)}_{4M}(u), \quad \text{(A31)}$$

normalized as $\int du\phi^{(g)}_{4M}(u) = 1$. After some simple algebra one obtains the following equation for the moments of $\delta\psi^{(s)}_{4M}(u)$:

$$\int_0^1 du(2u-1)^n \delta\psi_{4M}^{(s)}(u) = \frac{1}{4}\frac{1+(-1)^n}{(n+1)(n+2)}\int_0^1 du[1-(2u-1)^{n+2}]\frac{\phi_{4M}^{(g)}(u)}{u\bar{u}}, \tag{A32}$$

which can be solved for any given twist-four gluon DA. A remarkable feature of this equation is that the resulting distribution $\delta\psi_{4M}^{(s)}(u)$ depends on the shape of $\phi_{4M}^{(g)}(u)$ only very weakly. Using the asymptotic DA $\phi_{4M}^{(g)}(u) = 1$ one obtains

$$\delta\psi_{4M}^{(s)}(u) = -2[u\ln u + \bar{u}\ln\bar{u}], \tag{A33}$$

whereas for $\phi_{4M}^{(g)}(u) = 6u(1-u)$ one gets $\delta\psi_{4M}^{(s)}(u) = 6u(1-u)$ as well. The numerical difference between the two expressions is very small; see Fig. 6. The effect of the anomalous contribution is therefore mainly to redefine the normalization of the meson mass correction proportional to the twist-two DA, the second term in (A30), to

$$-2m_M^2 f_M^{(s)}\phi_M^{(s)}(u) + 2a_M\delta\psi_{4M}^{(s)}(u) \simeq -2(m_M^2 f_M^{(s)} - a_M)\phi_M^{(s)}(u) = -2h_M^{(s)}\phi_M^{(s)}(u) \tag{A34}$$

so that it matches the normalization of the pseudoscalar twist-three DA $\phi_{3M}^{(s)p}(u)$ (29). In this way the condition $\int du\psi_{4M}^{(s)}(u) = 0$ is restored.

The complete calculation of such contributions to the twist-four DA is complicated as it requires reevaluation of all operator identities. Hence relations between the parameters, e.g. Eq. (A8) will be modified. This is a large calculation that is beyond the scope of this work. Instead, we will assume that the same substitution,

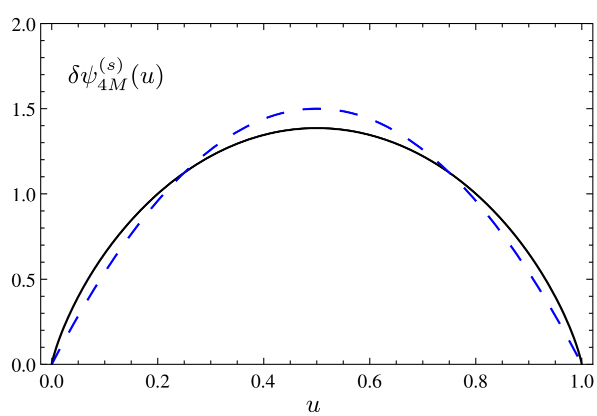

FIG. 6 (color online). The anomalous contribution to the twist-four DA $\psi_{4M}^{(s)}(u)$ (A33) compared to the asymptotic leading-twist DA $6u(1-u)$ (dashed line).

$$m_M^2 f_M^{(s)} \mapsto h_M^{(s)} = m_M^2 f_M^{(s)} - a_M \tag{A35}$$

can be applied for all occurrences of pseudoscalar meson masses m_M^2 in the flavor-octet higher-twist corrections. The ansatz (A35) is attractive as it guarantees that the higher-twist effects and therefore also the transition FFs at low momentum transfer obey the same FKS mixing scheme as is assumed for the leading twist. As we demonstrate in the text, this assumption does not contradict the existing data.

APPENDIX B: SCALE DEPENDENCE O THE LEADING-TWIST DAs TO NLO ACCURACY

1. Flavor-octet DAs

The scale dependence of the Gegenbauer coefficients in the expansion of the flavor-octet contributions to the η, η' DAs is the same as for the pion DA. One obtains [83–89]

$$c_n^{(8)}(\mu) = c_n^{(8)}(\mu_0)E_n^{\rm NLO}(\mu,\mu_0) + \frac{\alpha_s(\mu)}{2\pi}\sum_{k=0}^{n-2} c_k^{(8)}(\mu_0)E_k^{\rm LO}(\mu,\mu_0)d_n^k(\mu,\mu_0). \tag{B1}$$

The renormalization group (RG) factor $E_n^{\rm NLO}(\mu,\mu_0)$ in this expression is given by

$$E_n^{\rm NLO}(\mu,\mu_0) = \left[\frac{\alpha_s(\mu)}{\alpha_s(\mu_0)}\right]^{\gamma_n^{(0)}/\beta_0} \times \left\{1 + \frac{\alpha_s(\mu)-\alpha_s(\mu_0)}{2\pi\beta_0}\left(\gamma_n^{(1)} - \frac{\beta_1}{2\beta_0}\gamma_n^{(0)}\right)\right\}. \tag{B2}$$

The corresponding LO factor $E_n^{\rm LO}(\mu,\mu_0)$ is obtained by keeping the first term only in the braces.

Here $\beta_0(\beta_1)$ and $\gamma_n^{(0)}(\gamma_n^{(1)})$ are the LO (NLO) coefficients of the QCD β function and the anomalous dimensions, respectively:

$$\beta(\alpha_s) = \mu^2\frac{d\alpha_s}{d\mu^2} = -\alpha_s\left[\beta_0\frac{\alpha_s}{4\pi} + \beta_1\left(\frac{\alpha_s}{4\pi}\right)^2 + \ldots\right], \tag{B3}$$

$$\left[\mu^2\frac{\partial}{\partial\mu^2} + \beta(\alpha_s)\frac{\partial}{\partial\alpha_s} + \frac{1}{2}\gamma_n(\alpha_s)\right]c_n^{(8)} = 0,$$
$$\gamma_n(\alpha_s) = \gamma_n^{(0)}\frac{\alpha_s}{2\pi} + \gamma_n^{(1)}\left(\frac{\alpha_s}{2\pi}\right)^2 + \ldots. \tag{B4}$$

The first two coefficients of the beta function are

$$\beta_0 = 11 - \frac{2}{3}n_f, \qquad \beta_1 = 102 - \frac{38}{3}n_f, \tag{B5}$$

whereas the LO flavor-nonsinglet anomalous dimensions are given by

$$\gamma_n^{(0)} = C_F\left[4\psi(n+2) + 4\gamma_E - 3 - \frac{2}{(n+1)(n+2)}\right], \tag{B6}$$

where $\psi(x) = d\ln\Gamma(x)/dx$.

The NLO anomalous dimensions can most easily be obtained using the FeynCalc *Mathematica* package [90]. For convenience we present explicit expressions fo $n = 2, 4$ that are used in our calculations ($\gamma_0^{(1)} = 0$):

$$\gamma_2^{(1)} = \frac{17225}{486} - \frac{415}{162}n_f,$$
$$\gamma_4^{(1)} = \frac{331423}{6750} - \frac{7783}{2025}n_f. \tag{B7}$$

The off-diagonal mixing coefficients d_n^k in Eq. (B1) are given by the following expression:

$$d_n^k(\mu,\mu_0) = r_{nk}(\mu,\mu_0)M_n^k,$$
$$r_{nk}(\mu,\mu_0) = \frac{-1}{\gamma_n^{(0)} - \gamma_k^{(0)} - \beta_0}\left\{1 - \left[\frac{\alpha_s(\mu)}{\alpha_s(\mu_0)}\right]^{\frac{\gamma_n^{(0)}-\gamma_k^{(0)}-\beta_0}{\beta_0}}\right\}. \tag{B8}$$

The matrix M_n^k is defined as

$$M_n^k = \frac{(k+1)(k+2)(2n+3)}{(n+1)(n+2)}[\gamma_k^{(0)} - \gamma_n^{(0)}] \times\left\{\frac{4C_F A_n^k - \gamma_k^{(0)} - \beta_0}{(n-k)(n+k+3)} + 2C_F\frac{A_n^k - \psi(n+2) + \psi(1)}{(k+1)(k+2)}\right\} \tag{B9}$$

where

$$A_n^k = \psi\left(\frac{n+k+4}{2}\right) - \psi\left(\frac{n-k}{2}\right) + 2\psi(n-k) - \psi(n+2) - \psi(1). \tag{B10}$$

For convenience, we give the numerical values of the nonvanishing coefficients M_n^k for $n \le 4$:

$$M_2^0 = \frac{455}{162} - \frac{35}{81}n_f,$$
$$M_4^0 = \frac{143}{405} - \frac{286}{2025}n_f,$$
$$M_4^2 = \frac{6688}{1215} - \frac{836}{2025}n_f. \tag{B11}$$

2. Flavor-singlet DAs

The renormalization-group equations for the flavor-singlet quark and gluon DAs can be inferred from [91]. They are more compact in matrix notation. To this end we introduce the vector of Gegenbauer coefficients

$$\vec{c}_n = \begin{pmatrix} c_n^{(1)} \\ c_n^{(g)} \end{pmatrix}. \tag{B12}$$

Then

$$\vec{c}_n(\mu) = \mathcal{T}_n^{-1}\mathcal{E}_n^{\rm NLO}(\mu,\mu_0)\mathcal{T}_n\vec{c}_n(\mu_0) + \frac{\alpha_s(\mu)}{2\pi}\sum_{k=0,2,\ldots}^{n-2}\mathcal{T}_n^{-1}\mathcal{D}_n^k(\mu,\mu_0)\mathcal{E}_k^{\rm LO}(\mu,\mu_0)\mathcal{T}_k\vec{c}_k(\mu_0), \tag{B13}$$

where $\mathcal{E}_n^{\rm NLO(LO)}(\mu,\mu_0)$ and $\mathcal{D}_n^k(\mu,\mu_0)$ are 2×2 matrices that we will specify in what follows and

$$\mathcal{T}_n = {\rm diag}\left(\frac{3(n+1)(n+2)}{2(2n+3)}, \frac{5n(n+1)(n+2)(n+3)}{24(2n+3)}\right) \tag{B14}$$

is the transformation matrix from the local operator basis of Ref. [91] to the basis of Gegenbauer coefficients defined in Eqs. (16) and (20).

Let

$$\boldsymbol{\gamma}_n^{(i)} = \begin{pmatrix} {}^{qq}\gamma_n^{(i)} & {}^{qg}\gamma_n^{(i)} \\ {}^{gq}\gamma_n^{(i)} & {}^{gg}\gamma_n^{(i)} \end{pmatrix} \tag{B15}$$

be the matrix of anomalous dimensions where the superscript refers to the order of perturbation theory. The leading-order expressions are ($n \ge 2$)

$${}^{qq}\gamma_n^{(0)} = C_F\left[4\psi(n+2) + 4\gamma_E - 3 - \frac{2}{(n+1)(n+2)}\right],$$
$${}^{qg}\gamma_n^{(0)} = -n_f\frac{12}{(n+1)(n+2)},$$
$${}^{gq}\gamma_n^{(0)} = -C_F\frac{n(n+3)}{3(n+1)(n+2)},$$
$${}^{gg}\gamma_n^{(0)} = N_c\left[4\psi(n+2) + 4\gamma_E - \frac{8}{(n+1)(n+2)}\right] - \beta_0. \tag{B16}$$

The eigenvalues of the LO anomalous dimension matrix $\boldsymbol{\gamma}_n^{(0)}$ read

$$\gamma_n^{\pm} = \frac{1}{2}\left[{}^{qq}\gamma_n^{(0)} + {}^{gg}\gamma_n^{(0)} \pm \sqrt{({}^{qq}\gamma_n^{(0)} - {}^{gg}\gamma_n^{(0)})^2 + 4\,{}^{qg}\gamma_n^{(0)}\,{}^{gq}\gamma_n^{(0)}}\right]. \tag{B17}$$

Then

$$\mathcal{E}_n^{\rm LO}(\mu,\mu_0) = \mathbf{P}_n^+\left[\frac{\alpha_s(\mu)}{\alpha_s(\mu_0)}\right]^{\frac{\gamma_n^+}{\beta_0}} + \mathbf{P}_n^-\left[\frac{\alpha_s(\mu)}{\alpha_s(\mu_0)}\right]^{\frac{\gamma_n^-}{\beta_0}}, \qquad \text{(B18)}$$

where $\mathbf{P}_n^\pm$ are projectors on the eigenstates of the evolution equation

$$\mathbf{P}_0^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathbf{P}_0^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\mathbf{P}_n^\pm = \pm\frac{1}{\gamma_n^+ - \gamma_n^-}(\boldsymbol{\gamma}_n^{(0)} - \gamma_n^\mp \mathbb{1}), \qquad n \geq 2.$$

$$\mathbf{P}_n^+ + \mathbf{P}_n^- = \mathbf{1}, \qquad (\mathbf{P}_n^\pm)^2 = \mathbf{P}_n^\pm, \qquad \mathbf{P}_n^+\mathbf{P}_n^- = 0. \qquad \text{(B19)}$$

Further

$$\mathcal{E}_n^{\rm NLO}(\mu,\mu_0) = \sum_{a,b=\pm}\left[\delta_{ab}\mathbf{P}_n^a + \frac{\alpha_s(\mu)}{2\pi}\mathcal{R}_{nn}^{ab}(\mu,\mu_0)\mathbf{P}_n^a\Gamma_n\mathbf{P}_n^b\right] \times \left[\frac{\alpha_s(\mu)}{\alpha_s(\mu_0)}\right]^{\frac{\gamma_n^b}{\beta_0}} \qquad \text{(B20)}$$

and

$$\mathcal{D}_n^k(\mu,\mu_0) = \sum_{a,b=\pm}\mathcal{R}_{nk}^{ab}(\mu,\mu_0)\mathbf{P}_n^a\boldsymbol{\mathcal{M}}_n^k\mathbf{P}_k^b, \qquad \text{(B21)}$$

where

$$\boldsymbol{\Gamma}_n = \boldsymbol{\gamma}_n^{(1)} - \frac{\beta_1}{2\beta_0}\boldsymbol{\gamma}_n^{(0)} \qquad \text{(B22)}$$

and

$$\mathcal{R}_{nk}^{ab}(\mu,\mu_0) = \frac{-1}{\gamma_n^a - \gamma_k^b - \beta_0}\left\{1 - \left[\frac{\alpha_s(\mu)}{\alpha_s(\mu_0)}\right]^{\frac{\gamma_n^a-\gamma_k^b-\beta_0}{\beta_0}}\right\}. \qquad \text{(B23)}$$

The NLO anomalous dimensions matrices for $n = 2, 4$ are given by [92]

$$\boldsymbol{\gamma}_2^{(1)} = \begin{pmatrix} \frac{17225}{486} - \frac{745}{324}n_f - 4n_f & -\frac{43}{216}n_f \\ -\frac{7295}{2916} - \frac{25}{243}n_f & \frac{447}{8} - \frac{437}{81}n_f - 4n_f \end{pmatrix},$$

$$\boldsymbol{\gamma}_4^{(1)} = \begin{pmatrix} \frac{331423}{6750} - \frac{37963}{10125}n_f - 4n_f & \frac{22127}{13500}n_f \\ -\frac{288421}{91125} - \frac{1316}{6075}n_f & \frac{31744}{375} - \frac{93788}{10125}n_f - 4n_f \end{pmatrix} \qquad \text{(B24)}$$

where the terms $-4n_f$ on the diagonal are due to the factorization of the scale-dependent coupling $f_M^{(1)}$ in the definition of the DAs; cf. Eq. (15). The matrices $\boldsymbol{\mathcal{M}}_n^k$, $k < n \leq 4$ that describe mixing between different orders in the conformal (Gegenbauer) expansion are given by

$$\boldsymbol{\mathcal{M}}_2^0 = \begin{pmatrix} \frac{65}{9} - \frac{4}{9}n_f & 32n_f - 6\pi^2 n_f \\ -\frac{175}{27} - \frac{10}{27}n_f & -1080 + 120\pi^2 - \frac{10}{3}n_f \end{pmatrix},$$

$$\boldsymbol{\mathcal{M}}_4^0 = \begin{pmatrix} \frac{13}{9} - \frac{14}{45}n_f & \frac{226}{5}n_f - 6\pi^2 n_f \\ -\frac{1414}{135} - \frac{56}{135}n_f & 399\pi^2 - \frac{18753}{5} - \frac{56}{15}n_f \end{pmatrix},$$

$$\boldsymbol{\mathcal{M}}_4^2 = \begin{pmatrix} \frac{2128}{243} - \frac{259}{405}n_f & \frac{49}{30}n_f \\ -\frac{4214}{1215} - \frac{196}{1215}n_f & \frac{539}{15} - \frac{98}{405}n_f \end{pmatrix}. \qquad \text{(B25)}$$

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