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$O(\alpha_s^2)$ and $O(\alpha_s^3)$ heavy flavor contributions to transversity at $Q^2 \gg m^2$

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In deep-inelastic processes the heavy flavor Wilson coefficients factorize for $Q^2 \gg m^2$ into the light-flavor Wilson coefficients of the corresponding process and the massive operator matrix elements (OMEs). We calculate the $O(\alpha_s^2)$ and $O(\alpha_s^3)$ massive OME for the flavor nonsinglet transversity distribution. At $O(\alpha_s^2)$ the OME is obtained for general values of the Mellin variable N, while at $O(\alpha_s^3)$ the moments $N = 1$ to 13 are computed. The terms $\propto T_F$ of the 3-loop transversity anomalous dimension are obtained and results in the literature are confirmed. We discuss the relation of these contributions to the Soffer bound for transversity.

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I. INTRODUCTION

The transversity distribution $\Delta_T f(x, Q^2)$ is one of the three possible quarkonic twist-2 parton distributions besides the unpolarized quark density $f(x, Q^2)$ and the longitudinally polarized density $\Delta f(x, Q^2)$. Unlike the latter distributions, it cannot be measured in inclusive deeply inelastic scattering since the corresponding contribution is $\propto m_q^2/Q^2$, [1], with m_q a light quark mass and Q^2 the virtuality of the exchanged gauge boson. It can be extracted from deep-inelastic scattering studying isolated meson production, also called semi-inclusive deeply inelastic scattering (SIDIS), [2,3], and in the polarized Drell-Yan process [3–5].[1] Measurements of the transversity distribution in different polarized hard scattering processes are currently performed or in preparation [7]. In the past, phenomenological models for the transversity distribution were developed based on baglike models, chiral models, light-cone models, spectator models, and nonperturbative QCD calculations, cf. Sec. 8, Ref. [6]. The main behavior of the distributions is that they vanish by some power law both at small and large values of Bjorken x and exhibit a shifted bell-like shape. First attempts to extract the distributions out of data were made in Ref. [8]. The moments of the transversity distribution can be measured in lattice simulations, which help to constrain it *ab initio*. The first results were given in Ref. [9]. From these investigations there is evidence, that the up-quark distribution is positive while the down-quark distribution is negative, with first moments between 0.85…1.0 and −0.20… − 0.24, respectively.

The scaling violations of the transversity distribution were explored in leading-, [5,10–12],[2] and next-to-leading order, [14–16].[3] In Ref. [11] also the method proposed in [18] was used to calculate the anomalous dimension. At three-loop order the moments $N = 1$ to 8 for the anomalous dimension are known [19]. For the calculation of the scattering cross sections also the corresponding Wilson coefficients have to be known. In the case of SIDIS these corrections have not yet been calculated. For the transversely polarized Drell-Yan process the $O(\alpha_s)$ Wilson coefficient was derived in Ref. [16] based on [20] and at higher orders the contributions due to soft resummation are available [21].

The scattering cross sections dominated by the transversity distribution receive heavy flavor corrections, although transversity itself is a flavor nonsinglet distribution. These contributions reside in the corresponding Wilson coefficients. In deep-inelastic processes the heavy flavor Wilson coefficients factorize into massive operator matrix elements (OMEs) and the light-flavor Wilson coefficients at large enough momentum transfer $Q^2 \gg m^2$, as was shown in Ref. [22], with m the heavy quark mass. In this way all contributions except the power corrections $(m^2/Q^2)^k$, $k \geq 1$ can be calculated. The massive OMEs derive from the twist 2 operators emerging in the light-cone expansion between on-shell states and are process independent quantities. The formalism proposed in Ref. [22] has been applied successfully to calculate the asymptotic heavy flavor Wilson coefficients at $O(\alpha_s^2)$ [22–24] in unpolarized and polarized deep-inelastic scattering. For $F_L(x, Q^2)$ the asymptotic heavy flavor corrections to $O(\alpha_s^3)$ were calculated in Ref. [25]. A series of Mellin moments for the asymptotic heavy flavor Wilson coefficients contributing to the structure function $F_2(x, Q^2)$ at $O(\alpha_s^3)$ have recently been computed in Refs. [26,27].

In the present paper we apply this formalism to the tensor operator defining the flavor nonsinglet transversity distribution, and limit the consideration to contributions of twist 2 and the collinear parton model. We calculate the $O(\alpha_s^2)$ corrections for the flavor nonsinglet OME of transversity for general values of the Mellin variable N. At $O(\alpha_s^3)$ the OME is computed for individual Mellin moments $N = 1$ to 13. The 2-loop calculation verifies the T_F terms of the transversity anomalous dimension of former

[1] For a review see Ref. [6].
[2] The small x limit of the LO anomalous dimension was calculated in [13].
[3] For calculations in the nonforward case see [11,17].

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next-to-leading order (NLO) calculations [14–16]. In the 3-loop calculation we obtain the moments for the complete 2-loop anomalous dimension, which appears in the double pole term in the dimensional parameter $\varepsilon = D - 4$. Furthermore, the T_F contributions to the 3-loop anomalous dimension are obtained from the single pole term, which can be compared to the results in [19] for $N = 1$ to 8, while the T_F terms of the anomalous dimension for $N = 9$ to 13 are new. The results for the massive OME for transversity given in the present paper are related to future lattice simulations with $(2 + 1 + 1)$-, resp. $(2 + 1)$-dynamical fermions. The heavy flavor contributions are also of relevance for the Soffer bound for transversity [28].

The paper is organized as follows: In Sec. II we summarize the main relations for semi-inclusive scattering cross sections in the leading twist approximation from which the transversity distribution can be determined. Here, as in the case of inclusive deep-inelastic scattering, tagging on charm mesons allows to measure the charm contribution directly in high-luminosity experiments. The method to calculate the heavy flavor corrections in the asymptotic region is briefly described. In Sec. III, we calculate the $O(\alpha_s^2)$ massive operator matrix element. The Mellin moments of the OME at $O(\alpha_s^3)$ are computed in Sec. IV. In Sec. V, we discuss the heavy flavor contributions to the Soffer bound and Sec. VI contains the conclusions. In the Appendix, we summarize the T_F parts of the 3-loop anomalous dimension for transversity and the moments of the constant part $O(\varepsilon^0)$ of the unrenormalized $O(\alpha_s^3)$ massive OME for the Mellin moments $N = 1$ to 13. For details concerning the calculation and renormalization of massive nonsinglet OMEs we refer to Ref. [26].

II. BASIC FORMALISM

The transversity distribution

$$\Delta_T f(x, Q^2) \equiv f^{\uparrow}(x, Q^2) - f^{\downarrow}(x, Q^2) \tag{1}$$

contributes to a large variety of scattering processes, cf. [6]. Here, $\uparrow(\downarrow)$ denote the transverse spin directions. Equation (1) describes the transversity distribution obtained in the light-cone expansion at twist 2 or in the collinear parton model. For other phenomenological applications one may introduce $k_\perp$ effects for this distribution, [6]. This, however, has consequences for the twist expansion and the renormalization of the corresponding processes, when calculating them to higher orders. We will therefore restrict the analysis to the level of twist 2 and consider only processes which are free of $k_\perp$ effects, or after these were integrated out in the final state.

For semi-inclusive deeply inelastic charged lepton-nucleon scattering $lN \to l'h + X$ the Born cross section, after the $\mathbf{P}_{h\perp}$ integration, is given by, [6],

$$\frac{d^3\sigma}{dxdydz} = \frac{4\pi\alpha_{\rm em}^2 s}{Q^4} \sum_{a=q,\bar{q}} e_a^2 x \Big\{ \frac{1}{2}[1 + (1-y)^2] F_a(x, Q^2) \times \tilde{D}_a(z, Q^2) - (1-y)|\mathbf{S}_\perp||\mathbf{S}_{h\perp}| \times \cos(\phi_S + \phi_{S_h}) \Delta_T F_a(x, Q^2) \Delta_T \tilde{D}_a(z, Q^2) \Big\}. \tag{2}$$

Here, in addition to the Bjorken variables x and y, the fragmentation variable z occurs. $\mathbf{S}_\perp$ and $\mathbf{S}_{h\perp}$ are the transverse spin vectors of the incoming nucleon N and the measured hadron h. The angles ϕ_{S,S_h} are measured in the plane perpendicular to the $\gamma^* N$ (z) axis between the x axis and the respective vector. The transversity distribution can be obtained from Eq. (2) for a transversely polarized hadron h by measuring its polarization. The functions F_i, $\tilde{D}_i$, $\Delta_T F_i$, $\Delta_T \tilde{D}_i$ are given by

$$F_i(x, Q^2) = \mathcal{C}_i(x, Q^2) \otimes f_i(x, Q^2), \tag{3}$$

$$\tilde{D}_i(z, Q^2) = \tilde{\mathcal{C}}_i(z, Q^2) \otimes D_i(z, Q^2), \tag{4}$$

$$\Delta_T F_i(x, Q^2) = \Delta_T \mathcal{C}_i(x, Q^2) \otimes \Delta_T f_i(x, Q^2), \tag{5}$$

$$\Delta_T \tilde{D}_i(z, Q^2) = \Delta_T \tilde{\mathcal{C}}_i(z, Q^2) \otimes \Delta_T D_i(z, Q^2). \tag{6}$$

Here, $\otimes$ denotes the Mellin convolution, D_i, $\Delta_T D_i$ are the fragmentation functions and $\mathcal{C}_i$, $\tilde{\mathcal{C}}_i$, $\Delta_T \mathcal{C}_i$, $\Delta_T \tilde{\mathcal{C}}_i$ are the corresponding space- and time-like Wilson coefficients. The Wilson coefficient for transversity, $\Delta_T \mathcal{C}_i(x, Q^2)$, contains light ($\Delta_T C_i$) and heavy flavor ($\Delta_T H_i$) contributions

$$\Delta_T \mathcal{C}_i(x, Q^2) = \Delta_T C_i(x, Q^2) + \Delta_T H_i(x, Q^2). \tag{7}$$

For brevity we dropped arguments like m^2, the factorization scale, μ^2, and the number of light flavors, N_f, in Eq. (7).

Equation (2) holds for spin-1/2 hadrons in the final state, but the transversity distribution may also be measured in the lepto-production process of spin-1 hadrons, [29]. In this case, the $\mathbf{P}_{h\perp}$-integrated Born cross section reads

$$\frac{d^3\sigma}{dxdydz} = \frac{4\pi\alpha^2}{xyQ^2} \sin(\phi_S + \phi_{S_{\rm LT}}) |\mathbf{S}_\perp||S_{\rm LT}|(1-y) \times \sum_{i=q,\bar{q}} e_i^2 x \Delta_T F_i(x, Q^2) \hat{H}_{i,1,{\rm LT}}(z, Q^2). \tag{8}$$

Here, the polarization state of a spin-1 particle is described by a tensor with five independent components, [30]. $\phi_{\rm LT}$ denotes the azimuthal angle of $\vec{S}_{\rm LT}$, with

$$|S_{\rm LT}| = \sqrt{(S_{\rm LT}^x)^2 + (S_{\rm LT}^y)^2}. \tag{9}$$

$\hat{H}_{a,1,{\rm LT}}(z, Q^2)$ is a T- and chirally odd twist-2 fragmentation function at vanishing $k_\perp$. Process (8) has the advantage that the transverse polarization of the produced hadron can be measured from its decay products.

The transversity distribution can also be measured in the transversely polarized Drell-Yan process using the polarization asymmetry, see Refs. [16,20,21]. However, the SIDIS processes have the advantage that in high-luminosity experiments, cf. [31], the heavy flavor contributions can be tagged like in deep-inelastic scattering. This is not the case for the Drell-Yan process, where the heavy flavor effects appear as inclusive radiative corrections in the Wilson coefficients. We will therefore mainly consider SIDIS in the following.

As was shown in Ref. [22], in the region $Q^2 \gg m^2$ all nonpower contributions to the heavy quark Wilson coefficients obey factorization relations. In the general flavor nonsinglet case one obtains for N_f light and one heavy quark

$$H_a^{\mathrm{asymp,NS}}\left(x, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2}\right) = C_{a,q}^{\mathrm{NS}}\left(x, \frac{Q^2}{\mu^2}, N_f + 1\right) \otimes A_{qq,Q}^{\mathrm{NS}}\left(x, \frac{m^2}{\mu^2}\right) - C_{a,q}^{\mathrm{NS}}\left(x, \frac{Q^2}{\mu^2}, N_f\right), \tag{10}$$

where $C_{a,q}^{\mathrm{NS}}$ is a light-flavor Wilson coefficient and $A_{qq,Q}^{\mathrm{NS}}$ is the corresponding massive operator matrix element, cf. [22,24,26], with

$$C_{a,q}^{\mathrm{NS}}\left(x, \frac{Q^2}{\mu^2}\right) = \delta(1-x) + \sum_{k=1}^{\infty} a_s^k(\mu^2) C_{a,q}^{(k),\mathrm{NS}}\left(x, \frac{Q^2}{\mu^2}\right), \tag{11}$$

$$A_{qq,Q}^{\mathrm{NS}}\left(x, \frac{m^2}{\mu^2}\right) = \langle q|O^{\mathrm{NS}}|q\rangle = \delta(1-x) + \sum_{k=2}^{\infty} a_s^k(\mu^2) A_{qq,Q}^{(k),\mathrm{NS}}\left(x, \frac{m^2}{\mu^2}\right). \tag{12}$$

Here, $a_s(\mu^2) = \alpha_s(\mu^2)/(4\pi)$ denotes the strong coupling constant and $|q\rangle$ are light quark states, with on-shell momenta. The local flavor nonsinglet twist-2 operator for transversity is given by

$$O_{q,r}^{\mathrm{TR,NS},\mu,\mu_1,\ldots,\mu_N}(z) = \frac{1}{2} i^{N-1} S\left[\bar{q}(z)\sigma^{\mu\mu_1} D^{\mu_2} \ldots D^{\mu_N} \frac{\lambda_r}{2} q(z)\right] - \text{Trace Terms}, \tag{13}$$

with $\sigma^{\mu\nu} = (i/2)[\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu]$, λ_r the Gell-Mann matrices for $SU(3)_{\mathrm{flavor}}$, D^ν the covariant derivative in QCD, $q(\bar{q})$ denote the quark and antiquark fields, and the operator S symmetrizes the Lorentz indices. Note that in Eq. (10) the heavy quark degrees of freedom are all contained in the process independent OMEs.

In case of transversity one obtains the following representation for the heavy-flavor Wilson coefficient [4] after expanding Eq. (10) up to $O(a_s^3)$

$$\Delta_T H_q^{\mathrm{asym}}(N_f + 1) = a_s^2(N_f + 1)[\Delta_T A_{qq,Q}^{(2),\mathrm{NS}} + \Delta_T \hat{C}_q^{(2)}(N_f)] + a_s^3(N_f + 1) \times [\Delta_T A_{qq,Q}^{(3),\mathrm{NS}}(N_f + 1) + \Delta_T A_{qq,Q}^{(2),\mathrm{NS}} \Delta_T C_q^{(1)} + \Delta_T \hat{C}_q^{(3)}(N_f)]. \tag{14}$$

Here, we made the N_f dependence explicit and use the notation

$$\hat{f}(N_f) = f(N_f + 1) - f(N_f). \tag{15}$$

We dropped all arguments like x, N, m^2, μ^2, which are understood implicitly. Additionally, Eq. (14) is written in Mellin space, in which we will work from now on, if not stated otherwise. The assignment of the differing arguments in N_f in Eq. (14) is necessary to project onto the heavy quark part.

Following Ref. [26] we consider the Green's function $\hat{G}_{\mu,q,Q}^{ij,\mathrm{TR,NS}}$, which is obtained by contracting the matrix element of the local operator (13) with the source term $J_N = \Delta^{\mu_1} \ldots \Delta^{\mu_N}$

$$\bar{u}(p,s) G_{\mu,q,Q}^{ij,\mathrm{TR,NS}} \lambda_r u(p,s) = J_N \langle q_i(p) \mid O_{q,r;\mu,\mu_1,\ldots,\mu_N}^{\mathrm{TR,NS}} \mid q^j(p)\rangle_Q, \tag{16}$$

where p and s denote the 4-vectors of the momentum and spin of the external light quark line, $u(p,s)$ is the corresponding bi-spinor, $\Delta.\Delta = 0$, and Q labels the heavy quark contribution. The unrenormalized Green's function has the following Lorentz structure:

$$\hat{G}_{\mu,q,Q}^{ij,\mathrm{TR,NS}} = \delta_{ij}(\Delta.p)^{N-1}\left(\Delta_\rho \sigma^{\mu\rho} \Delta_T \hat{\hat{A}}_{qq,Q}^{\mathrm{NS}}\left(\frac{\hat{m}^2}{\mu^2}, \varepsilon, N\right) + c_1\Delta^\mu + c_2 p^\mu + c_3\gamma^\mu \not{p} + c_4 \not{\Delta}\not{p}\Delta^\mu + c_5 \not{\Delta}\not{p} p^\mu\right), \tag{17}$$

with unphysical constants $c_k|_{k=1\ldots5}$ and $\hat{m}$ the unrenormalized heavy quark mass. The unrenormalized massive OME is then obtained in Mellin space via the projection

[4] Apparently, the light-flavor Wilson coefficients for SIDIS were not yet calculated even at $O(a_s)$, although this calculation and the corresponding soft exponentiation should be straightforward.

$$\Delta_T \hat{\hat{A}}^{\rm NS}_{qq,Q}\left(\frac{\hat{m}^2}{\mu^2}, \varepsilon, N\right) = -i\frac{\delta^{ij}}{4N_c(\Delta.p)^{N+1}(D-2)} \times \{{\rm Tr}[\not\Delta \not p p^\mu \hat{G}^{ij,{\rm TR,NS}}_{\mu,q,Q}] - \Delta.p{\rm Tr}[p^\mu \hat{G}^{ij,{\rm TR,NS}}_{\mu,q,Q}] + i\Delta.p{\rm Tr}[\sigma^{\mu\rho}p^\rho \hat{G}^{ij,{\rm TR,NS}}_{\mu,q,Q}]\}. \quad (18)$$

Here, N_c denotes the number of colors. For the renormalization procedure and different steps to the final representation of the massive OME in the $\overline{\rm MS}$ scheme we refer to Ref. [26]. Note that the renormalization of the heavy quark mass is carried out in the on-mass-shell scheme.

III. THE $O(a_s^2)$ MASSIVE OPERATOR MATRIX ELEMENT

After mass renormalization the massive flavor nonsinglet OME for transversity at $O(a_s^2)$ is given by [22,24]

$$\Delta_T \hat{A}^{(2),\rm NS}_{qq,Q}(N) = S_\varepsilon^2\left(\frac{m^2}{\mu^2}\right)^\varepsilon \left\{\frac{1}{\varepsilon^2}[\beta_{0,Q}\gamma_{qq}^{(0),\rm TR}] + \frac{1}{\varepsilon}\left[\frac{1}{2}\hat{\gamma}_{qq}^{(1),\rm TR}\right] + a_{qq,Q}^{(2),\rm TR} + \varepsilon\bar{a}_{qq,Q}^{(2),\rm TR}\right\}. \quad (19)$$

Here, we dropped all arguments on the right-hand side. S_ε is the spherical factor that occurs due to dimensional regularization and is set to one in the $\overline{\rm MS}$ scheme. $\gamma_{qq}^{(k),\rm TR}(N)$ denote the $(k+1)$-loop anomalous dimensions for the nonsinglet composite operator (13). Note that as in Ref. [26] we define the anomalous dimension corresponding to an operator Z factor via

$$\gamma = \mu\frac{\partial}{\partial\mu}\ln(Z(\mu)). \quad (20)$$

$\beta_{0,Q}$ denotes the heavy flavor contribution to the β function in lowest order,

$$\beta_{0,Q} = -\frac{4}{3}T_F, \quad (21)$$

with $T_F = 1/2$. Equation (19) has been expanded up to $O(\varepsilon)$ since the coefficient $\bar{a}_{qq,Q}^{(2),\rm TR}$ enters the 3-loop OME via renormalization. The renormalized OME is given in Mellin space by

$$\Delta_T A^{(2),{\rm NS},\overline{\rm MS}}_{qq,Q}(N) = \frac{\beta_{0,Q}\gamma_{qq}^{(0),\rm TR}}{4}\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{\hat{\gamma}_{qq}^{(1),\rm TR}}{2}\ln\left(\frac{m^2}{\mu^2}\right) + a_{qq,Q}^{(2),\rm TR} - \frac{\beta_{0,Q}\gamma_{qq}^{(0),\rm TR}}{4}\zeta_2 \quad (22)$$

in the $\overline{\rm MS}$ scheme and ζ_k, $k \geq 2$, $k \in \mathbf{N}$ denotes the Riemann ζ function at integer arguments. The calculation of the 2-loop OME in terms of Feynman-parameter integrals is straightforward, see [24]. For the anomalous dimensions $\gamma_{qq}^{(0),\rm TR}$ and $\hat{\gamma}_{qq}^{(1),\rm TR}$ we obtain

$$\gamma_{qq}^{(0),\rm TR}(N) = 2C_F[-3+4S_1], \quad (23)$$

$$\hat{\gamma}_{qq}^{(1),\rm TR}(N) = \frac{32}{9}C_F T_F\left[3S_2 - 5S_1 + \frac{3}{8}\right], \quad (24)$$

with $C_F = (N_c^2-1)/(2N_c)$, confirming earlier results, [14–16]. Here, $S_k \equiv S_k(N)$ denote the single harmonic sums, [32]. The finite and $O(\varepsilon)$ contributions of the unrenormalized OME, Eq. (19), read

$$a_{qq,Q}^{(2),\rm TR}(N) = C_F T_F\left\{-\frac{8}{3}S_3 + \frac{40}{9}S_2 - \left[\frac{224}{27} + \frac{8}{3}\zeta_2\right]S_1 + 2\zeta_2 + \frac{(24+73N+73N^2)}{18N(N+1)}\right\}, \quad (25)$$

$$\bar{a}_{qq,Q}^{(2),\rm TR}(N) = C_F T_F\left\{-\left[\frac{656}{81} + \frac{20}{9}\zeta_2 + \frac{8}{9}\zeta_3\right]S_1 + \left[\frac{112}{27} + \frac{4}{3}\zeta_2\right]S_2 - \frac{20}{9}S_3 + \frac{4}{3}S_4 + \frac{1}{6}\zeta_2 + \frac{2}{3}\zeta_3 + \frac{(-144-48N+757N^2+1034N^3+517N^4)}{216N^2(N+1)^2}\right\}. \quad (26)$$

The renormalized 2-loop massive OME (22) then becomes

$$\Delta_T A^{(2),{\rm NS},\overline{\rm MS}}_{qq,Q}(N) = C_F T_F\left\{\left[-\frac{8}{3}S_1 + 2\right]\ln^2\left(\frac{m^2}{\mu^2}\right) + \left[-\frac{80}{9}S_1 + \frac{2}{3} + \frac{16}{3}S_2\right]\ln\left(\frac{m^2}{\mu^2}\right) - \frac{8}{3}S_3 + \frac{40}{9}S_2 - \frac{224}{27}S_1 + \frac{24+73N+73N^2}{18N(N+1)}\right\}. \quad (27)$$

Corresponding quantities for vector currents were calculated in Refs. [22,24]. In the limit $N \to \infty$ $\gamma_{qq}^{(0)}(N)$, $\hat{\gamma}_{qq}^{(1)}(N)$, $a_{qq,Q}^{(2)}(N)$, $\bar{a}_{qq,Q}^{(2)}(N)$, and $A_{qq,Q}^{(2)}(N)$ in the vector and transversity case approach each other. This has also been observed for the 2-loop transversity anomalous dimension in Ref. [14].

IV. THE $O(a_s^3)$ MASSIVE OPERATOR MATRIX ELEMENT

The renormalized OME for transversity at $O(a_s^3)$ has the same structure as the flavor nonsinglet OME in the case of vector currents, [26]. In Mellin space it is given by

$$\Delta_T A_{qq,Q}^{(3),\mathrm{NS},\overline{\mathrm{MS}}}(N) = -\frac{\gamma_{qq}^{(0),\mathrm{TR}}\beta_{0,Q}}{6}(\beta_0 + 2\beta_{0,Q})\ln^3\left(\frac{m^2}{\mu^2}\right) + \frac{1}{4}\{2\gamma_{qq}^{(1),\mathrm{TR}}\beta_{0,Q} - 2\hat{\gamma}_{qq}^{(1),\mathrm{TR}}(\beta_0 + \beta_{0,Q}) + \beta_{1,Q}\gamma_{qq}^{(0),\mathrm{TR}}\}\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{1}{2}\{\hat{\gamma}_{qq}^{(2),\mathrm{TR}} - (4a_{qq,Q}^{(2),\mathrm{TR}} - \zeta_2\beta_{0,Q}\gamma_{qq}^{(0),\mathrm{TR}})(\beta_0 + \beta_{0,Q}) + \gamma_{qq}^{(0),\mathrm{TR}}\beta_{1,Q}^{(1)}\}\ln\left(\frac{m^2}{\mu^2}\right) + 4\bar{a}_{qq,Q}^{(2),\mathrm{TR}}(\beta_0 + \beta_{0,Q}) - \gamma_{qq}^{(0)}\beta_{1,Q}^{(2)} - \frac{\gamma_{qq}^{(0),\mathrm{TR}}\beta_0\beta_{0,Q}\zeta_3}{6} - \frac{\gamma_{qq}^{(1),\mathrm{TR}}\beta_{0,Q}\zeta_2}{4} + 2\delta m_1^{(1)}\beta_{0,Q}\gamma_{qq}^{(0),\mathrm{TR}} + \delta m_1^{(0)}\hat{\gamma}_{qq}^{(1),\mathrm{TR}} + 2\delta m_1^{(-1)}a_{qq,Q}^{(2),\mathrm{TR}} + a_{qq,Q}^{(3),\mathrm{TR}} \quad (28)$$

in the $\overline{\mathrm{MS}}$ scheme, performing mass renormalization in the on-mass-shell scheme. Here, the expansion coefficients of the β function and the mass renormalization constants are, cf. [26,33,34],

$$\beta_0 = \frac{11}{3}C_A - \frac{4}{3}T_F N_f, \quad (29)$$

$$\beta_{1,Q} = -4\left(\frac{5}{3}C_A + C_F\right)T_F, \quad (30)$$

$$\beta_{1,Q}^{(1)} = -\frac{32}{9}T_F C_A + 15 T_F C_F, \quad (31)$$

$$\beta_{1,Q}^{(2)} = -\frac{86}{27}T_F C_A - \frac{31}{4}T_F C_f - \zeta_2 T_F\left(\frac{5}{3}C_A + C_F\right), \quad (32)$$

$$\delta m_1^{(-1)} = 6C_F, \quad (33)$$

$$\delta m_1^{(0)} = -4C_F, \quad (34)$$

$$\delta m_1^{(1)} = \left(4 + \frac{3}{4}\zeta_2\right)C_F, \quad (35)$$

with $C_A = N_c$, and the NLO anomalous dimension $\gamma_{qq}^{(1),\mathrm{TR}}$ reads, cf. [14–16],

$$\gamma_{qq}^{(1),\mathrm{TR}}(N) = C_F^2(4S_2 - 8S_1 - 1) + 8C_F\left(C_F - \frac{C_A}{2}\right)\times\left[-4S_1S_2 - 8S_1S_{-2} + S_1 - 4S_3 - 4S_{-3} + \frac{5}{2}S_2 + 8S_{-2,1} - \frac{1-(-1)^N}{N(N+1)} - \frac{1}{4}\right] + C_F C_A\left(-16S_1S_2 - \frac{58}{3}S_2 + \frac{572}{9}S_1 - \frac{20}{3}\right) + C_F T_F N_f\left(\frac{32}{3}S_2 - \frac{160}{9}S_1 + \frac{4}{3}\right). \quad (36)$$

All contributions to Eq. (28) are known for general values of N, except of $\hat{\gamma}_{qq}^{(2),\mathrm{TR}}$ and $a_{qq,Q}^{(3),\mathrm{TR}}$, the constant contribution to the unrenormalized 3-loop massive OME. Similarly to the vector case, Ref. [26], we calculate $\Delta_T A_{qq,Q}^{(3),\mathrm{NS},\overline{\mathrm{MS}}}(N)$ for a fixed number of Mellin moments. The Feynman diagrams were generated by a code based on QGRAF [35] and the color algebra was performed using COLOR.H [36]. The computation is based on FORM [37] codes using MATAD [38]. Since the projector in Eq. (18)

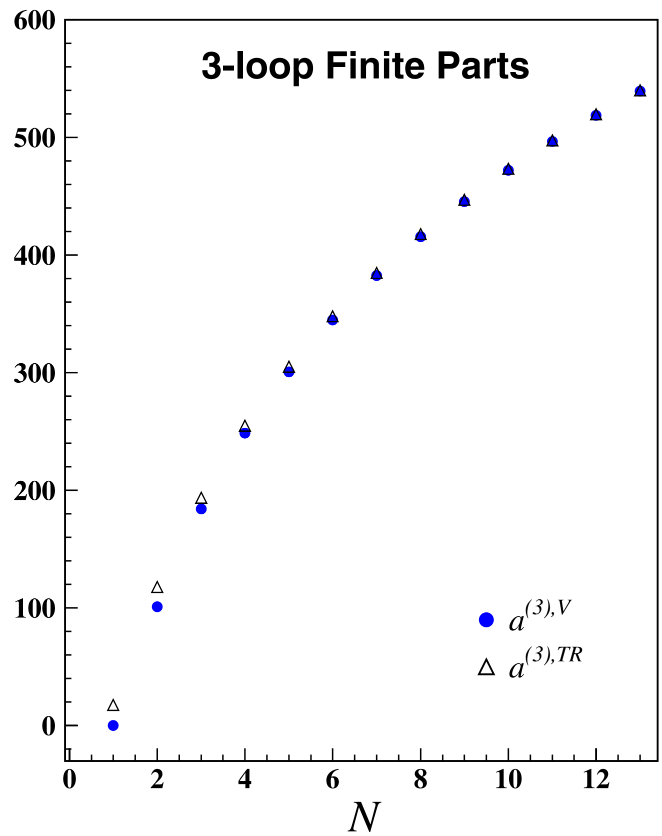

FIG. 1 (color online). The constant part $a_{qq,Q}^{(3)}$ of the unrenormalized flavor nonsinglet massive 3-loop OME in the vector case [26] and for transversity for $N_f = 3$.

has to be applied we can calculate the moments $N = 1$ to 13, i.e. one moment less than in the vector case in Ref. [26], given the complexity of the problem and the computer resources presently available. The computation time amounted to about nine days. The contributions to the 3-loop transversity anomalous dimension, $\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(N)$, and the constant part of the unrenormalized massive transversity OME $a_{qq,Q}^{(3),\mathrm{TR}}(N)$ are given in the Appendix. In Fig. 1 the numerical values of $a_{qq,Q}^{(3),\mathrm{TR}}(N)$ are compared to those of $a_{qq,Q}^{(3),\mathrm{V}}(N)$, Ref. [26]. As has been observed at $O(a_s^2)$ already, for larger values of N both quantities approach each other at $O(a_s^3)$. This also applies to $\hat{\gamma}_{qq}^{(2),(\mathrm{V},\mathrm{TR})}(N)$.

The present calculation confirms the T_F parts of the transversity 3-loop anomalous dimension, which was calculated for $N = 1$ to 8 in Ref. [19] for the first time. We also present the moments $N = 9$ to 13. As a by-product of the present calculation the complete NLO anomalous dimension [14–16] is confirmed for the moments $N = 1$ to 13.

Finally, we show as examples the first moments of the $\overline{\mathrm{MS}}$-renormalized $O(a_s^3)$ massive transversity OME. Unlike the case for the vector current, the first moment does not vanish, since there is no conservation law to enforce this. One obtains

$$\begin{aligned}\Delta_T A_{qq,Q}^{(3),\mathrm{NS},\overline{\mathrm{MS}}}(1) = C_F T_F \Big\{ & \Big(\frac{44}{27}C_A - \frac{16}{27}T_F(N_f+2)\Big)\ln^3\Big(\frac{m^2}{\mu^2}\Big) + \Big(\frac{32}{3}C_F - \frac{106}{9}C_A - \frac{104}{27}T_F\Big)\ln^2\Big(\frac{m^2}{\mu^2}\Big) \\ & + \Big[\Big(\frac{233}{9} + 16\zeta_3\Big)C_F + \Big(-\frac{2233}{81} - 16\zeta_3\Big)C_A - \frac{604}{81}N_f T_F - \frac{496}{81}T_F\Big]\ln\Big(\frac{m^2}{\mu^2}\Big) \\ & + \Big(-\frac{16}{3}B_4 + 24\zeta_4 - \frac{278}{9}\zeta_3 + \frac{7511}{81}\Big)C_F + \Big(\frac{8}{3}B_4 - 24\zeta_4 + \frac{437}{27}\zeta_3 - \frac{34135}{729}\Big)C_A \\ & + \Big(-\frac{6556}{729} + \frac{128}{27}\zeta_3\Big)T_F N_f + \Big(\frac{2746}{729} - \frac{224}{27}\zeta_3\Big)T_F\Big\},\end{aligned} \tag{37}$$

$$\begin{aligned}\Delta_T A_{qq,Q}^{(3),\mathrm{NS},\overline{\mathrm{MS}}}(2) = C_F T_F \Big\{ & \Big(\frac{44}{9}C_A - \frac{16}{9}T_F(N_f+2)\Big)\ln^3\Big(\frac{m^2}{\mu^2}\Big) + \Big(-\frac{34}{3}C_A - 8T_F\Big)\ln^2\Big(\frac{m^2}{\mu^2}\Big) \\ & + \Big[(15 + 48\zeta_3)C_F + \Big(-\frac{73}{9} - 48\zeta_3\Big)C_A - \frac{196}{9}N_f T_F - \frac{496}{27}T_F\Big]\ln\Big(\frac{m^2}{\mu^2}\Big) \\ & + \Big(-16B_4 + 72\zeta_4 - \frac{310}{3}\zeta_3 + \frac{4133}{27}\Big)C_F + \Big(8B_4 - 72\zeta_4 + \frac{533}{9}\zeta_3 - 56\Big)C_A \\ & + \Big(-\frac{1988}{81} + \frac{128}{9}\zeta_3\Big)T_F N_f + \Big(\frac{338}{27} - \frac{224}{9}\zeta_3\Big)T_F\Big\},\end{aligned} \tag{38}$$

with

$$\begin{aligned}B_4 &= -4\zeta_2\ln^2(2) + \tfrac{2}{3}\ln^4(2) - \tfrac{13}{2}\zeta_4 + 16\,\mathrm{Li}_4(\tfrac{1}{2}) \\ &\approx -1.7\,628\,000\,871.\end{aligned} \tag{39}$$

The structure of the massive OME is similar to the result for the unpolarized case, cf. Ref. [26], Eq. (5.57). We checked the moments $N = 1$ to 4 keeping the complete dependence on the gauge-parameter ξ and find that it cancels in the final result. We observe that the massive OME do not depend on ζ_2,[5] as is also the case for the various massive OMEs, which were calculated for vector currents in Ref. [26]. The results for the massive OME for the moments $N = 1$ to 13 and the quantities listed in the Appendix are attached to this paper in FORM format.

Since the light-flavor Wilson coefficients for the processes from which the transversity distribution can be extracted are not known to 2- and 3-loop order, phenomenological studies on the effect of the heavy flavor contributions cannot yet be performed. However, our results can be used in comparisons with upcoming lattice simulations of operator matrix elements with (2 + 1 + 1)-dynamical fermions including the charm quark.

V. REMARKS ON THE SOFFER BOUND

If the Soffer inequality [28]

$$|\Delta_T f(x, Q_0^2)| \leq \tfrac{1}{2}[f(x, Q_0^2) + \Delta f(x, Q_0^2)] \tag{40}$$

holds for the nonperturbative parton distribution functions at a given scale Q_0^2 one may check its generalization at the level of the corresponding structure functions. In the light-flavor case this has been investigated to $O(a_s)$ for the Drell-Yan process in Ref. [16]. For the heavy-flavor corrections

[5]The combination of multiple zeta values B_4 is characteristic for quantities depending on a single mass scale. In this specific combination ζ values at even integer argument contribute.

studied in the present paper one investigates

$$|\Delta_T F(x, Q^2)| \le \tfrac{1}{2}[F(x, Q^2) + \Delta F(x, Q^2)], \qquad (41)$$

where the structure functions are given in Eqs. (3), (5), and (7) and by corresponding relations in the longitudinally polarized case. One may try to separate the evolution effects in the parton distribution functions from those of the Wilson coefficients.

The solution of the nonsinglet evolution equation for the parton distribution $f^{\rm NS}(N, Q_0^2)$ in Mellin space for N_f massless flavors reads to 3-loop order, cf. [39],

$$\begin{aligned} f^{\rm NS}(N, Q^2) &= E(N, Q^2, Q_0^2) f^{\rm NS}(N, Q_0^2) = \left(\frac{a}{a_0}\right)^{\gamma_{qq}^{(0),\rm NS}(N)/\beta_0} \hat{E}(N, Q^2, Q_0^2) f^{\rm NS}(N, Q_0^2) \\ &= \left(\frac{a}{a_0}\right)^{\gamma_{qq}^{(0),\rm NS}(N)/\beta_0} \Bigg\{ 1 - \frac{1}{\beta_0}(a - a_0)\left[-\gamma_{qq}^{(1),\rm NS}(N) + \frac{\beta_1}{\beta_0}\gamma_{qq}^{(0),\rm NS}(N)\right] \\ &\quad - \frac{1}{2\beta_0}(a^2 - a_0^2)\left[-\gamma_{qq}^{(2),\rm NS}(N) + \frac{\beta_1}{\beta_0}\gamma_{qq}^{(1),\rm NS}(N) - \left(\frac{\beta_1^2}{\beta_0^2} - \frac{\beta_2}{\beta_0}\right)\gamma_{qq}^{(0),\rm NS}(N)\right] \\ &\quad + \frac{1}{2\beta_0^2}(a - a_0)^2\left(\gamma_{qq}^{(1),\rm NS}(N) - \frac{\beta_1}{\beta_0}\gamma_{qq}^{(0),\rm NS}(N)\right)^2\Bigg\} f^{\rm NS}(N, Q_0^2), \end{aligned} \qquad (42)$$

where $a_0 = a(Q_0^2)$ and

$$\beta_1 = \tfrac{34}{3}C_A^2 - 4C_F T_F N_f - \tfrac{20}{3}C_A T_F N_f, \qquad (43)$$

$$\begin{aligned} \beta_2 &= \tfrac{2857}{54}C_A^3 + 2C_F^2 T_F N_f - \tfrac{205}{9}C_F C_A T_F N_f - \tfrac{1415}{27}C_A^2 T_F N_f \\ &\quad + \tfrac{44}{9}C_F T_F^2 N_f^2 + \tfrac{158}{27}C_A T_F^2 N_f^2, \end{aligned} \qquad (44)$$

cf. [40]. The moments of the anomalous dimensions for vector currents are given in Ref. [41]. The evolution operator in the unpolarized and the longitudinally polarized case are the same due to a Ward identity. Therefore, it is sufficient to investigate the relation

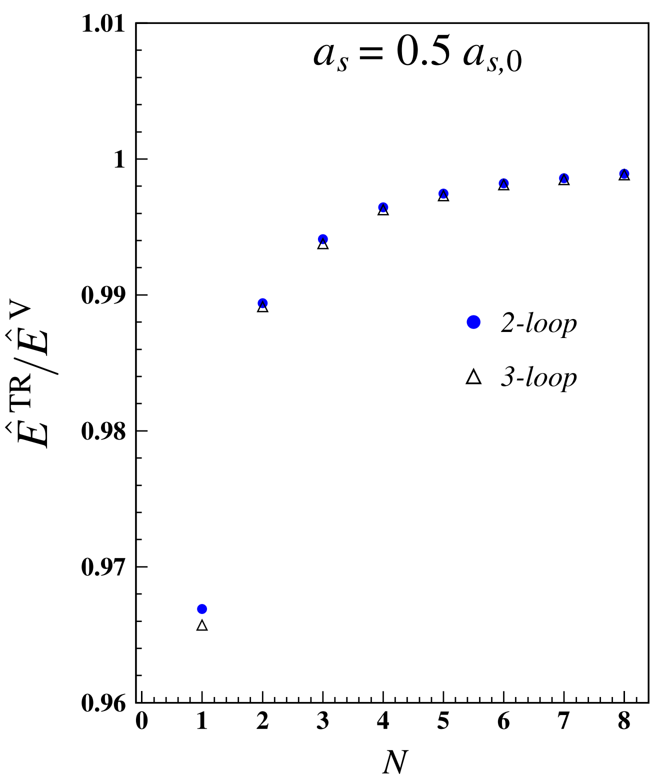

FIG. 2 (color online). Ratio of the evolution operators $\hat{E}^{\rm TR,V}(N)$, Eq. (42), expanded up to the $O(a_s)$ terms (2 loops) and the $O(a_s^2)$ terms (3 loops), respectively, as a function of the Mellin variable N, with $\alpha_{s,0} = 0.3$.

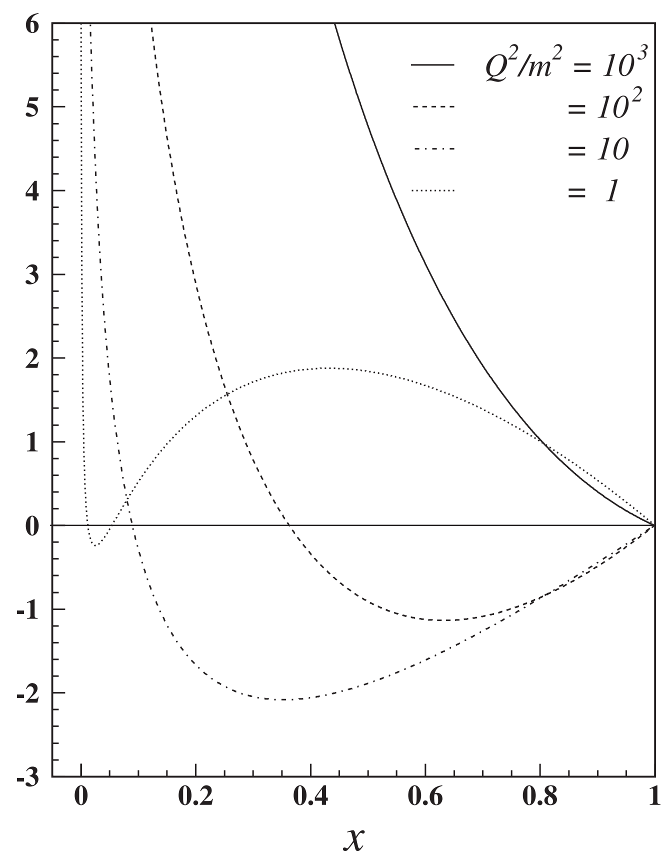

FIG. 3. Difference of the massive OMEs $A_{qq,Q}^{(2),\rm NS,\overline{MS}}(x) - \Delta_T A_{qq,Q}^{(2),\rm NS,\overline{MS}}(x)$, Eq. (46), for different ratios Q^2/m^2.

$$|\Delta_T E(N, Q^2)| \leq E^V(N, Q^2). \tag{45}$$

Up to the $O(a_s)$ corrections (NLO) the validity of this inequality was shown in [16]. Beyond this level only a finite number of Mellin moments can be compared for $\hat{E}^{\rm TR}(N, Q^2, Q_0^2)/\hat{E}^{\rm V}(N, Q^2, Q_0^2)$, for which the 3-loop transversity anomalous dimension is known [19], expanding up to $O(a_s^2)$. This quantity is shown in Fig. 2 for the 2- and 3-loop case. The corresponding correction preserves the Soffer bound for characteristic values of a_s.

Turning to the effect of the heavy-flavor Wilson coefficient in the asymptotic region, Eq. (14), we have to limit the investigation to the massive operator matrix elements since the corresponding light-flavor Wilson coefficients were not yet calculated. In Fig. 3 we show the difference

$$A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}(x) - \Delta_T A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}(x)$$
$$= C_F T_F (1-x)\left\{\frac{4}{3}\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{8}{3}\left(\ln(x) + \frac{11}{3}\right)\ln\left(\frac{m^2}{\mu^2}\right) + \frac{2}{3}\left[\ln^2(x) + \frac{22}{3}\ln(x) + \frac{116}{9}\right]\right\} \tag{46}$$

for a series of values $Q^2 = \mu^2$. At large scales $A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}(x) - \Delta_T A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}(x)$ is positive and descending toward $x \simeq 1$, while at lower scales also negative values are reached in the intermediate region of x. The difference is always positive in the small x region. To maintain the Soffer bound the light-flavor Wilson coefficients have to compensate the negative contributions. In Fig. 4 we show $A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}} - \Delta_T A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}$ in Mellin space, where also a sign change is obtained. The behavior of $A_{qq,Q}^{(3),{\rm NS},\overline{\rm MS}} - \Delta_T A_{qq,Q}^{(3),{\rm NS},\overline{\rm MS}}$, Fig. 5, is quite similar to that shown in Fig. 4 and a corresponding behavior of $A_{qq,Q}^{(3),{\rm NS},\overline{\rm MS}}(x) - \Delta_T A_{qq,Q}^{(3),{\rm NS},\overline{\rm MS}}(x)$ to the one found at $O(a_s^2)$ is expected. From the knowledge of the massive OMEs alone a conclusion on the validity of the Soffer bound at the level of the structure functions can not be drawn before the light-flavor Wilson coefficients have been computed.

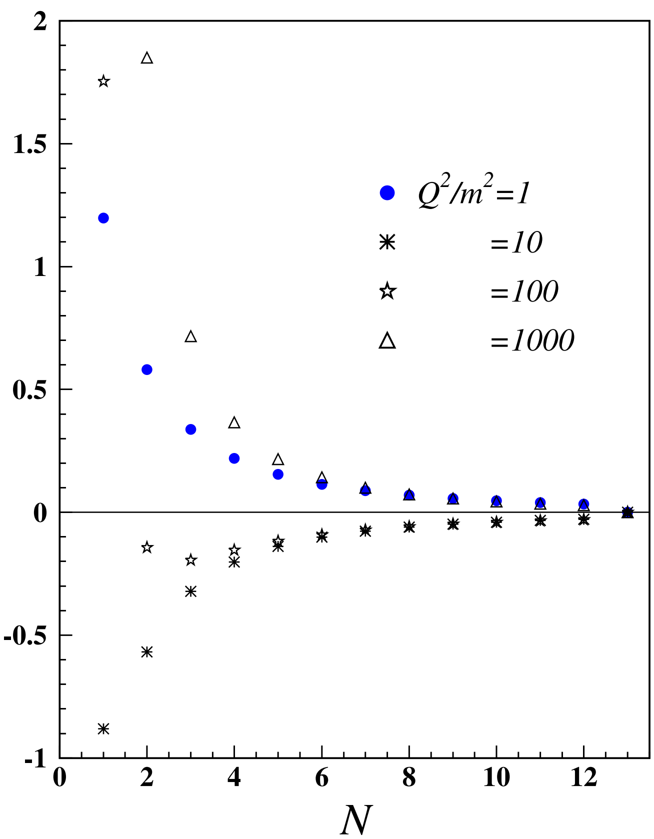

FIG. 4 (color online). Difference of the massive OMEs $A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}(N) - \Delta_T A_{qq,Q}^{(2),{\rm NS},\overline{\rm MS}}(N)$, Eq. (27), and Ref. [22], Eq. (3.35) for different ratios Q^2/m^2.

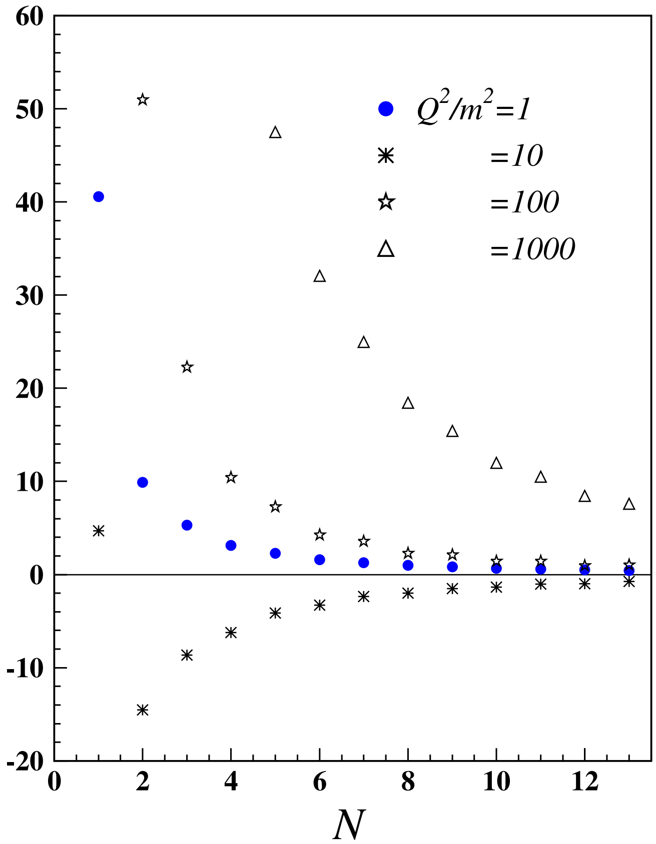

FIG. 5 (color online). Difference of the massive OMEs $A_{qq,Q}^{(3),{\rm NS},\overline{\rm MS}}(N) - \Delta_T A_{qq,Q}^{(3),{\rm NS},\overline{\rm MS}}(N)$, Eq. (28), and Ref. [26], Eq. (4.17) in the $\overline{\rm MS}$-scheme for different ratios Q^2/m^2.

VI. CONCLUSIONS

We calculated the flavor nonsinglet massive OME for transversity at 2-loop order and for the Mellin moments $N = 1$ to 13 at 3-loop order. For large scales $Q^2 \gg m^2$ the heavy flavor Wilson coefficient can be determined from the light-flavor Wilson coefficients and the respective process independent massive operator matrix element computed in the present paper. For flavor nonsinglet quantities the heavy flavor corrections start at $O(a_s^2)$. The measurement of the corresponding scattering cross sections requires high luminosity. In the present calculation we have verified the T_F parts of the 3-loop transversity anomalous dimension for the moments $N = 1$ to 8 and extended this part up to $N = 13$. As a general observation we found that both the anomalous dimension and the expansion coefficients in ε computed in the present calculation for transversity approach those in the vector case for large values of the Mellin parameter N. We investigated the compatibility of the results of the present calculation with the Soffer bound on the level of structure functions. While for the evolution operator the Soffer bound is obeyed to 3-loop order, a final conclusion cannot be drawn for the massive operator matrix element at $O(a_s^2)$ and $O(a_s^3)$ alone concerning the massive Wilson coefficients for the whole phase space, due to a sign change for $A_{qq,Q}^{\mathrm{NS},\overline{\mathrm{MS}}} - \Delta_T A_{qq,Q}^{\mathrm{NS},\overline{\mathrm{MS}}}$ at lower scales of Q^2 and medium values of x. A firm conclusion can only be drawn after the yet unknown massless Wilson coefficients have been computed.

ACKNOWLEDGMENTS

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APPENDIX

The T_F contributions to the 3-loop anomalous dimensions for $N = 1$ to 13 are given by

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(1) = C_F T_F\Big[-\tfrac{8}{3}T_F(2N_f+1) - \tfrac{2008}{27}C_A + \tfrac{196}{9}C_F + 32(C_F - C_A)\zeta_3\Big], \tag{A1}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(2) = C_F T_F\Big[-\tfrac{184}{27}T_F(2N_f+1) - \tfrac{2084}{27}C_A - 60C_F + 96(C_F - C_A)\zeta_3\Big], \tag{A2}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(3) = C_F T_F\Big[-\tfrac{2408}{243}T_F(2N_f+1) - \tfrac{19\,450}{243}C_A - \tfrac{25\,276}{243}C_F + \tfrac{416}{3}(C_F - C_A)\zeta_3\Big], \tag{A3}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(4) = C_F T_F\Big[-\tfrac{14\,722}{1215}T_F(2N_f+1) - \tfrac{199\,723}{2430}C_A - \tfrac{66\,443}{486}C_F + \tfrac{512}{3}(C_F - C_A)\zeta_3\Big], \tag{A4}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(5) = C_F T_F\Big[-\tfrac{418\,594}{30\,375}T_F(2N_f+1) - \tfrac{5\,113\,951}{60\,750}C_A - \tfrac{49\,495\,163}{303\,750}C_F + \tfrac{2944}{15}(C_F - C_A)\zeta_3\Big], \tag{A5}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(6) = C_F T_F\Big[-\tfrac{3\,209\,758}{212\,625}T_F(2N_f+1) - \tfrac{3\,682\,664}{42\,525}C_A - \tfrac{18\,622\,301}{101\,250}C_F + \tfrac{1088}{5}(C_F - C_A)\zeta_3\Big], \tag{A6}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(7) = C_F T_F\Big[-\tfrac{168\,501\,142}{10\,418\,625}T_F(2N_f+1) - \tfrac{1\,844\,723\,441}{20\,837\,250}C_A - \tfrac{49\,282\,560\,541}{243\,101\,250}C_F + \tfrac{8256}{35}(C_F - C_A)\zeta_3\Big], \tag{A7}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(8) = C_F T_F\Big[-\tfrac{711\,801\,943}{41\,674\,500}T_F(2N_f+1) - \tfrac{6\,056\,338\,297}{66\,679\,200}C_A - \tfrac{849\,420\,853\,541}{3\,889\,620\,000}C_F + \tfrac{8816}{35}(C_F - C_A)\zeta_3\Big], \tag{A8}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(9) = C_F T_F\Big[-\tfrac{20\,096\,458\,061}{1\,125\,211\,500}T_F(2N_f+1) - \tfrac{119\,131\,812\,533}{1\,285\,956\,000}C_A - \tfrac{24\,479\,706\,761\,047}{105\,019\,740\,000}C_F + \tfrac{83\,824}{315}(C_F - C_A)\zeta_3\Big], \tag{A9}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(10) = C_F T_F\Big[-\tfrac{229\,508\,848\,783}{12\,377\,326\,500}T_F(2N_f+1) - \tfrac{4\,264\,058\,299\,021}{45\,008\,460\,000}C_A - \tfrac{25\,800\,817\,445\,759}{105\,019\,740\,000}C_F + \tfrac{87\,856}{315}(C_F - C_A)\zeta_3\Big], \tag{A10}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(11) = C_F T_F\Big[-\tfrac{28\,677\,274\,464\,343}{1\,497\,656\,506\,500}T_F(2N_f+1) - \tfrac{75\,010\,870\,835\,743}{778\,003\,380\,000}C_A - \tfrac{396\,383\,896\,707\,569\,599}{1\,537\,594\,013\,340\,000}C_F + \tfrac{1\,006\,736}{3465}(C_F - C_A)\zeta_3\Big], \tag{A11}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(12) = C_F T_F\Big[-\tfrac{383\,379\,490\,933\,459}{19\,469\,534\,584\,500}T_F(2N_f+1) - \tfrac{38\,283\,693\,844\,132\,279}{389\,390\,691\,690\,000}C_A - \tfrac{1\,237\,841\,854\,306\,528\,417}{4\,612\,782\,040\,020\,000}C_F + \tfrac{1\,043\,696}{3465}(C_F - C_A)\zeta_3\Big], \tag{A12}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{TR}}(13) = C_F T_F\Big[-\tfrac{66\,409\,807\,459\,266\,571}{3\,290\,351\,344\,780\,500}T_F(2N_f+1) - \tfrac{6\,571\,493\,644\,375\,020\,121}{65\,807\,026\,895\,610\,000}C_A - \tfrac{36\,713\,319\,015\,407\,141\,570\,017}{131\,745\,667\,845\,011\,220\,000}C_F + \tfrac{14\,011\,568}{45\,045}(C_F - C_A)\zeta_3\Big]. \tag{A13}$$

The constant parts $a_{qq,Q}^{(3),\mathrm{TR}}(N)$ of the massive 3-loop OME for $N = 1$ to 13 are given by

$$a_{qq,Q}^{(3),\mathrm{TR}}(1) = C_F T_F\Big[\Big(\tfrac{481}{27}\zeta_3 + \tfrac{8}{3}B_4 - 24\zeta_4 - \tfrac{61}{27}\zeta_2 - \tfrac{26\,441}{1458}\Big)C_A + \Big(-\tfrac{52}{27}\zeta_2 + \tfrac{112}{27}\zeta_3 - \tfrac{15\,850}{729}\Big)N_f T_F + \Big(-\tfrac{104}{27}\zeta_2 - \tfrac{6548}{729} - \tfrac{256}{27}\zeta_3\Big)T_F + \Big(-\tfrac{278}{9}\zeta_3 + \tfrac{49}{3}\zeta_2 + \tfrac{15\,715}{162} - \tfrac{16}{3}B_4 + 24\zeta_4\Big)C_F\Big], \tag{A14}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(2) = C_F T_F\Big[\Big(\frac{577}{9}\zeta_3 + 8B_4 - 72\zeta_4 + \frac{1}{3}\zeta_2 + \frac{1043}{162}\Big)C_A + \Big(-4\zeta_2 + \frac{112}{9}\zeta_3 - \frac{4390}{81}\Big)N_f T_F + \Big(-8\zeta_2 - \frac{1388}{81} - \frac{256}{9}\zeta_3\Big)T_F + \Big(-\frac{310}{3}\zeta_3 + 33\zeta_2 + \frac{10255}{54} - 16B_4 + 72\zeta_4\Big)C_F\Big], \tag{A15}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(3) = C_F T_F\Big[\Big(\frac{40001}{405}\zeta_3 + \frac{104}{9}B_4 - 104\zeta_4 + \frac{121}{81}\zeta_2 + \frac{327967}{21870}\Big)C_A + \Big(-\frac{452}{81}\zeta_2 + \frac{1456}{81}\zeta_3 - \frac{168704}{2187}\Big)N_f T_F + \Big(-\frac{904}{81}\zeta_2 - \frac{52096}{2187} - \frac{3328}{81}\zeta_3\Big)T_F + \Big(-\frac{1354}{9}\zeta_3 + \frac{3821}{81}\zeta_2 + \frac{1170943}{4374} - \frac{208}{9}B_4 + 104\zeta_4\Big)C_F\Big], \tag{A16}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(4) = C_F T_F\Big[\Big(\frac{52112}{405}\zeta_3 + \frac{128}{9}B_4 - 128\zeta_4 + \frac{250}{81}\zeta_2 + \frac{4400353}{218700}\Big)C_A + \Big(-\frac{554}{81}\zeta_2 + \frac{1792}{81}\zeta_3 - \frac{20731907}{218700}\Big)N_f T_F + \Big(-\frac{1108}{81}\zeta_2 - \frac{3195707}{109350} - \frac{4096}{81}\zeta_3\Big)T_F + \Big(-\frac{556}{3}\zeta_3 + \frac{4616}{81}\zeta_2 + \frac{56375659}{174960} - \frac{256}{9}B_4 + 128\zeta_4\Big)C_F\Big], \tag{A17}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(5) = C_F T_F\Big[\Big(\frac{442628}{2835}\zeta_3 + \frac{736}{45}B_4 - \frac{736}{5}\zeta_4 + \frac{8488}{2025}\zeta_2 + \frac{1436867309}{76545000}\Big)C_A + \Big(-\frac{15962}{2025}\zeta_2 + \frac{10304}{405}\zeta_3 - \frac{596707139}{5467500}\Big)N_f T_F + \Big(-\frac{31924}{2025}\zeta_2 - \frac{92220539}{2733750} - \frac{23552}{405}\zeta_3\Big)T_F + \Big(-\frac{47932}{225}\zeta_3 + \frac{662674}{10125}\zeta_2 + \frac{40410914719}{109350000} - \frac{1472}{45}B_4 + \frac{736}{5}\zeta_4\Big)C_F\Big], \tag{A18}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(6) = C_F T_F\Big[\Big(\frac{172138}{945}\zeta_3 + \frac{272}{15}B_4 - \frac{816}{5}\zeta_4 + \frac{10837}{2025}\zeta_2 + \frac{807041747}{53581500}\Big)C_A + \Big(-\frac{17762}{2025}\zeta_2 + \frac{3808}{135}\zeta_3 - \frac{32472719011}{267907500}\Big)N_f T_F + \Big(-\frac{35524}{2025}\zeta_2 - \frac{5036315611}{133953750} - \frac{8704}{135}\zeta_3\Big)T_F + \Big(-\frac{159296}{675}\zeta_3 + \frac{81181}{1125}\zeta_2 + \frac{14845987993}{36450000} - \frac{544}{15}B_4 + \frac{816}{5}\zeta_4\Big)C_F\Big], \tag{A19}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(7) = C_F T_F\Big[\Big(\frac{27982}{135}\zeta_3 + \frac{688}{35}B_4 - \frac{6192}{35}\zeta_4 + \frac{620686}{99225}\zeta_2 + \frac{413587780793}{52509870000}\Big)C_A + \Big(-\frac{947138}{99225}\zeta_2 + \frac{1376}{45}\zeta_3 - \frac{1727972700289}{13127467500}\Big)N_f T_F + \Big(-\frac{1894276}{99225}\zeta_2 - \frac{268946573689}{6563733750} - \frac{22016}{315}\zeta_3\Big)T_F + \Big(-\frac{8454104}{33075}\zeta_3 + \frac{90495089}{1157625}\zeta_2 + \frac{12873570421651}{29172150000} - \frac{1376}{35}B_4 + \frac{6192}{35}\zeta_4\Big)C_F\Big], \tag{A20}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(8) = C_F T_F\Big[\Big(\frac{87613}{378}\zeta_3 + \frac{2204}{105}B_4 - \frac{6612}{35}\zeta_4 + \frac{11372923}{1587600}\zeta_2 - \frac{91321974347}{112021056000}\Big)C_A + \Big(-\frac{2030251}{198450}\zeta_2 + \frac{4408}{135}\zeta_3 - \frac{29573247248999}{210039480000}\Big)N_f T_F + \Big(-\frac{2030251}{99225}\zeta_2 - \frac{4618094363399}{105019740000} - \frac{70528}{945}\zeta_3\Big)T_F + \Big(-\frac{9020054}{33075}\zeta_3 + \frac{171321401}{2058000}\zeta_2 + \frac{1316283829306051}{2800526400000} - \frac{4408}{105}B_4 + \frac{6612}{35}\zeta_4\Big)C_F\Big], \tag{A21}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(9) = C_F T_F\Big[\Big(\frac{9574759}{37422}\zeta_3 + \frac{20956}{945}B_4 - \frac{20956}{105}\zeta_4 + \frac{16154189}{2041200}\zeta_2 - \frac{17524721583739067}{1497161413440000}\Big)C_A + \Big(-\frac{19369859}{1786050}\zeta_2 + \frac{41912}{1215}\zeta_3 - \frac{2534665670688119}{17013197880000}\Big)N_f T_F + \Big(-\frac{19369859}{893025}\zeta_2 - \frac{397003835114519}{8506598940000} - \frac{670592}{8505}\zeta_3\Big)T_F + \Big(-\frac{85698286}{297675}\zeta_3 + \frac{131876277049}{1500282000}\zeta_2 + \frac{1013649109952401819}{2041583745600000} - \frac{41912}{945}B_4 + \frac{20956}{105}\zeta_4\Big)C_F\Big], \tag{A22}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(10) = C_F T_F\Big[\Big(\frac{261607183}{935550}\zeta_3 + \frac{21964}{945}B_4 - \frac{21964}{105}\zeta_4 + \frac{618627019}{71442000}\zeta_2 - \frac{176834434840947469}{7485807067200000}\Big)C_A + \Big(-\frac{4072951}{357210}\zeta_2 + \frac{43928}{1215}\zeta_3 - \frac{321908083399769663}{2058596943480000}\Big)N_f T_F + \Big(-\frac{4072951}{178605}\zeta_2 - \frac{50558522757917663}{1029298471740000} - \frac{702848}{8505}\zeta_3\Big)T_F + \Big(-\frac{3590290}{11907}\zeta_3 + \frac{137983320397}{1500282000}\zeta_2 + \frac{11669499797141374121}{22457421201600000} - \frac{43928}{945}B_4 + \frac{21964}{105}\zeta_4\Big)C_F\Big], \tag{A23}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(11) = C_F T_F\Big[\Big(\frac{3687221539}{12162150}\zeta_3 + \frac{251684}{10395}B_4 - \frac{251684}{1155}\zeta_4 + \frac{149112401}{16038000}\zeta_2 - \frac{436508000489627050837}{11775174516705600000}\Big)C_A + \Big(-\frac{514841791}{43222410}\zeta_2 + \frac{503368}{13365}\zeta_3 - \frac{40628987857774916423}{249090230161080000}\Big)N_f T_F + \Big(-\frac{514841791}{21611205}\zeta_2 - \frac{6396997235105384423}{124545115080540000} - \frac{8053888}{93555}\zeta_3\Big)T_F + \Big(-\frac{452259130}{1440747}\zeta_3 + \frac{191230589104127}{1996875342000}\zeta_2 + \frac{177979311179110818909401}{328799103812625600000} - \frac{503368}{10395}B_4 + \frac{251684}{1155}\zeta_4\Big)C_F\Big], \tag{A24}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(12) = C_F T_F\Big[\Big(\frac{85827712409}{8644482000}\zeta_2 - \frac{245210883820358086333}{4783664647411650000} + \frac{260924}{10395}B_4 - \frac{260924}{1155}\zeta_4 + \frac{3971470819}{12162150}\zeta_3\Big)C_A + \Big(-\frac{7126865031281296825487}{42096248897222520000} + \frac{521848}{13365}\zeta_3 - \frac{535118971}{43222410}\zeta_2\Big)N_f T_F + \Big(-\frac{8349568}{93555}\zeta_3 - \frac{535118971}{21611205}\zeta_2 - \frac{1124652164258976877487}{21048124448611260000}\Big)T_F + \Big(\frac{260924}{1155}\zeta_4 + \frac{2396383721714622551610173}{4274388349564132800000} - \frac{468587596}{1440747}\zeta_3 - \frac{521848}{10395}B_4 + \frac{198011292882437}{1996875342000}\zeta_2\Big)C_F\Big], \tag{A25}$$

$$a_{qq,Q}^{(3),\mathrm{TR}}(13) = C_F T_F\Big[\Big(\frac{15\,314\,434\,459\,241}{1\,460\,917\,458\,000}\zeta_2 - \frac{430\,633\,219\,615\,523\,278\,883\,051}{6\,467\,514\,603\,300\,550\,800\,000} + \frac{3\,502\,892}{135\,135}B_4 - \frac{3\,502\,892}{15\,015}\zeta_4 + \frac{327\,241\,423}{935\,550}\zeta_3\Big)C_A + \Big(-\frac{1\,245\,167\,831\,299\,024\,242\,467\,303}{7\,114\,266\,063\,630\,605\,880\,000} + \frac{7\,005\,784}{173\,745}\zeta_3 - \frac{93\,611\,152\,819}{7\,304\,587\,290}\zeta_2\Big)N_f T_F + \Big(-\frac{112\,092\,544}{1\,216\,215}\zeta_3 - \frac{93\,611\,152\,819}{3\,652\,293\,645}\zeta_2 - \frac{196\,897\,887\,865\,971\,730\,295\,303}{3\,557\,133\,031\,815\,302\,940\,000}\Big)T_F + \Big(\frac{3\,502\,892}{15\,015}\zeta_4 + \frac{70\,680\,445\,585\,608\,577\,308\,861\,582\,893}{122\,080\,805\,651\,901\,196\,900\,800\,000} - \frac{8\,173\,5983\,092}{243\,486\,243}\zeta_3 - \frac{7\,005\,784}{135\,135}B_4 + \frac{449\,066\,258\,795\,623\,169}{4\,387\,135\,126\,374\,000}\zeta_2\Big)C_F\Big]. \quad \text{(A26)}$$

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