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Subtraction method for NLO corrections in Monte-Carlo event generators for leptoproduction

John Collins

Physics Department, Penn State University
104 Davey Laboratory, University Park PA 16802, USA
E-mail: collins@phys.psu.edu

Abstract: In the case of the gluon-fusion process in deep-inelastic leptoproduction, I explicitly show how to incorporate NLO corrections in a Monte-Carlo event generator by a subtraction method. I calculate the parton densities to be used by the event generator in terms of $\overline{\rm MS}$ densities. The method is generalizable. A particular motivation for treating the gluon-fusion process is to treat diffractive deep-inelastic scattering properly, since in diffractive scattering the gluon density dominates the quark densities. I also propose a modified algorithm for treating parton kinematics in event generators; the new algorithm results in much simpler formulae for the NLO corrections. A disadvantage of the new method is that some of the generated events may have negative weights. However, an adjustable cut-off function is present in the formalism, and this permits a renormalization-group-like transformation that can be used to at least reduce the proportion of events with negative weights.

Keywords: QCD, NLO Computations, Deep Inelastic Scattering.

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Contents

1. Introduction

In an event generator for leptoproduction[1] one has a choice of generating events either by using the lowest-order parton model process or using the next-to-leading order (NLO) hard scattering matrix elements (for photon-gluon fusion, etc). The first case is suitable for the total DIS cross section, where one neglects the NLO subprocesses, since they represent order α_s corrections to the basic process. The second case is suitable, for example, when two-jet production is to be calculated.

Ideally, one wants to include both the LO and the NLO terms to get good accuracy. The problem is particularly acute in *diffractive* DIS, since the gluon density

[1] Of course, exactly similar considerations apply to event generators for other processes.

is substantially larger than the quark density. Thus the gluon-induced NLO subprocess is not necessarily smaller than the LO parton model process. This implies that inclusion of the photon-gluon term is mandatory to get a sensible phenomenology. However, the initial-state showering associated with the LO process already includes part of the photon-gluon process, and it is not at all obvious how the two terms are to be combined.

In this paper, I explain how to consistently use both terms in an event generator-like LEPTO [1] or RAPGAP [2] that uses the algorithm constructed by Bengtsson and Sjöstrand [3] for initial-state showering. As a consequence of their method for treating the exact parton kinematics, the resulting formulae have a non-linear dependence on the parton densities. Therefore, I also propose an alternative leading-order algorithm for which the corresponding NLO corrections have a conventional structure.

With the exception of the recent paper by Friberg and Sjöstrand [4], previous attempts, e.g. [5, 6], at incorporating NLO corrections have tended to implement them by a reweighting of the events generated by showering from the LO matrix elements. In contrast, the subtraction method that I describe involves generating two classes of events. One class is made from the LO parton-model process by showering the initial- and final- state quarks, exactly as at present. The second class of events is generated by starting with a photon-gluon fusion process, and showering the partons, again exactly as at present, but with one exception. The exception is that the hard cross section for the photon-gluon fusion subprocess is equipped with a subtraction that correctly compensates the double counting between the two classes of events; the subtraction removes that part of the photon-gluon fusion term that is included in the LO parton model plus showering calculation. My method is rather similar to the one outlined by Friberg and Sjöstrand in [4].

Of course, there is no physical distinction between the two classes of events; they populate the same regions of state space, and the events differ only in how the program generates them. Indeed the relative contributions of the two classes of events can be changed by changing the cutoff on the virtuality of lines in the parton showering. A change of this cut-off amounts to a renormalization-group transformation, and does not affect the physical cross section, aside from the error due to uncalculated higher-order corrections.

There is a contrast with the standard subtraction method used in analytic calculations. In that method an infinite number of positive weighted events is generated from the basic photon-gluon fusion graphs. The subtraction term gives an infinite number of events with negative weights and somewhat different kinematics. Although the infinities cancel in the integral over the hadronic final states, the integrand is totally unsuitable for use in an event generator. The new method does the subtractions point-by-point in the integrand, so that a Monte-Carlo integration is entirely satisfactory.

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It is true that a finite number of events with finite negative weights may be generated with my algorithm. This is at least a potential disadvantage, particularly if it is desired to compare the results directly with data. I will discuss this problem in more detail in section 5. There I will show how to overcome this problem, to a large extent, by adjustment of a cut-off function that is present in any Monte-Carlo algorithm. I will also explain that if an event generator gives a small number of negative weighted events, this is not necessarily a severe disadvantage.

Since an important immediate application is to deal with the problem of the large gluon density in diffractive DIS, I give results for the photon-gluon fusion process. This case is technically simple because there are no soft gluon effects and no virtual graphs. However, the method is capable of being generalized.

In section 2, I summarize the basic algorithm used in the event generator at LO, and then compute the corresponding first-order term for the photon-gluon fusion process. Then in section 3, I explain the observation of Bengtsson and Sjöstrand [3] that the intended kinematics for the target hadron are not correctly reproduced. After reviewing the implementation of their correction to the kinematics, I obtain the corrected first-order cross section, from which I compute the subtracted gluon-fusion cross section. This forms the primary quantitative result of this paper: it is intended to be directly implemented in an event generator. The parton densities are not in the $\overline{\mathrm{MS}}$ scheme, so I show how to relate them to the ordinary $\overline{\mathrm{MS}}$ parton densities. Unfortunately the resulting formulae are rather complicated; in fact, they are non-linear functionals of the parton densities. So in section 4, I present a new algorithm for treating the parton kinematics and show that the resulting NLO corrections are simpler and more conventional than with the Bengtsson-Sjöstrand algorithm. In section 5, I discuss the problem that events with negative weights may be generated, and show how they may be at least reduced in number. Finally, I summarize the directions for future work in section 6.

2. Basic Monte-Carlo algorithm

2.1 Algorithm

I first review the algorithm [3] used in LEPTO or RAPGAP. Only the first part of the algorithm will be relevant for our later discussions:[2]

1. Generate values of x and y (and hence Q) from the LO cross section for DIS:

$$\frac{d\sigma}{dx\,dy} = K F_2(x, Q^2)\,, \tag{2.1}$$

[2]I describe the algorithm for the case of fully inclusive DIS. The case of diffractive DIS is handled by changing the proton to a Pomeron, by replacing the variable x by β, etc.

with

$$K = \frac{4\pi\alpha_{\rm em}^2}{sx^2y^2}\left(1 - y + \frac{y^2}{2}\right), \tag{2.2}$$

and

$$F_2 = \sum_a e_a^2 x f_a(x, Q^2)\,. \tag{2.3}$$

Here, the sum is over all flavors of quarks and antiquarks, and f_a is the parton probability density.

2. Generate a virtuality Q_1^2 for the incoming quark a, a longitudinal momentum fraction z_1 for the first branching, and an azimuthal angle ϕ for this branching. The distributions arise from the Sudakov form factor

$$\begin{aligned} S_a\left(x, Q^2_{\rm max}, Q_1^2\right) = \exp\Bigg\{ -\int_{Q_1^2}^{Q^2_{\rm max}} \frac{dQ'^2}{Q'^2}\frac{\alpha_s\left(Q'^2\right)}{2\pi} \times \\ \times \sum_c \int_x^1 \frac{dz}{z} P_{c\to ab}\left(z\right)\frac{f_c(x/z, Q'^2)}{f_a(x, Q'^2)}\Bigg\}\,. \end{aligned} \tag{2.4}$$

Here $Q^2_{\rm max}$ is normally set equal to Q^2. The Sudakov form factor is the probability that the virtuality of the struck quark is less than Q_1^2.

3. Iterate the branching for all initial-state and final-state partons until no further branchings are possible.

4. Generate 4-vectors for the momenta of all the generated partons.

2.2 First-order term in Monte-Carlo

Our aim in this paper is to calculate the NLO contribution to deep-inelastic scattering from gluon-fusion graphs like figure 1. The result is to be accurate for the case that the incoming gluon, of momentum p_3, has virtuality and transverse momentum small compared with Q, and that the intermediate quark, of momentum p_1, has a virtuality of order Q^2. To avoid double counting, it is necessary to subtract the contribution in this region that is obtained from the showering algorithm applied to the initial- and final-state partons of the LO partonic cross section.

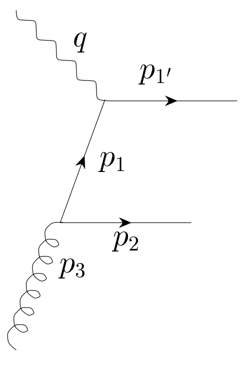

Figure 1: Photon-gluon fusion.

This contribution is obtained by multiplying the lowest-order cross section, from eqs. (2.1)–(2.3), by the the first-order term in the expansion of the Sudakov form factor (2.4) in powers of $\alpha_s(Q^2)$. This is made differential in the momenta of the particles involved, and the gluon-induced term is selected:

$$\frac{d\sigma}{dx\,dy\,dQ_1^2\,dz_1\,d\phi} = K\sum_a e_a^2\frac{\alpha_s\left(Q^2\right)}{4\pi^2 Q_1^2}C\left(Q_1^2\right)P(z_1)\frac{x}{z_1}f_g\left(x/z_1,Q^2\right). \qquad (2.5)$$

Here the splitting kernel is for $g \to$ quark + antiquark: $P(z_1) = P_{g\to q\bar{q}}(z_1) = \frac{1}{2}(1 - 2z_1 + 2z_1^2)$. Note that because we are doing a strict expansion in powers of $\alpha_s(Q^2)$, the scale argument of the parton density is Q^2. The function $C(Q_1^2)$ is a cut-off function that gives the maximum value of Q_1^2. To reproduce the upper limit on the Q'^2 integral in the Sudakov form factor, eq. (2.4), one sets $C(Q_1^2) = \theta(Q^2 - Q_1^2)$. However, as explained in the introduction, one can envisage changing the cut-off function.

One might worry that a full Sudakov form factor should appear in eq. (2.5), to represent the actual physical suppression of the cross section at low Q_1^2. In fact, the Sudakov form factor should not be used in this formula, since the raison d'être of (2.5) is to be a subtraction term for the NLO contribution to the cross section. The unsubtracted NLO contribution — eq. (3.20) below — has the same singularity and lacks a Sudakov factor. The subtraction will cancel the singularity — see eq. (3.21) — to leave an NLO term that is dominantly in the region of large Q_1^2. Thus a strict expansion to lowest order in $\alpha_s(Q^2)$ is appropriate, and a resummation of higher-order terms, such as is represented by the Sudakov form factor, is not needed.

3. Bengtsson and Sjöstrand algorithm

Bengtsson and Sjöstrand [3] give a prescription for the 4-momenta of the partons, and we now apply it to our first-order calculation. In this scheme, the 4-vectors for the momenta q, p_1 and p_3 of the virtual photon, the intermediate quark and the incoming gluon obey the following requirements:

1. q^μ is the correct value of the photon's momentum.

2. The proton is to be moving in the $-z$ direction.

3. $p_1^2 = -Q_1^2$.

4. $(p_1+q)^2 = (p_3-p_1)^2 = p_3^2 = 0$.

5. $z_1 = \dfrac{p_1\cdot(p_1+q)}{p_3\cdot(p_3+q)}$.

In the $\gamma^* g$ center-of-mass frame, we therefore have

$$q^\mu = \frac{Q(1-Q_1^2/Q^2)}{2\sqrt{z_1(1-z_1-Q_1^2/Q^2)}}\left(1-\frac{2z_1}{1-Q_1^2/Q^2},\mathbf{0}_T,1\right), \qquad (3.1)$$

$$
\begin{aligned}
p_{1'}^{\mu} &= \frac{Q\sqrt{1-z_1-Q_1^2/Q^2}}{2\sqrt{z_1}} \times \\
&\times \left(1, \frac{2Q_1}{Q}\frac{\sqrt{z_1\left[1-(1+z_1)Q_1^2/Q^2\right]}}{1-Q_1^2/Q^2}\mathbf{n}_T, 1-\frac{2z_1Q_1^2/Q^2}{1-Q_1^2/Q^2}\right),
\end{aligned} \tag{3.2}
$$

$$
\begin{aligned}
p_{2}^{\mu} &= \frac{Q\sqrt{1-z_1-Q_1^2/Q^2}}{2\sqrt{z_1}} \times \\
&\times \left(1, -\frac{2Q_1}{Q}\frac{\sqrt{z_1\left[1-(1+z_1)Q_1^2/Q^2\right]}}{1-Q_1^2/Q^2}\mathbf{n}_T, -1+\frac{2z_1Q_1^2/Q^2}{1-Q_1^2/Q^2}\right),
\end{aligned} \tag{3.3}
$$

$$
p_3^{\mu} = \frac{Q\,(1-Q_1^2/Q^2)}{2\sqrt{z_1(1-z_1-Q_1^2/Q^2)}}\,(1, \mathbf{0}_T, -1)\,. \tag{3.4}
$$

Here $\mathbf{n}_T$ is a unit transverse vector in the direction defined by the azimuthal angle ϕ. The components are in the order $(0, \text{transverse}, z)$.

We now transform the cross section in eq. (2.5) into convenient variables for a hard scattering describing photon-gluon fusion.

The scattering angle obeys

$$
\cos\theta = \frac{p_1^z + q^z}{p_1^0 + q^0} = 1 - \frac{2z_1Q_1^2/Q^2}{1-Q_1^2/Q^2}\,. \tag{3.5}
$$

The fractional momentum of the gluon is defined in [3] to be

$$
x_3 = \frac{p_3\cdot(p_3+q)}{p\cdot q} = \frac{x}{z_1}\left(1-\frac{Q_1^2}{Q^2}\right), \tag{3.6}
$$

where p^{μ} is the proton's momentum. Up to a correction of order m^2/Q^2, this definition agrees with the definition in terms of light-front variables: $x_3 = (p_3^0 - p_3^z)/(p^0 - p^z)$, since the gluon is on-shell with zero transverse momentum.

We will also use the inverse transformation, to give Q_1^2 and z_1 in terms of x_3 and θ:

$$
\frac{Q_1^2}{Q^2} = (1-\cos\theta)\,\frac{x_3}{2x}\,, \qquad z_1 = \frac{x}{x_3} - \frac{1}{2}\,(1-\cos\theta)\,. \tag{3.7}
$$

The Jacobian of the transformation is

$$
\frac{\partial(x_3, \cos\theta)}{\partial(z_1, Q_1^2)} = \frac{2x}{z_1 Q^2}\,, \tag{3.8}
$$

Then the cross section is:

$$\frac{d\sigma^{(\mathrm{BS1})}_{\mathrm{shower}}}{dx\,dy\,dx_3\,d\cos\theta\,d\phi} = K\sum_a e_a^2 \frac{\alpha_s\left(Q^2\right)}{4\pi^2} C\left(Q_1^2\right) \times \\ \times \frac{1}{1-\cos\theta}\, P\left(\frac{x}{x_3} - \frac{1}{2}(1-\cos\theta)\right) \frac{x}{x_3} f_g\left(x/z_1, Q^2\right) . \tag{3.9}$$

The superscript on the cross section is "BS1" rather than "BS". This anticipates that we will be forced to change the algorithm; it is the modified cross section that will be denoted by a superscript "BS".

3.1 Inconsistency in kinematics

Observe that in eq. (3.9) the fractional momentum argument of the gluon density is x/z_1 rather than the actual fractional momentum of the gluon, x_3.

This is a symptom of the inconsistency explained by Bengtsson and Sjöstrand [3]. The problem can be seen quite dramatically by applying our first-order calculation to the case of a gluon target. In that case the density of gluons is a delta-function: $f_g(x_3, Q_1^2) = \delta(x_3 - 1)$, and the generated value of z_1 is x, from eq. (2.5). But then the definitions of the parton 4-momenta imply that the fractional momentum of the gluon is $x_3 = 1 - Q_1^2/Q^2$ — see eq. (3.6) — instead of the correct value of $x_3 = 1$.

3.2 Parton model

What has gone wrong can be explained by examining the derivation of the parton-model formula. We consider graphs for deep inelastic scattering that have the form of figure 2. For our purposes we can ignore polarization effects, so that the contribution of this graph to the structure function is

$$F = \frac{Q^2}{2\pi} \int \frac{d^4 p_1}{(2\pi)^4} L(p, p_1)\, H\left(q^2, p_1^2, p_{1'}^2\right) U\left(p_{1'}^2\right) . \tag{3.10}$$

Here L represents the lower part of the graph, H represents the hard scattering, and U represents the upper part of the graph, The overall factor Q^2 in the definition of the structure function ensures that it obeys Bjorken scaling, and the overall factor $1/2\pi$ gives it the standard normalization

We now use light-front coordinates [defined by $V^\mu = (V^+, V^-, \mathbf{v}_\perp)$, with $V^\pm = (V^0 \pm V^z)/\sqrt{2}$]:

$$p^\mu = \left(m^2/2p^-, p^-, \mathbf{0}_\perp\right) , \tag{3.11}$$

$$q^\mu = \left(Q^2/2xp^-, -xp^-, \mathbf{0}_\perp\right) , \tag{3.12}$$

$$p_1^\mu = \left(p_1^+, \xi p^-, \mathbf{p}_{1,\perp}\right) , \tag{3.13}$$

$$p_{1'}^\mu = \left((Q^2 + xm^2)/2xp^-, (\xi - x)p^-, \mathbf{p}_{1,\perp}\right) . \tag{3.14}$$

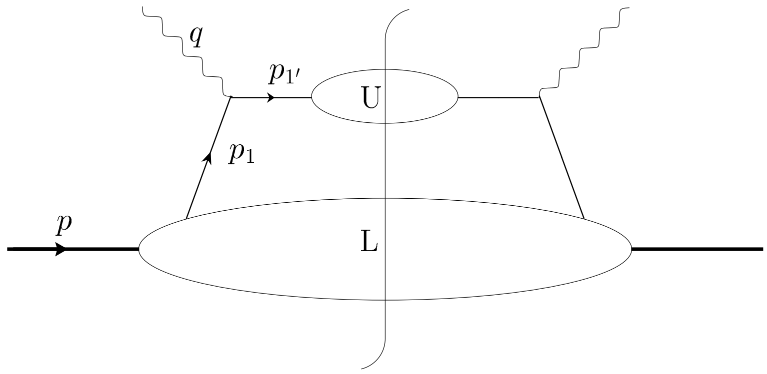

Figure 2: The parton model for deep inelastic scattering is derived from cut graphs of this form.

The parton-model approximation to the graph is obtained by making approximations that are appropriate if the incoming and outgoing quarks, p_1 and p'_1 have small transverse momenta and virtualities, relative to Q. To make this quantitative, we let the magnitudes of $p^2_{1\perp}$, p^2_1, and $p^2_{1'}$ be M^2. Then $\xi = x + O(M^2/Q^2)$. Up to a power-suppressed correction, we can replace H by its value with massless quarks, $H(q^2, 0, 0)$, and we can replace the value of $p_1^- = \xi p^-$ in L by xp^-. A shift in the integration over ξ then gives the factorized form:

$$
\begin{aligned}
F &= \left[xp^- \int \frac{dp_1^+ d^2\mathbf{p}_{1,\perp}}{(2\pi)^4} L\left(p, \left(p_1^+, xp^-, \mathbf{p}_{1,\perp}\right)\right) \right] H(q^2, 0, 0) \left[\int \frac{dp_{1'}^2}{2\pi} \, dU\left(p_{1'}^2\right) \right] + \\
&\quad + O\left(M^2/Q^2\right) \\
&= f(x) H(q^2, 0, 0) D + O(M^2/Q^2) \,. \qquad (3.15)
\end{aligned}
$$

Here the parton density $f(x)$ is defined by the usual light-front operator. The fragmentation function D is the integral over the discontinuity of a propagator, so that it is equal to unity if the integral is convergent.

The above derivation is exactly correct in a super-renormalizable field theory, for then all the integrals over virtualities are convergent in the approximated integral. In a real theory, like QCD, there are ultra-violet divergences that need to be renormalized. The correct physics is obtained in the factorization theorem which shows that the above result is valid up to higher-order corrections in $\alpha_s(Q^2)$.

3.3 Correction to the kinematics of initial-state showering

In the parton-model formula (3.15), the hard scattering has been replaced by a massless approximation with zero transverse momentum. Moreover, in the usual way of estimating the graph, the quark entering the fragmentation function is given zero transverse momentum, and it is given a minus component of momentum equal to $(\xi - x)p^-$. For a calculation of the inclusive cross section this use of approximated kinematics is correct, since the hadronic final-state is integrated over. But for the exclusive calculation, as in an event generator, the use of approximated kinematics is wrong, and it results in the inconsistent kinematics noted in section 3.1.

The inconsistency is in the definitions of the variable specifying the longitudinal momentum of the quark p_1. Bengtsson and Sjöstrand [3] effectively[3] define this variable by

$$x_1 = \frac{p_1 \cdot (p_1 + q)}{p \cdot q} \,. \tag{3.16}$$

In contrast, the calculation of the Sudakov form factor in eq. (2.4) assumes that the fractional momentum of the struck quark equals the Bjorken variable x, an assumption that is only valid in the limit that transverse momenta, masses and virtualities are negligible with respect to Q.

Hence the inconsistency arises because we have specified the fractional momentum of p_1 in two ways. On the one hand the momentum p_1^μ is determined once one has specified the virtualities of all the lines, the z_1 variable for the first branching, and the fractional momentum of the incoming parton. On the other hand we asserted that the fractional momentum of p_1 is the parton model value, i.e. that it equals the Bjorken variable x. There are several ways one can correct the inconsistency:

- Change the value of the fractional momentum of p_1 to the correct value. This is the prescription of Bengtsson and Sjöstrand [3]. We will use it for the remainder of this section. It is implemented in LEPTO and RAPGAP, and it requires a modified Sudakov form factor.

- Only generate the value of Bjorken x after the values of the fractional momenta are generated. In this approach one cannot choose to generate events with a specified value of x.

- Remove the requirement on the fractional momentum of p_1, while keeping the unmodified Sudakov form factor. Here one generates the fractional momentum variables for all lines except p_1, and then determines p_1 without putting any explicit requirement on its fractional momentum. This is the prescription I will implement in section 4.

I now explain the Bengtsson and Sjöstrand method. They first make an explicit definition equivalent to eq. (3.16):

$$x_1 = x \left(1 + \frac{m_{1'}^2 - Q_1^2}{Q^2} \right) . \tag{3.17}$$

[3]They actually define a variable z for the relative longitudinal momenta of neighboring partons in the showering. Their definition implies that the longitudinal momentum fraction of the struck quark is given by eq. (3.16). Note that the formula is not in its most satisfactory form. It would appear more consistent to replace the denominator by $p \cdot (p+q)$. This results in small changes, of relative size xm^2/Q^2. To keep agreement with the formulae used in [3], I do not make this further change.

Here, $m_{1'}^2 = p_{1'}^2$ and $Q_1^2 = -p_1^2$. They then write a modified Sudakov form factor:

$$S_a^{(\mathrm{BS})}\left(x, Q_{\max}^2, Q_1^2, m_{1'}^2\right) = \exp\left\{ -\int_{Q_1^2}^{Q_{\max}^2} \frac{dQ'^2}{Q'^2} \frac{\alpha_s(Q'^2)}{2\pi} \times \right.$$
$$\left. \times \sum_c \int_{x_1}^1 \frac{dz}{z} P_{c\to ab}(z) \frac{f_c(x_1/z, Q'^2)}{f_a(x_1, Q'^2)} \right\}. \quad (3.18)$$

At first sight, this modified Sudakov factor is not satisfactory, since it depends on the virtuality of the outgoing jet. This results in a non-factorizing cross section, whereas one usually assumes that the showering on different lines can be performed independently. In fact, there is no problem as regards the calculation. One simply has to perform the generation of the virtuality of the outgoing quark before one performs the initial-state showering. A practical alternative is to use the original Sudakov factor to generate events and then to reweight the events by the ratio of the form factors. All the necessary variables to define the modified Sudakov factor (3.18) are available when the reweighting is done. An actual reweighting may be done, or the generated events may be vetoed with the appropriate probability.

As we will see, the method also results in formulae for NLO cross sections that are non-linear in the parton densities. Similarly, the relations between parton densities for the event generator and in the $\overline{\mathrm{MS}}$ scheme are non-linear. Although the complication in the formulae must be regarded as a disadvantage, the disadvantage is not fatal.

A more fundamental concern is that the dependence of the Sudakov form factor on the virtuality of the final-state parton may signal that the form factor is not universal between different processes. Since the dependence is only on a single variable, one might hope that the problem is tractable.

3.4 Modification to first-order gluon-fusion

The modification in the Sudakov factor entails two changes in the cross section formula (3.9). One is that $f(x/z_1)$ must be replaced by $f(x_3)$, and the other is that a factor $f_a(x)/f_a(x_1)$ must be inserted, where $x_1 = x(1 - Q_1^2/Q^2)$. Thus the first-order cross section implemented in the event generator is

$$\frac{d\sigma_{\text{shower}}^{(\mathrm{BS})}}{dx\, dy\, dx_3\, d\cos\theta\, d\phi} = K \sum_a e_a^2 \frac{\alpha_s\left(Q^2\right)}{4\pi^2} C\left(Q_1^2\right) \frac{x}{x_3} f_g(x_3, Q^2) \frac{f_a(x)}{f_a(x_1)} \times$$
$$\times \frac{1}{1-\cos\theta} P\left(\frac{x}{x_3} - \frac{1}{2}(1-\cos\theta)\right), \quad (3.19)$$

where the fractional momentum of the gluon in the gluon density is now the same as in the calculation of its 4-momentum.

The extra factor of $f_a(x)/f_a(x_1)$ looks quite unusual. Nevertheless it does represent what is actually implemented[4] in the code for LEPTO and RAPGAP, following the prescription of [3]. This factor does go to unity when $Q_1^2 \ll Q^2$, as is necessary if the showering is to be correct in the collinear limit. However our purpose is to derive the NLO correction to the event generator, and for that we must use the actually implemented cross section when Q_1^2 is of order Q^2.

3.5 Photon-gluon fusion with subtraction

From standard references (e.g. [7]), we find that the unsubtracted photon-gluon fusion contribution to F_2 gives a cross section

$$\begin{aligned}
\frac{d\sigma_{\text{unsubtracted}}\,(F_2 \text{ part})}{dx\,dy\,dx_3\,d\!\cos\theta\,d\phi} &= \\
&= K \sum_{\text{quarks } a} e_a^2 \frac{\alpha_s\,(Q^2)}{4\pi^2} \frac{x}{x_3} f_g(x_3, Q^2) \times \\
&\quad \times \left\{ P(z) \left[\frac{1}{1-\cos\theta} + \frac{1}{1+\cos\theta} \right] - \frac{1}{2} + 3z(1-z) \right\}, \quad (3.20)
\end{aligned}$$

where $z = x/x_3$. Notice that the sum is over quark, but not antiquark flavors.

We must now subtract the $O(\alpha_s)$ term from the showering, eq. (3.19), for both quarks and antiquarks. The antiquark term can be treated as a quark term with θ replaced by $\pi - \theta$. This gives

$$\begin{aligned}
\frac{d\sigma^{(\text{BS})}_{\text{hard}}(F_2 \text{ part})}{dx\,dy\,dx_3\,d\!\cos\theta\,d\phi} &= \\
&= K \sum_{\text{quarks } a} e_a^2 \frac{\alpha_s\,(Q^2)}{4\pi^2} \frac{x}{x_3} f_g(x_3, Q^2) \times \\
&\quad \times \left\{ \frac{1}{1-\cos\theta} \left[P(z) - C(-t) \frac{f_a(x)}{f_a(x_1)} P\left(z - \frac{1}{2}(1-\cos\theta) \right) \right] + \right. \\
&\quad + \frac{1}{1+\cos\theta} \left[P(z) - C(-u) \frac{f_{\bar{a}}(x)}{f_{\bar{a}}(x_1)} P\left(z - \frac{1}{2}(1+\cos\theta) \right) \right] - \\
&\quad \left. - \frac{1}{2} + 3z(1-z) \right\}. \quad (3.21)
\end{aligned}$$

Here again $z = x/x_3$, $x_1 = x(1-Q_1^2/Q^2)$, and $P(z) = \frac{1}{2}(1-2z+2z^2)$. The virtualities in the cut-off function are $-t = Q^2(1-\cos\theta)x_3/2x$ and $-u = Q^2(1+\cos\theta)x_3/2x$.

Observe how the redefinition of the kinematics of the parton showers has resulted in a formula for the NLO correction that is non-linear in the parton densities. In principle this is not incorrect. However, the structure of the formula is much different to what one usual deals with, and is more complicated.

[4]Private communication from H. Jung and T. Sjöstrand.

For completeness, here follows the corresponding contribution to the cross section that results from the photon-gluon fusion part of F_L:

$$\frac{d\sigma_{\rm hard}(F_L \text{ part})}{dx\,dy\,dx_3\,d\cos\theta\,d\phi} = -\frac{Ky^2}{2-2y+y^2} \times \\ \times \sum_{\text{quarks } a} e_a^2 \frac{\alpha_s\,(Q^2)}{4\pi^2} \frac{x}{x_3} f_g(x_3, Q^2)\, 2z(1-z)\,. \tag{3.22}$$

The complete gluon-fusion contribution to the cross section is the sum of (3.21) and (3.22).

In the above calculations, there is an arbitrary cut-off function $C(Q_1^2)$. To implement an event generator with the standard Sudakov form factor, one should set $C(Q_1^2) = \theta(Q^2 - Q_1^2)$. However, the derivation of the leading-order formalism does not require this choice; the purpose of the derivation is only to obtain the correct cross section when $Q_1^2 \ll Q^2$. Another choice of the cut-off function which is unity at small Q_1^2 would also be valid.

Now the aim of computing higher-order corrections, such as eq. (3.21) is to obtain the correct cross section when large virtualities are involved. So any change in the cut-off function is compensated by the corresponding changes in the subtraction terms, up to errors of yet higher order in $\alpha_s(Q^2)$. So there is a kind of renormalization-group invariance under changes in the cut-off function. If we were able to calculate the cross section to all orders in α_s, then the cross section would be exactly invariant under changes in $C(Q_1^2)$.

Although the cut-off function is arbitrary, it is not completely arbitrary if we are to do useful calculations. We must choose it so that higher-order corrections, such as eq. (3.21), are not excessively large. Thus the standard case $C(Q_1^2) = \theta(Q^2 - Q_1^2)$ is a simple rational choice. However, if one examines the ranges of virtualities actually involved, one may well find that some other choice is better.

Indeed, there is no need to restrict one's attention to sharp cutoffs. A smoother function, like

$$C(Q_1^2) = \begin{cases} 1 - AQ_1^2/Q^2 & \text{if } Q_1^2 < Q^2/A, \\ 0 & \text{otherwise} \end{cases} \tag{3.23}$$

might even be better, since then one could for example choose it to track the typical behavior of a higher-order correction. In this formula A is an adjustable parameter. *If the cut-off function is changed, then one must also redefine the Sudakov form factor.* Such a change is likely to be particularly useful in connection with the problem that eq. (3.21) does not automatically give a positive cross section.

This will be discussed further in section 5, where I will show that the use of a suitable cut-off function can at least substantially reduce the number of negative-weighted events, and where I will also discuss the extent how the use of a formula that contains a negative cross section is not necessarily incompatible with its use in an event generator.

3.6 Comparison with $\overline{\mathrm{MS}}$ scheme

Once one has a systematic algorithm for treating NLO corrections in event generators, it is both possible and necessary to answer the question of what scheme is being used for the parton densities. The numerical values of the parton densities can be changed at order α_s and beyond by a change of scheme. Thus it is necessary to know the actual scheme being used in order that the cross section is actually known to the claimed accuracy of α_s. Moreover, standard fits to parton densities are typically made in the $\overline{\mathrm{MS}}$ scheme; it is necessary to translate these to the scheme used in the event generator.

It does not seem to me to be possible to modify the Monte-Carlo algorithm to use $\overline{\mathrm{MS}}$ densities directly, since the algorithm explicitly uses the dependence on parton 4-momentum of the parton correlation function in the target. In contrast, the definition of the $\overline{\mathrm{MS}}$ densities involves an integral over all values of the transverse momentum and virtuality, followed by a renormalization of the consequent ultra-violet divergence. So one must resign oneself to the fact that the event generator uses parton densities that are in effect tailored to its algorithm.

A fundamental way of approaching this issue would be to deduce, from derivation of the Monte-Carlo algorithm, the operators that define its parton densities.

But here I will take a lower-level approach, which is to integrate the Monte-Carlo cross section over the hadronic final states and then to require that the result be the same as the cross section in the standard factorization approach with $\overline{\mathrm{MS}}$ parton densities.

In this approach one must be concerned that the relation between the parton densities might be process dependent. In fact, the process dependence cancels. For example, the same unsubtracted photon-gluon cross-section eq. (3.20) occurs in both the Monte-Carlo calculation and the $\overline{\mathrm{MS}}$ calculation, and so it cancels out when one subtracts the two formulae for the same physical cross section to obtain the relation between the parton densities.

First we take the formula for the structure function with $\overline{\mathrm{MS}}$ parton densities [7]. Now our aim is to compute a process-independent relation between parton densities, and we want a result for each flavor of quark and not just the combination that appears in the usual electromagnetic F_2. So it is convenient to replace the actual cross section by one in which the photon couples only to one flavor of quark, with unit coupling:

$$\begin{aligned} F_2^a\left(x, Q^2\right) = {} & x f_a^{(\overline{\mathrm{MS}})}(x, \mu^2) + \\ & + \frac{\alpha_s\left(\mu^2\right)}{2\pi} \int_x^1 dx_3 \frac{x}{x_3} f_g^{(\overline{\mathrm{MS}})}(x_3, \mu^2) \left[P(z) \ln \frac{Q^2(1-z)}{\mu^2 z} - \frac{1}{2} + 4z(1-z) \right] + \\ & + \text{first-order quark terms } + O\left(\alpha_s^2\right), \end{aligned} \tag{3.24}$$

where $z = x/x_3$, the same as in the formula for the hard scattering. This must equal the same structure function given by the Monte-Carlo calculation. From the order α_s calculation in eq. (3.21), we find

$$
\begin{aligned}
F_2^a(x,Q^2) = x f_a^{(\mathrm{BS})}\left(x,Q^2\right) + \\
&+ \frac{\alpha_s\left(Q^2\right)}{2\pi}\int_x^1 dx_3 \int_{-1}^1 d\!\cos\theta \frac{x}{x_3} f_g(x_3,Q^2) \times \\
&\times \left\{ \frac{1}{1-\cos\theta}\left[P(z) - C(-t)\frac{f_a(x)}{f_a(x_1)} P\left(z - \frac{1}{2}(1-\cos\theta)\right)\right] - \right. \\
&\quad \left. -\frac{1}{4} + \frac{3}{2} z(1-z) \right\} \\
&+ \text{first-order quark terms} + O\left(\alpha_s^2\right) . \qquad (3.25)
\end{aligned}
$$

Here $-t = Q^2(1-\cos\theta)x_3/2x$, and $x_1 = x - \frac{1}{2}x_3(1-\cos\theta)$. Because of the dependence on $f_a(x_1)$, it is not possible to do the integral over $\cos\theta$ analytically. The superscript on the quark density indicates that it is in the scheme appropriate for the Bengtsson-Sjöstrand algorithm.

It follows immediately that

$$
\begin{aligned}
x f_a^{(\mathrm{BS})}(x,Q^2) = x f_a^{(\overline{\mathrm{MS}})}(x,\mu^2) + \\
&+ \frac{\alpha_s(\mu^2)}{2\pi}\int_x^1 dx_3 \frac{x}{x_3} f_g^{(\overline{\mathrm{MS}})}(x_3,\mu^2) \times \\
&\times \left\{ P(z)\ln\frac{Q^2(1-z)}{\mu^2} + z(1-z) - 2\int_{-1}^1 \frac{d\!\cos\theta}{1-\cos\theta} \times \right. \\
&\quad \left. \times \left[P(z) - C(-t)\frac{f_a(x)}{f_a(x_1)} P\left(z - \frac{1}{2}(1-\cos\theta)\right)\right] \right\} + \\
&+ \text{first-order quark terms } + O\left(\alpha_s^2\right) . \qquad (3.26)
\end{aligned}
$$

This is clearly a rather unpleasant formula. However it is necessitated by the algorithm currently used in the event generators.

4. New algorithm for parton kinematics

The formulae generated in the preceding sections are rather complicated and have non-linear dependence on the parton densities. This is a result of the particular choice made in [3] for handling the kinematics of the off-shell struck quark. So I now propose an alternative algorithm which will result in much more pleasant properties for the cross section and the parton densities.

Consider first how the 4-momenta of the partons are generated. In figure 3 is shown a general shower. The showering algorithm generates a specification of the partons. The specification consists of (a) the flavor of each parton, (b) the virtuality of each parton, (c) the fractional momentum z_{2n+1} for each branching, and (d) an azimuthal angle for the transverse momentum of each branching. The fractional momentum of each space-like line is specified as

$$x_{2n+1} = \frac{x}{\prod_{i=0}^{n-1} z_{2i+1}}\,, \tag{4.1}$$

so that $x_3 = x/z_1$, $x_5 = x/(z_1 z_3)$, etc. In reconstructing the 4-momenta, Bengtsson and Sjöstrand tell us to use

$$\frac{p_{2n+1}\cdot(p_{2n+1}+q)}{p\cdot q} = x_{2n+1}\,. \tag{4.2}$$

If we apply these equations for all n from 0 upwards, we get the previously explained inconsistency. The resolution proposed by Bengtsson and Sjöstrand was to change the formula, (4.1); they made a consistent definition of a fractional momentum x_{2n+1} as the right-hand side of eq. (4.1) times $[1+(m_1'^2 - Q_1^2)/Q^2]$, and they used the modified Sudakov form factor (3.18).

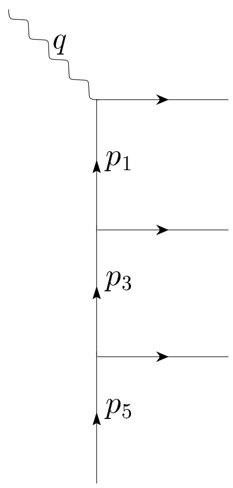

Figure 3: Generic initial-state shower.

An alternative which generates simpler formulae is as follows:

1. Generate virtualities for the partons and fractional momenta for the branchings from the unmodified Sudakov form factor eq. (2.4).

2. Use eq. (4.1) to compute the fractional momenta, *except in the case* $n = 0$, i.e. except for computing x_1.

3. Similarly, use eq. (4.2) for all p_{2n+1}, except for p_1.

4. The momentum p_1 is now completely determined, given the virtualities and the azimuthal angles.

The inconsistency is eliminated because we have dropped one equation, for the longitudinal momentum of p_1. Bengtsson and Sjöstrand, in contrast, changed the computation of every x_{2n+1} so that the two conditions for p_1 are consistent.

The price of the new procedure is that the definition of the longitudinal momentum fraction, eq. (4.2) is not applied universally. The reward, as we will see, is that the formulae for the cross sections etc. are now of a conventional form that is linear in the parton densities and that is therefore considerably simpler.

Both procedures are correct; they simply represent alternative prescriptions for computing the 4-momenta of the partons from the scalar values generated by the algorithm.

4.1 First-order term for showering

Since the showers are generated from the unmodified Sudakov factor, eq. (2.4), the cross section for the showering at order α_s is given by the unmodified eq. (2.5). The parton momenta are given by simpler formulae than eqs. (3.1)–(3.4):[5]

$$q^\mu = \frac{Q}{2\sqrt{z_1(1-z_1)}}\left(1-2z_1, \mathbf{0}_T, 1\right), \tag{4.3}$$

$$p_{1'}^\mu = \frac{Q\sqrt{1-z_1}}{2\sqrt{z_1}}\left(1, \mathbf{n}_T\sin\theta, \cos\theta\right), \tag{4.4}$$

$$p_2^\mu = \frac{Q\sqrt{1-z_1}}{2\sqrt{z_1}}\left(1, -\mathbf{n}_T\sin\theta, -\cos\theta\right), \tag{4.5}$$

$$p_3^\mu = \frac{Q}{2\sqrt{z_1(1-z_1)}}\left(1, \mathbf{0}_T, -1\right). \tag{4.6}$$

Here, we now have

$$\cos\theta = 1 - \frac{2z_1 Q_1^2}{Q^2}, \tag{4.7}$$

so that

$$\sin\theta = \frac{2Q_1}{Q}\sqrt{z_1\left(1 - z_1\frac{Q_1^2}{Q^2}\right)}. \tag{4.8}$$

The change of variables is now to $\cos\theta$ defined by eq. (4.7) and to $x_3 = x/z_1$. This gives

$$\frac{d\sigma^{(\mathrm{new})}_{\mathrm{shower}}}{dx\, dy\, dx_3\, d\cos\theta\, d\phi} = K\sum_a e_a^2\frac{\alpha_s\left(Q^2\right)}{4\pi^2}\frac{C(Q_1^2)}{1-\cos\theta}P\left(\frac{x}{x_3}\right)\frac{x}{x_3}f_g(x_3, Q^2). \tag{4.9}$$

4.2 NLO term with subtraction

The hard scattering cross section with its subtraction is changed to

$$\begin{aligned}
&\frac{d\sigma^{(\mathrm{new})}_{\mathrm{hard}}(F_2\ \mathrm{part})}{dx\, dy\, dx_3\, d\cos\theta\, d\phi} = \\
&\quad = K\sum_{\mathrm{quarks}\, a} e_a^2\frac{\alpha_s\left(Q^2\right)}{4\pi^2}\frac{x}{x_3}f_g(x_3, Q^2)\times \\
&\qquad \times\left\{\frac{P(z)\Big[1 - C(-t)\Big]}{1-\cos\theta} + \frac{P(z)\Big[1 - C(-u)\Big]}{1+\cos\theta} - \frac{1}{2} + 3z(1-z)\right\},
\end{aligned} \tag{4.10}$$

where $z = x/x_3$, $-t = Q^2(1-\cos\theta)x_3/2x$ and $-u = Q^2(1+\cos\theta)x_3/2x$. Notice the considerable simplification compared with the previous scheme.

[5] In the list of requirements above eq. (3.1), we only need to modify the formula for z_1, which now becomes $z_1 = Q^2/2p_3\cdot(p_3+q)$.

4.3 Relation to $\overline{\mathrm{MS}}$ parton densities

From eq. (4.10) it follows that the structure function F_2^a is

$$
\begin{aligned}
F_2^a\left(x, Q^2\right) = {} & x f_a^{(\mathrm{new})}(x, Q^2) + \\
& + \frac{\alpha_s\left(Q^2\right)}{2\pi} \int_x^1 dx_3 \frac{x}{x_3} f_g^{(\mathrm{new})}(x_3, Q^2) \left[P(z)\ln(1/z) - \frac{1}{2} + 3z(1-z)\right] + \\
& + \text{first-order quark terms } + O\left(\alpha_s^2\right) ,
\end{aligned}
\tag{4.11}
$$

where again $z = x/x_3$. Comparison with the structure function expressed in terms of the $\overline{\mathrm{MS}}$ densities, eq. (3.24), gives

$$
\begin{aligned}
x f_a^{(\mathrm{new})}(x, Q^2) = {} & x f_a^{(\overline{\mathrm{MS}})}(x, \mu^2) + \\
& + \frac{\alpha_s(\mu^2)}{2\pi} \int_x^1 dx_3 \frac{x}{x_3} f_g^{(\overline{\mathrm{MS}})}(x_3, \mu^2) \left[P(z)\ln\frac{Q^2(1-z)}{\mu^2} + z(1-z)\right] + \\
& + \text{first-order quark terms } + O\left(\alpha_s^2\right) .
\end{aligned}
\tag{4.12}
$$

This is clearly much more tractable than the previous version.

5. Negative weighted events

The subtracted NLO cross sections eqs. (3.21) and (4.10) are not automatically positive. This is not unphysical, since these formulae only give a component of the cross-section. However it is a problem for an event generator when one generates separate classes of LO and NLO events.

The problem is not necessarily fatal. For example, suppose one wishes to make a histogram of a differential cross section. Then one can choose to generate weighted events (which if necessary can be passed through a detector simulation, etc). The contents of each bin of the histogram are obtained as a weighted sum of events, and there is no need to require that individual events have positive weights.

What would cause a real disaster would be to have a relatively small final answer being obtained by a cancellation of large numbers of positive-weighted events and large numbers of negative-weighted events. This is not the case for the algorithm proposed in this paper, but it is the case for some kinds of analytic calculation.

Nevertheless, one often prefers to be able to generate unweighted events, for then one can genuinely simulate real experimental data. This can be done on the basis of generation of weighted events, by standard Monte-Carlo techniques, but only if all the weights are positive.

Luckily there is freedom in the proposed method to reduce the number of negative-weighted events, by the choice of the cutoff function $C(Q_1^2)$. Not only can the position of the cutoff be changed from its standard value Q^2, but the shape of the function can be changed, for example to the form in eq. (3.23). Appropriate changes in the showering algorithm will be needed, as explained in section 3.5. At low Q_1^2, the cut-off function goes to unity, so that collinear limits are unchanged. But the smoother form of cutoff reduces the amount that is subtracted from the bare cross section at large t or u in eqs. (3.21) and (4.10). For a suitable cut-off function, the result is therefore to reduce the number of negative-weighted events, if not eliminate them completely.

Even if one cannot eliminate absolutely all the negative-weighted events, it should be enough for practical purposes if only a small fraction of the generated events have negative weights.

6. Future work

In the context of diffractive deep-inelastic scattering, the NLO corrections calculated in this paper are clearly the most urgently needed. Because the gluon density is substantially larger than the quark densities, these particular corrections are not numerically suppressed in the way that would otherwise be expected of NLO corrections. The first new result is the calculation of the gluon-induced contribution to the hard scattering [eqs. (3.21) and (4.10)]. The second new result is the gluon-induced part of the relation between the parton densities to be used in the event generator and the $\overline{\rm MS}$ parton densities [eqs. (3.26) and (4.12)].

We saw that within the conventional scheme for performing initial-state showering, the NLO corrections are unusually complicated non-linear functionals of the parton densities. This is an inevitable consequence of the algorithm chosen in [3] for imposing consistent parton kinematics. Therefore, in section 4, I proposed an alternative algorithm for computing the parton 4-momenta. The change in algorithm entails a change in the scheme that defines the parton densities used in the event generator. Different numerical values of the parton densities are to be used in each scheme, and these numerical values differ from the $\overline{\rm MS}$ parton densities that are obtained in the standard global analyses.

Further calculations and theoretical developments that are needed include:

1. Calculation at order α_s of the quark-induced subprocesses.

2. Numerical calculations of the parton densities from the standard fits, which use the $\overline{\rm MS}$ scheme.

3. Extension of the cross section calculations to include weak boson exchange.

4. Extension of the methods to handle other processes in hadron-hadron collisions and e^+e^- annihilation.

5. Non-leading corrections to the showering.

6. Investigation of the non-positivity of the NLO term in the cross sections: Can it be eliminated by a suitable choice of the cut-off function? How acceptable is it if an NLO term is negative?

7. Handling more general processes will require a proper treatment of the soft region. Technically, I see this as the most difficult problem.

8. The NLO corrections are valid when the virtuality of the intermediate quark, Q_1^2, is of order Q^2. There is no singularity at $Q_1^2 = 0$, so the contribution from $Q_1^2 \ll Q^2$ is suppressed by a power of Q^2. Even so, events are generated for all values of Q_1^2, down to $Q_1^2 = 0$. Thus one may need to modify the Monte-Carlo algorithm to handle this kinematic region.

9. One of the treatments of the kinematics of off-shell partons entails a redefinition of the Sudakov form factor in a way that appears non-universal. It needs to be understood whether this non-universality is genuine or whether it is only apparent.

10. It would be useful to understand the relation of the Monte-Carlo formalism to definitions of the parton densities that involve explicit parton transverse momentum. Compare Mrenna's work [6].

11. Would it be useful to find a way of computing the hard scattering coefficients with off-shell matrix elements? There are obviously non-trivial issues of gauge invariance that would arise.

12. Which of the algorithms for calculating the parton 4-momenta is better? Is there a yet better algorithm?

Acknowledgments

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Erratum

In the original version of this paper, the variable x_1 in eq. (3.21) was used twice with different meanings. This equation and its surrounding paragraph should be modified to read as follows:

We must now subtract the $O(\alpha_s)$ term associated with the showering, eq. (3.19), for both quarks and antiquarks. The antiquark term can be treated as a quark term with θ replaced by $\pi - \theta$. This gives

$$\begin{aligned}\frac{d\sigma^{(\mathrm{BS})}_{\mathrm{hard}}(F_2\ \mathrm{part})}{dx\,dy\,dx_3\,d\cos\theta\,d\phi} = K \sum_{\mathrm{quarks}\ a} e_a^2 \frac{\alpha_s(Q^2)}{4\pi^2}\frac{x}{x_3} f_g(x_3,Q^2)\times \\ \times\left\{\frac{1}{1-\cos\theta}\left[P(z) - C(-t)\frac{f_a(x)}{f_a(x_{1t})}P\left(z-\frac{1}{2}(1-\cos\theta)\right)\right]+\right. \\ +\frac{1}{1+\cos\theta}\left[P(z) - C(-u)\frac{f_{\bar a}(x)}{f_{\bar a}(x_{1u})}P\left(z-\frac{1}{2}(1+\cos\theta)\right)\right] \\ \left. -\frac{1}{2}+3z(1-z)\right\}. \end{aligned} \tag{3.21}$$

Here again $z = x/x_3$, and $P(z) = \frac{1}{2}(1-2z+2z^2)$. The virtualities in the cut-off function are $-t = Q^2(1-\cos\theta)x_3/2x$ and $-u = Q^2(1+\cos\theta)x_3/2x$; these are used to give $x_{1t} = x(1+t/Q^2)$ and $x_{1u} = x(1+u/Q^2)$.

There were two errors in eq. (3.26), which should read as follows

$$\begin{aligned} xf_a^{(\mathrm{BS})}(x,Q^2) = xf_a^{(\overline{\mathrm{MS}})}(x,\mu^2) + \frac{\alpha_s(\mu^2)}{2\pi}\int_x^1 dx_3 \frac{x}{x_3} f_g^{(\overline{\mathrm{MS}})}(x_3,\mu^2)\times \\ \times\left\{P(z)\ln\left(\frac{Q^2(1-z)}{\mu^2 z}\right) + z(1-z) - \right. \\ \left. -\int_{-1}^1 \frac{d\cos\theta}{1-\cos\theta}\left[P(z) - C(-t)\frac{f_a(x)}{f_a(x_1)}P\left(z-\frac{1}{2}(1-\cos\theta)\right)\right]\right\} + \\ + \text{first-order quark terms} + O(\alpha_s^2)\,. \end{aligned} \tag{3.26}$$

Added acknowledgments

I thank S. Schilling for pointing out the above errors in the originally published version of this paper.