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A MONTE CARLO METHOD TO CALCULATE THE QCD EVOLUTION OF STRUCTURE FUNCTIONS
WITH THE INCLUSION OF HEAVY QUARK EFFECTS

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A B S T R A C T

A Monte Carlo method is presented for the calculation of the QCD evolution of structure functions. Its application is discussed in detail in the framework of the LLA, but it can also be used with modified parton decay probability functions including higher order effects. For heavy quark production, threshold constraints can be correctly taken into account, and one obtains results which at low Q^2 are consistent with those of the photon-gluon fusion model.

A quantitative verification of the predictions of Quantum Chromodynamics (QCD) for the evolution of structure functions in deep inelastic scattering requires an extended range of Q^2 and a high accuracy of the data, which only counter experiments appear able to provide. On the other hand, the conventional and theoretically easy way of using moments for such a verification is not suitable for counter data. Because of limited acceptance, too much of the moments is often left unmeasured, and trying to avoid this by combining different sets of data is not a healthy remedy because of the presence of normalization problems.

Techniques for calculating the Q^2 evolution at fixed x predicted by QCD have already been presented in the literature¹⁾, but they have shortcomings. The principal one is the inability for all of them to take into account the effects of new thresholds (in particular, charm production) which are clearly present in the data. These effects appear to be described rather well, at presently available Q^2 , by the photon-gluon fusion model^{2,3)}. The latter, however, constitutes only an $O(\alpha_s)$ approximation, and cannot be applied at large Q^2 . The difficulty encountered with the above techniques when treating the emission of heavy quarks is due to the fact that they use as starting point the evolution equations, in which it is hard to incorporate phase space constraints associated with the massiveness of the quanta.

In this note we present a simple Monte Carlo method which bypasses the use of the evolution equations and in which phase space constraints can be easily incorporated. If the emission of massive quarks is neglected, its results represent, with any wanted accuracy, the solution of the evolution equations for structure functions in their standard form. Although we discuss here only its implementation in the leading logarithm approximation (LLA), higher order corrections can be included in it by the use of modified parton decay probability functions. The method is essentially an adaptation to the (spacelike) case of structure functions of the Monte Carlo cascade introduced for the calculation of jet properties [see Ref. 4); see also Ref. 5) for related considerations].

The basic quantities which determine the Q^2 evolution of structure functions are the elementary emission probabilities:

$$dP_E^q = \frac{\alpha_s(Q^2)}{2\pi} \frac{dQ^2}{Q^1} \int_{\epsilon}^{1-\epsilon} dz P_{q,qG}(z) \quad (1)$$

for a quark leg, and the same with $P_{q,qG}(z)$ replaced by $[P_{G,GG}(z) + \sum_{i=1}^{N_f} P_{G,q\bar{q}}(z)]$ for a gluon leg. Here $P_{q,qG}(z)$, $P_{G,GG}(z)$ and $P_{G,q\bar{q}}(z)$ are the standard real emission probability functions (i.e., with no regularizing δ term, and therefore positive definite^{*)}; $\alpha_s(Q^2) = (b \log(Q^2/\Lambda^2))^{-1}$, $b = (33 - 2N_f)/(12\pi)$; ϵ is an infra-red cut-off and the limit $\epsilon \rightarrow 0$ is understood (at the end of the calculation). dP_E^q represents the probability that when increasing the phase space from Q^2 to $Q^2 + dQ^2$ a quantum is emitted. If, to fix the ideas, we consider a quark leg, both possibilities are included for the two secondaries: a spacelike quark and a timelike gluon, or a spacelike gluon and a timelike quark. To study the Q^2 evolution, one follows only spacelike quanta, but since both possibilities are included in the emission, one has in practice to follow a cascade. When a quark emits, one picks up a spacelike quark with a fraction z of the momentum of the parent distributed according to $P_{q,qG}(z)$, and a spacelike gluon distributed according to $P_{q,qG}(1-z)$. The only difference with respect to a conventional exclusive cascade is that the sum of the momenta of the two spacelike quanta is not necessarily equal to the momentum of the parent (this is relevant when discussing phase space limitations associated with the emission of heavy quarks).

If $q^i(x, Q^2)$ ($i = 1, 2, N_f$) and $G(x, Q^2)$ are the quark and gluon densities at Q^2 , when increasing the phase space by dQ^2 , $q^i(x, Q^2 + dQ^2)$ will pick up:

- i) quarks of species i which have not emitted in the added phase space, and the probability for this to happen is $1 - dP_E^q$;
- ii) quarks which have undergone emission, with probability given by dP_E^q ;
- iii) quarks emitted by gluons, with a probability given by Eq. (1) with $P_{q,qG}(z)$ replaced by $P_{G,q\bar{q}}(z)$. In sum:

$$\begin{aligned}
 q^i(x, Q^2 + dQ^2) = & \left[1 - \frac{\alpha_s(Q^2)}{2\pi} \frac{dQ^2}{Q^2} \int_{\epsilon}^{1-\epsilon} dz P_{q,qG}(z) \right] q^i(x, Q^2) \\
 & + \frac{\alpha_s(Q^2)}{2\pi} \frac{dQ^2}{Q^2} \int_0^1 dy \int_{\epsilon}^{1-\epsilon} dz P_{q,qG}(z) q^i(y, Q^2) \delta(x - yz) \\
 & + \frac{\alpha_s(Q^2)}{2\pi} \frac{dQ^2}{Q^2} \int_0^1 dy \int_{\epsilon}^{1-\epsilon} dz P_{G,q\bar{q}}(z) G(y, Q^2) \delta(x - yz)
 \end{aligned} \quad (2)$$

^{*)} $P_{q,qG}(z) = C_F (1+z^2)/(1-z)$, $P_{G,GG}(z) = C_A ((1-z)/z + z/(1-z) + z(1-z))$,
 $P_{G,q\bar{q}}(z) = (z^2 + (1-z)^2)/2$, $C_A = 3$, $C_F = 4/3$.

which is one of the Altarelli-Parisi⁶⁾ evolution equations. One similarly obtains the evolution equation for the gluon density. But in order to get the numerical answer, it is easier not to use these equations, and to refer directly to the elementary emission probability [Eq. (1)].

The probability that a quark leg, say, does not emit in the (finite) phase volume between Q_s^2 and $Q^2 + dQ^2$ ($\geq Q_s^2$) may be written as the product of probabilities

$$\Pi_{NE}^q(Q_s^2, Q^2 + dQ^2) = \Pi_{NE}^q(Q_s^2, Q^2) (1 - dP_E^q) \quad (3)$$

This represents a simple differential equation which may be written as

$$d \log (\Pi_{NE}^q(Q_s^2, Q^2)) = -dP_E^q \quad (4)$$

Integrating both sides, and requiring $\Pi_{NE}^q(Q_s^2, Q_s^2) = 1$, one obtains

$$\Pi_{NE}^q(Q_s^2, Q^2) = \exp\left(-\int_{Q_s^2}^{Q^2} dP_E^q\right) = \exp\left(-(Y - Y_s)/\tau_q\right) \quad (5)$$

where τ_q is a constant

$$1/\tau_q = \frac{1}{2\pi b} \int_{\epsilon}^{1-\epsilon} dz P_{q,qG}(z) \quad (6)$$

and $Y = \log[\log(Q^2/\Lambda^2)]$.

The probability $d\Pi_E^q(Q_s^2, Q^2)$ that the first emission of a quark leg in its evolution from Q_s^2 occurs between Q^2 and $Q^2 + dQ^2$ is given by the product of two probabilities:

- i) that there is no emission between Q_s^2 and Q^2 ;

ii) that there is emission between Q^2 and $Q^2 + dQ^2$. That is:

$$d\Pi_E^q(Q_s^2, Q^2) = \Pi_{NE}^q(Q_s^2, Q^2) dP_E^q = -\frac{d}{dQ^2} [\Pi_{NE}^q(Q_s^2, Q^2)] dQ^2 \quad (7)$$

Equation (7), together with Eq. (5), (and the corresponding probabilities for gluons), provide the basic tools to calculate the Q^2 evolution of parton densities. Let us consider first the evolution of a non-singlet quantity, for which one has to follow only the spacelike quark after each emission.

The density function at Q^2 can be expressed in terms of a convolution of the density function at Q_0^2 times a kernel, which depends only on the difference of the corresponding evolution parameters:

$$q^{NS}(x, Q^2) = \int_x^1 dz \int_{x/z}^1 dy K^{NS}(z, Y-Y_0) q^{NS}(y, Q_0^2) \delta(x-zy) \quad (8)$$

Setting $q^{NS}(y, Q_0^2) = \delta(y-1)$, one realizes that $K^{NS}(x, Y-Y_0)$ represents the distribution at Q^2 of the quark momentum fraction with respect to that of the original quark at Q_0^2 . To calculate it, one can use a simple cascade scheme. Suppose one has a quark leg emitted at $Q^2 = Q_s^2$ and over-all momentum fraction x_s . Then go through the following cascade steps:

i) generate the Q_E^2 ($\geq Q_s^2$) at which the leg undergoes the next emission according to the distribution of Eq. (7). This means to generate the corresponding Y_E with

$$Y_E = Y_S - \log(RR) * \tau_q \quad (9)$$

where τ_q is defined in Eq. (6), and RR is a random number uniformly distributed between 0 and 1;

- ii) generate the $x_E = z x_s$ momentum fraction of the emitted quark, with z distributed according to $P_{q,qG}(z)$ between ϵ and $1 - \epsilon$;
- iii) set $Q_s^2 = Q_E^2$ and $x_s = x_E$ and go to step i) again.

If one is interested in the evolution between Q_0^2 and Q^2 , one enters the loop at step i) with $Q_s^2 = Q_0^2$ and $x_s = 1$, and one leaves it still at step i) when the generated Q_E^2 is $\geq Q^2$. The final quark contributes (with unitary weight) to the x distribution at Q^2 at the exit value for x_s . Generating N_{cas} cascades and dividing at the end the resulting distribution by N_{cas} gives the kernel for the evolution between Q_0^2 and Q^2 . The kernel depends only on $Y - Y_0$. If $K^{NS}(x, Y - Y_0)$ is needed for several values of $Q^2(Q_i^2, i=1, N)$, the same cascade developed between Q_0^2 and Q_N^2 can also be used for the other intermediate values of Q^2 . For each Q_i^2 the quark is recorded in the distribution for $K^{NS}(x, Y_i - Y_0)$ at the x_s for which, at step i), the condition $Q_E^2 \geq Q_i^2$ is first met (see Fig. 1, following only the valence quark).

The CPU time required for the execution of the corresponding Fortran programme is rather small. With $Q_0^2 = 2 \text{ GeV}^2$, $Q^2 = 200 \text{ GeV}^2$, $\Lambda = 0.3 \text{ GeV}$, $\epsilon = 0.001$, one obtains 10,000 cascades in three seconds of CDC7600. We have verified that the analytically calculated behaviour of moments up to $N = 10$ is reproduced within the expected statistical accuracy (e.g., $\leq 0.3\%$ with 100,000 cascades).

For the calculation of kernels describing the evolution of the singlet and gluon densities, one uses exactly the same procedure (starting from a quark or a gluon according to the kernel). But now at each emission one has to follow two secondaries (Fig. 1). Although, as we have said above, the sum of the x 's of the two secondaries is not necessarily equal to that of the parent, to economize on time one can, of course, treat the branching as an exclusive one and thus generate at step ii) just one z (this does not apply though to the case of heavy quark emission, see below). When fitting experimental data, one is not interested in the evaluation of the kernels for $x < x_{min}$, where x_{min} is the lowest Bjorken x measured. This means that quanta generated with $x < x_{min}$ during the cascade can be disposed of. The average multiplicity of gluons of which one must keep track at each stage is given by the zero moment (N_G) of the gluon density function. For an initial gluon, its evolution can be obtained by the analogue of Eq. (1) for the gluon density function. Neglecting finite terms in the z probability functions (which leads to an overestimation) and taking into account the cancellation of the $(1-z)^{-1}$ divergences between the "virtual" and the "real emission" terms, one obtains the equation:

$$\begin{aligned}
 N_G(Q^2) &= \frac{\alpha_s(Q^2)}{2\pi} \left[\int_{x_{\min}}^1 dz \frac{2C_A}{z} \right] N_G(Q^2) \frac{dQ^2}{Q^2} \\
 &= \frac{C_A}{\pi b} (-\log x_{\min}) N_G(Q^2) dY
 \end{aligned}
 \tag{10}$$

whose solution is

$$N_G(Q^2) = \text{EXP} \left[-\frac{C_A}{\pi b} (-\log x_{\min}) Y \right] \simeq e^{6.8 Y}
 \tag{11}$$

for $x_{\min} = 0.01$.

With $Q_0^2 = 2 \text{ GeV}^2$, $Q^2 = 200 \text{ GeV}^2$, $\Lambda = 0.3 \text{ GeV}$, Eq. (11) gives $N_G \simeq 12$. Actually, N_G is about half of that. Therefore one is very far from having computer storage problems at presently available Q^2 . Cascades for singlet and gluon densities are of course longer to compute than non-singlet ones (about an order of magnitude more at currently available Q^2). But since the sea which is developed represents only a small fraction of the total result, for most of the applications it is not necessary to attain the same statistical accuracy as for the non-singlet case. Anyway, errors in the final results can easily be estimated using kernels determined with two different initializations of the random number generator.

Heavy quark production. The Monte Carlo approach allows us to easily incorporate phase space constraints arising in heavy quark production. When emission of a massive parton occurs, the following kinematic bound must be satisfied⁴⁾:

$$K_1^2 - \frac{K_2^2}{z} - \frac{K_R^2}{1-z} \geq 0
 \tag{12}$$

Here K_1^2 , K_2^2 and K_R^2 are the square masses of the parent and of the two secondaries respectively, with the understanding $K_1^2, K_2^2 < 0$ ($|K_2^2| \geq |K_1^2|$), $K_R^2 \geq M^2$,

M being the mass of the heavy quark; z is the momentum fraction of the parent taken out by the secondary spacelike leg. This leads to an upper bound for z given by

$$(1-z) \left(\frac{|K_2^2|}{z} - |K_1^2| \right) \geq M^2 \quad (13)$$

In the Monte Carlo approach one can take into account this bound in the following way. If a parton leg undergoes an emission in which a heavy quark is produced, and if the generated z of the spacelike secondary does not satisfy Eq. (13), the parent keeps on evolving as if nothing had happened. The effect is substantial only for a gluon converting into a heavy quark-antiquark pair, and can be neglected for a heavy quark emitting a (hard) spacelike gluon.

On top of it one can impose an over-all threshold condition. Suppose that at the final Q^2 one has a parton with momentum fraction x originating from an emission (somewhere in the cascade) involving a heavy quark. To register it, one can then require:

$$s = Q^2(1-x)/x \geq s_{\text{threshold}} \quad (14)$$

where s is the c.m.s. energy of the current - target parton system. $s_{\text{threshold}}$ is to be identified with $4M^2$ in an electromagnetic process, and with M^2 in a weak process. This condition can be rewritten as $x \leq x_0 = Q^2/(Q^2 + s_{\text{threshold}})$.

The photon-gluon fusion (γG) model³⁾ (see Fig. 2), appears to have some success in describing charm production phenomena in electromagnetic processes²⁾. This is to be compared with the poor performance of conventional LLA approaches based on the Altarelli-Parisi evolution of the charmed sea²⁾. The basic reason is that the γG model correctly incorporates threshold behaviour. Since it is just an $O(\alpha_s)$ approximation its validity is limited to small Q^2 , where associated emission of gluons can be neglected. In Fig. 3, we compare the charmed sea contribution to the structure function $F^{c,c}(x)$ for a gluon target (the square-charge factor $4/9$ appropriate for charmed quarks is not included) as calculated with the Monte Carlo method, with that resulting from the γG model. We use in both cases the prescription $\alpha_s(Q^2 + 4M^2)$ for the running coupling constant. We

also show what happens when in the Monte Carlo the threshold condition is replaced by slow rescaling "à la Barnett" ⁷⁾ [still maintaining Eq. (13)]. Taking into account that the recipe for the argument of the running coupling constant at low Q^2 is somewhat arbitrary, and that in any case threshold behaviour is treated in an effective way, not properly taking into account bound state effects, one can conclude that the γG model and the LLA with threshold constraints give compatible results for the absolute rate (Fig. 3a). With $\langle x_{c,\bar{c}} \rangle \equiv \int x F^{c,\bar{c}}(x) dx / \int F^{c,\bar{c}}(x) dx$, one feels better the difference among the various treatments. The LLA Monte Carlo with the threshold condition properly enforced gives the same results as the γG model up to $Q^2 \approx 100 \text{ GeV}^2$ ($\Lambda = 0.3 \text{ GeV}$ has been assumed in the calculation). Beyond that, one clearly sees the effects of unduly neglecting in the γG model the emission of extra gluons.

For actual fits to the data, the evolution kernel for charmed quark production should be computed separately, because of the different argument used in the running coupling constant. The kernel in this case is no longer just a function of the evolution parameter Y , but it explicitly depends also on Λ .

Higher order effects. The application of the Monte Carlo method is not limited to the LLA. Higher order effects may be included using the correspondingly modified parton decay probability functions, which have been recently obtained by a number of authors ⁸⁾. The basic structure of the Monte Carlo cascade remains unaltered, but the evolution in Q^2 and the degradation in x are no longer independent, since z distributions depend now on Q^2 . Also the quantity in Eq. (5) will not have a simple analytic form and a numerical tabulation will be required as for the case of timelike evolution. However, these are just technical points, not hard to deal with.

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FIGURE CAPTIONS

- Fig. 1 : Schematic picture of the LLA evolution cascade initiated by a quark (solid lines for quarks, dashed lines for gluons).
- Fig. 2 : Basic diagrams for charm production treated in the LLA and with the photon-gluon fusion model.
- Fig. 3 : a) Integrated contributions for the charm-anticharm sea to the e.m. structure function for a gluon target calculated according to the photon-gluon fusion model and with the LLA Monte Carlo;
b) Q^2 behaviour of $\langle x_{c,\bar{c}} \rangle = \int x F^{c,\bar{c}}(x) dx / \int F^{c,\bar{c}}(x) dx$.

Fig. 1

Fig. 2

Fig. 3