HIERARCHICALLY ORGANIZED ITERATIVE SOLUTIONS OF THE EVOLUTION EQUATIONS IN QCD *

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The task of Monte Carlo simulation of the evolution of the parton distributions in QCD and of constructing new parton shower Monte Carlo algorithms requires new way of organizing solutions of the QCD evolution equations, in which quark–gluon transitions on the one hand and quark–quark or gluon–gluon transitions (pure gluonstrahlung) on the other hand, are treated separately and differently. This requires certain reorganization of the iterative solutions of the QCD evolution equations and leads to what we refer to as a *hierarchic iterative solutions* of the evolution equations. We present three formal derivations of such a solution. Results presented here are already used in the other recent works to formulate new MC algorithms for the parton-shower-like implementations of the QCD evolution equations. They are primarily of the non-Markovian type. However, such a solution can be used for the Markovian-type MCs as well. We also comment briefly on the relation of the presented formalism to similar methods used in other branches of physics.

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1. Introduction to the problem

The standard QCD evolution equation

$$\partial_t D_k(t,x) = \sum_j \mathcal{P}_{kj}(t,\cdot)\otimes D_j(t,\cdot)(x)\,,$$

$$f(\cdot)\otimes g(\cdot)(x) \equiv \int_0^1 dx_1 dx_2 \delta(x-x_1x_2) f(x_1)g(x_2) \equiv \int_x^1 \frac{dx_2}{x_2} f\Big(\frac{x}{x_2}\Big) g(x_2)\,, \quad (1)$$

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describes response of the parton distribution function (PDF) $D_k(t,x)$ to a change of the large energy scale $Q = \exp(t)$. Variable x is identified as a fraction of the hadron momentum carried by parton of the type k (quark, gluon). Evolution kernel $\mathcal{P}$ is calculable within perturbative QCD.

The above evolution equation (1) is an important ingredient in many QCD perturbative calculations. It can be solved using variety of the numerical methods, including Monte Carlo method. The knowledge of $D_k(t_0,x)$ at certain initial t_0, is required for solving evolution equation at other $t > t_0$. The initial PDF is fitted to experimental data.

The principal aim of this work is to derive the following analytical solution of the above QCD evolution equations

$$\begin{aligned} D_k(t,x) \;=\; & \int_0^1 dz' dx_0 G^B_{kk}(t,t_0,z') D_k(t_0,x_0)\delta(x-z'x_0) + \sum_{n=1}^{\infty} \int_0^1 dx_0 \\ & \times \sum_{k_{n-1},\ldots,k_1,k_0} \left[\prod_{j=1}^{n} \int_{t_0}^{t} dt_j \Theta(t_j - t_{j-1}) \right] \int_0^1 dz'_{n+1} \left[\prod_{i=1}^{n} \int_0^1 dz'_i dz_i \right] \\ & \times G^B_{kk}(t,t_n,z'_{n+1}) \left[\prod_{i=1}^{n} \mathcal{P}^A_{k_i k_{i-1}}(t_i,z_i) G^B_{k_{i-1}k_{i-1}}(t_i,t_{i-1},z'_i) \right] \\ & \times D_{k_0}(t_0,x_0)\delta\left(x - x_0 \prod_{i=1}^{n} z_i \prod_{i=1}^{n+1} z'_i \right), \qquad k_n = k\,, \end{aligned} \tag{2}$$

where we have isolated flavour conserving (bremsstrahlung) part of the kernel[1] $\mathcal{P}^B_{kj} \equiv \delta_{kj}\mathcal{P}_{kk}$ from the total kernel, $\mathcal{P}_{kj} = \mathcal{P}^A_{kj} + \mathcal{P}^B_{kj}$, and $G^B_{kk}(t_1,t_0,z)$ is the solution of the following simplified evolution equation, similar to Eq. (1),

$$\partial_t G^B_{kk}(t,t_0,z) = \mathcal{P}^B_{kk}(t,\cdot) \otimes G^B_{kk}(t,t_0,\cdot)(z)\,, \tag{3}$$

see Section 2.2.2 for the details. The boundary condition is $G^B_{kk}(t_0,t_0,z) = \delta(1-z)$. See also Fig. 1 for graphical representation.

It is important to provide formal proof of Eq. (2), because it is a critical ingredient in several new Monte Carlo algorithms of the non-Markovian type described in Refs. [1] and [2], and possibly in other works as well.

Let us now explain in details notation used in Eqs. (1)–(3). In function $D_k(t,x)$ variable $1 \geq x \geq 0$ is the fraction of the hadron momentum carried by the parton of the type $k = G, q_i, \bar{q}_i$, *i.e.* gluon, quark or antiquark, at the high energy scale Q, conveniently translated into the "evolution time"

[1] Since $\mathcal{P}^A_{kk} = 0$, only flavour changing indices $k_i \neq k_{i-1}$ enter in the flavour sum in Eq. (2).

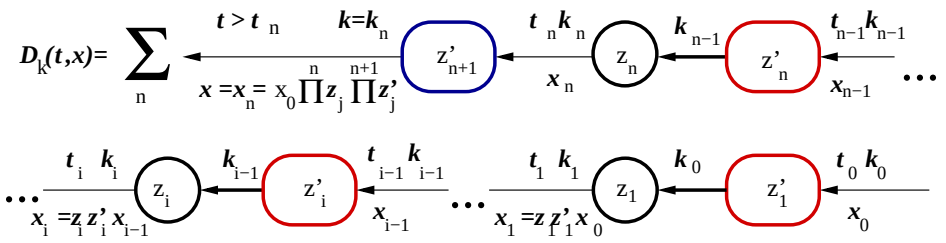


Fig. 1. Kinematics in the 2-level emission tree of Eq. (2).

variable $t = \ln Q$. In QCD the PDF represents the wave function of the hadron close to the light-cone. See Ref. [3] for an expert discussion on the precise meaning of PDF in QCD, in a wide context of the so-called *factorization theorems* [4–6] in the gauge Quantum Field Theories.

In this work we shall restrict ourselves to the most common QCD evolution equations of the DGLAP type [7], with the kernel splitting functions incorporating the QCD coupling constant (for the sake of the simplicity of notation)

$$\mathcal{P}_{kj}(t,z) = \frac{\alpha(t)}{\pi} P_{kj}(t,z)\,. \tag{4}$$

The QCD kernel functions are singular, with singularities of the type $(\ln(1-z)^n/(1-z))_+$. We shall typically regularize them with the help of an explicit small infrared (IR) cutoff parameter ε as follows:

$$\begin{aligned} \mathcal{P}_{kj}(t,z) &= -\mathcal{P}^{\delta}_{kk}(t,\varepsilon)\delta_{kj}\delta(1-z) + \mathcal{P}^{\Theta}_{kj}(t,z)\,, \\ \mathcal{P}^{\Theta}_{kj}(t,z) &= \mathcal{P}_{kj}(t,z)\Theta(1-z-\varepsilon)\,. \end{aligned} \tag{5}$$

The infinitesimal parameter ε can be t-dependent, without any loss of generality in the following treatment. The important Sudakov formfactor $\Phi_k(t,t_0)$ is directly related to the virtual part of the kernels:

$$\Phi_k(t,t_0) = \int_{t_0}^{t} dt' \mathcal{P}^{\delta}_{kk}(t',\varepsilon)\,. \tag{6}$$

Finally the (bremsstrahlung-type) auxiliary distribution

$$G^{B}_{kk}(t,t_0,z) \;=\; \delta(1-z)e^{-\Phi_k(t,t_0)}$$

$$+\sum_{n=1}^{\infty}\left[\prod_{i=1}^{n}\int_{t_0}^{t} dt_i\Theta(t_i-t_{i-1})\int_0^1 dz_i\right]e^{-\Phi_k(t,t_n)}$$
$$\times\left[\prod_{i=1}^{n}\mathcal{P}_{kk}^{\Theta}(t_i,z_i)e^{-\Phi_k(t_i,t_{i-1})}\right]\delta(z-\prod_{i=1}^{n}z_i) \qquad (7)$$

is an iterative[2] solution of the flavour-diagonal evolution equation of Eq. (3). See also Fig. 2 for graphical representation of the above gluonstrahlung segment of the evolution.

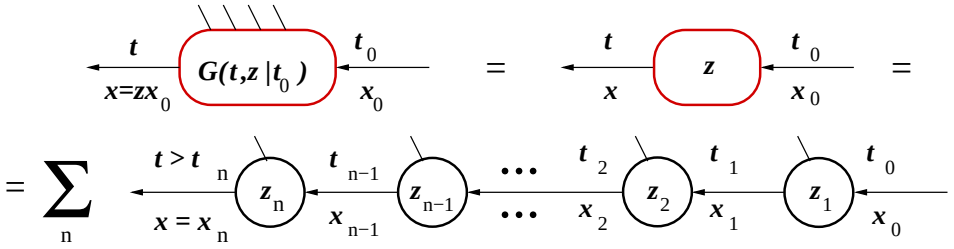


Fig. 2. Kinematics in the pure bremsstrahlung emission tree of Eq. (7).

2. The solutions

If our only aim was to prove the correctness of Eq. (2) as a solution of Eq. (1), then the simplest approach would be just to substitute it into this equation and check with a little bit of algebra that indeed it is the solution. Our aims are however more general: *(i)* to derive Eq. (2) in a more systematic way, *(ii)* to understand better its relation to the other widely known and used iterative solutions of Eq. (1), *(iii)* to prove that its *exclusive* content, in terms of the fully differential distribution in all variables t_i and z_i, $i = 1, 2, ..., n$, for each n, is exactly the same as in other iterative solutions, commonly used in the MC approaches.

Having all the above in mind, let us proceed methodically, first with deriving solution of the evolution of Eq. (1), in terms of a time-ordered exponential, widely used in the literature. Next, we shall present first example of the derivation of Eq. (2) by means of reorganizing the evolution equation and solving it once again. Then, we shall present second example of the derivation, in which the above time-ordered exponential is algebraically reorganized (transformed) into Eq. (2). Finally the third derivation of Eq. (2) based on straightforward reorganization of the multiple sums and integrals will be included in the Appendix.

[2] We shall explain in the next section why we call it "iterative".

2.1. Time-ordered exponential

The solution of Eq. (1) can be established quickly and rigorously, for instance by means iteration, as a time-ordered exponential of the kernel operator $\mathcal{P}$ in the vector (linear) space indexed by one continuous variable x and one discrete k. More precisely, Eq. (1) in a more compact matrix notation reads

$$\partial_t \boldsymbol{D}(t) = \boldsymbol{P}(t)\boldsymbol{D}(t)\,, \tag{8}$$

and its solution in the same compact matrix notation is given by

$$\boldsymbol{D}(t) = \exp\left(\int_{t_0}^{t} \boldsymbol{P}(t')dt'\right)_T \boldsymbol{D}(t_0) = \boldsymbol{G}_P(t,t_0)D(t_0)\,, \tag{9}$$

where we employ the following well known *time-ordered exponential* evolution operator

$$\begin{aligned}\boldsymbol{G}_H(t,t_0) &= \boldsymbol{G}(H;t,t_0) = \exp\left(\int_{t_0}^{t} \boldsymbol{H}(t')dt'\right)_T \\ &= \boldsymbol{I} + \sum_{n=1}^{\infty}\prod_{i=1}^{n}\int_{t_0}^{t} dt_i \theta_{t_i>t_{i-1}}\boldsymbol{H}(t_i)\,,\end{aligned} \tag{10}$$

for $t \geq t_0$. Here and in the following we define $\prod_{i=1}^{n} A_i \equiv A_n A_{n-1}\ldots A_2 A_1$. Formula (10) is familiar to all readers of the Quantum Mechanics textbooks[3]. We define function $\theta_{x>y}$ to be equal 1 when $x > y$ and equal 0 otherwise.

The compact solution of Equation (9), can be translated into more traditional integro-tensorial notation, with explicit sums and integrals:

$$\begin{aligned}D_k(t,x) &= \left\{\left[\exp\left(\int_{t_0}^{t} dt'\boldsymbol{P}(t',\cdot)\otimes\right)\right]_T \boldsymbol{D}(t_0,\cdot)\right\}_k \\ &= D_k(t_0,x) + \sum_{n=1}^{\infty}\sum_{k_{n-1}\ldots k_1 k_0}\int_0^1 dx_0 \\ &\quad\times\left[\prod_{j=1}^{n}\int_{t_0}^{t} dt_j\theta_{t_j>t_{j-1}}\int_0^1 dz_j \mathcal{P}_{k_j k_{j-1}}(z_i)\right] \\ &\quad\times D_{k_0}(t_0,x_0)\delta_{x=x_0\prod_{i=1}^{n} z_i}\,,\end{aligned} \tag{11}$$

[3] However, we do not require $\boldsymbol{H}$ to be hermitian and $\boldsymbol{G}$ to be unitary.

where $\delta_{x=y} \equiv \delta(x-y)$. We realize, that the above formula, although rigorous and very elegant, is useless for any practical evaluations, because it contains polynomials of the negative and singular terms coming from products of $-\mathcal{P}^{\delta}\delta(1-z)$ factors. In principle these inconvenient terms can be resummed (exponentiated) with the help of the direct but tedious algebra on the multiple flavour indices and z-integrals, in a similar way, as in the Appendix, to re-sum another part of the kernel. In the following section we shall do it using more elegant methods.

Having defined the time ordered exponential evolution operator $\boldsymbol{G}_H$, let us quote its basic features and extend its definition for the latter use. The well known rule[4]

$$\boldsymbol{G}_H(t,t_x)\boldsymbol{G}_H(t_x,t) = \boldsymbol{G}_H(t,t_0)\,, \qquad t \geq t_x \geq t_0 \tag{12}$$

helps to manipulate products of the time-ordered exponents. We may also define the inverse operator for the "backward evolution" ($t < t_0$) as follows

$$\boldsymbol{G}_H(t_0,t) \equiv \boldsymbol{G}_H^{-1}(t,t_0)\,, \qquad t < t_0\,, \tag{13}$$

where the inverse operator is constructed using $\boldsymbol{G}_H^{-1}(t,t_0) \equiv \boldsymbol{G}_{(-H)}(t,t_0)$. The algebraic proof that $\boldsymbol{G}_H^{-1}(t,t_0)\boldsymbol{G}_H(t,t_0) = \boldsymbol{I}$, using Eq. (10), we leave to the reader. The matrix elements of $\boldsymbol{G}^{-1}$ can be non-positive and highly singular. With help of the above definition validity of Eq. (12) can be extended to any t_x.

2.2. Derivation by reorganizing evolution equation

In the following we show how to resume singular $\mathcal{P}^{\delta}$ terms by going back to the evolution equation, reorganizing it and solving it once again. We are going to show this standard trick in a detail, because, subsequently, we shall generalize it to the case of an arbitrary part of the kernel (instead of the $\mathcal{P}^{\delta}$ part). It is essentially a warm-up example.

2.2.1. Resumming virtual part of the kernel — warm-up example

Inserting explicitly regularized kernel, our evolution equation takes the following form

$$\partial_t D_k(t,x) = -\mathcal{P}^{\delta}_{kk}(t)\; D_k(t,x) + \sum_j \mathcal{P}^{\ominus}_{kj}(t,\cdot) \otimes D_j(t,\cdot)(x)\,. \tag{14}$$

[4] Chapman–Kolmogorov–Smoluchowski–Einstein relation, see Ref. [8,9].

It can be transformed into

$$\partial_t\Big(e^{\Phi_k(t,t_0)}D_k(t,x)\Big) = \sum_j e^{\Phi_k(t,t_0)}\mathcal{P}^{\Theta}_{kj}(t,\cdot)e^{-\Phi_j(t,t_0)} \otimes e^{\Phi_j(t,t_0)}D_j(t,\cdot)(x)\,. \tag{15}$$

This integro-differential form is exposed in the QCD textbooks, see Ref. [10], and is also used in the numerical evaluation (evolution) of PDFs using non-Monte Carlo methods, for instance Ref. [11]. Changing slightly notation the above is transformed into

$$\begin{aligned}
\partial_t\tilde{D}_k(t,x) &= \sum_j \tilde{\mathcal{P}}^{\Theta}_{kj}(t,\cdot)\otimes\tilde{D}_j(t,\cdot)(x)\,,\\
\tilde{D}_k(t,x) &\equiv \exp(\Phi_k(t,t_0))D_k(t,x)\,,\\
\tilde{\mathcal{P}}^{\Theta}_{kj}(t,z) &\equiv \exp(\Phi_k(t,t_0))\mathcal{P}^{\Theta}_{kj}(t,z)\exp(-\Phi_j(t,t_0))\,,
\end{aligned} \tag{16}$$

or in an equivalent compact matrix formulation it reads

$$\partial_t\tilde{D}(t) = \tilde{\boldsymbol{P}}^{\Theta}(t)\tilde{D}(t)\,. \tag{17}$$

The time ordered solution

$$\tilde{D}(t) = \exp\left(\int_{t_0}^{t}\tilde{\boldsymbol{P}}^{\Theta}(t')dt'\right)_T \tilde{D}(t_0) = \boldsymbol{G}_{\tilde{\boldsymbol{P}}^{\Theta}}(t,t_0)\;\tilde{D}(t_0) \tag{18}$$

of the evolution equation is widely known and exploited routinely in many practical evaluations of solutions of the QCD evolution. It is usually written in the traditional integro-tensorial representation similarly as Eq. (11), in terms of the initial $D(t_0)$ and the product of $\mathcal{P}^{\Theta}$, taking the following familiar shape:

$$\begin{aligned}
D_k(t,x) &= e^{-\Phi_k(t,t_0)}D_k(t_0,x)\\
&\quad+\sum_{n=1}^{\infty}\sum_{k_0,\ldots,k_{n-1}}\left[\prod_{i=1}^{n}\int_{t_0}^{t}dt_i\Theta(t_i-t_{i-1})\int_0^1 dz_i\right]\\
&\quad\times e^{-\Phi_k(t,t_n)}\int_0^1 dx_0\left[\prod_{i=1}^{n}\mathcal{P}^{\Theta}_{k_ik_{i-1}}(t_i,z_i)e^{-\Phi_{k_{i-1}}(t_i,t_{i-1})}\right]\\
&\quad\times D_{k_0}(t_0,x_0)\delta\left(x-x_0\prod_{i=1}^{n}z_i\right)\,.
\end{aligned} \tag{19}$$

Trivial identity

$$e^{-\Phi_i(t_i,t_0)}e^{\Phi_i(t_{i-1},t_0)} = e^{-\Phi_i(t_i,t_{i-1})} \tag{20}$$

was also employed. The above solution of the evolution equation is used as a basic formula in the Monte Carlo evaluation of the PDFs using Markovian MC algorithms, see for example Ref. [2]. We shall refer to this solution as non-hierarchic iterative solution of the evolution equation.

Let us remind the reader, that in the above warm-up exercise we have resummed the relatively simple component $\mathcal{P}^B_{jk}(t,z) = -\delta_{jk}\mathcal{P}^\delta_{kk}(t)\delta(1-z)$ of the evolution kernel, which was completely diagonal, both in k and in z. In this special case $\boldsymbol{G}^{-1}_{\mathcal{P}^B}$ is trivially calculable, contrary to more general case of non-diagonal $\mathcal{P}^B$ discussed in the following.

Let us now come back to our principal aim, proving Eq. (2), where less trivial component of the kernel will be isolated/resummed.

2.2.2. Resuming gluonstrahlung — the real thing

In order to prove Eq. (2), we need to resum (exponentiate) the following part of the kernel

$$\mathcal{P}^B_{jk}(t,z) = \delta_{jk}\mathcal{P}_{kk}(t,z) = -\delta_{jk}\mathcal{P}^\delta_{kk}(t)\delta(1-z) + \delta_{jk}\mathcal{P}^\Theta_{kk}(t,z)\,, \tag{21}$$

which is diagonal in the flavour indices, but not in z. This part of the kernel is always IR divergent and generates multiple gluon emission process, that is *gluonstrahlung*. The remaining *flavour-changing* part of the full kernel is defined as $\mathcal{P}^A = \mathcal{P} - \mathcal{P}^B$. The original full evolution equation and its solution read

$$\begin{aligned} \partial\boldsymbol{D}(t) &= \Big(\boldsymbol{P}^A(t) + \boldsymbol{P}^B(t)\Big)\boldsymbol{D}(t)\,, \\ D(t) &= \exp\left(\int_{t_0}^{t}\Big(\boldsymbol{P}^A(t') + \boldsymbol{P}^B(t')\Big)dt'\right)_T \boldsymbol{D}(t_0)\,. \end{aligned} \tag{22}$$

At this point, the G-function of Eq. (7) can be identified with the following operator

$$\boldsymbol{G}_B(t,t_0) \equiv \boldsymbol{G}_{P^B}(t,t_0) = \exp\left(\int_{t_0}^{t}\boldsymbol{P}^B(t')dt'\right)_T\,, \tag{23}$$

where

$$\partial_t\boldsymbol{G}_B(t,t_0) = \boldsymbol{P}^B(t)\boldsymbol{G}_B(t,t_0)\,, \tag{24}$$

see also Eq. (3).

In order to derive Eq. (2) we proceed analogously as in the derivation of Eq. (19); we shall introduce $\boldsymbol{G}_B(t,t_0)$ in the evolution equation, similarly as we have introduced $\exp\left(\Phi_k(t,t_0)\right)$. The main complication will be in the non-commutative nature of $\boldsymbol{G}_B(t,t_0)$. Let us introduce in the evolution equation an auxiliary PDF

$$\tilde{\boldsymbol{D}}(t) = \boldsymbol{G}_B^{-1}(t,t_0)\boldsymbol{D}(t)\,, \qquad \boldsymbol{D}(t) = \boldsymbol{G}_B(t,t_0)\;\tilde{\boldsymbol{D}}(t)\,, \tag{25}$$

getting after the differentiation

$$\boldsymbol{G}_B(t,t_0)\;\partial\tilde{D}(t) + \Big(\partial\boldsymbol{G}_B(t,t_0)\Big)\tilde{D}(t) = \Big(\boldsymbol{P}^A(t)+\boldsymbol{P}^B(t)\Big)\boldsymbol{G}_B(t,t_0)\;\tilde{D}(t)\,. \tag{26}$$

After inserting Eq. (24) we obtain

$$\boldsymbol{G}_B(t,t_0)\partial\tilde{\boldsymbol{D}}(t) + \boldsymbol{P}^B(t)\boldsymbol{G}_B(t,t_0)\tilde{\boldsymbol{D}}(t) = \Big(\boldsymbol{P}^A(t)+\boldsymbol{P}^B(t)\Big)\boldsymbol{G}_B(t,t_0)\tilde{\boldsymbol{D}}(t)\,. \tag{27}$$

The term proportional to $\boldsymbol{P}^B$ gets eliminated

$$\boldsymbol{G}_B(t,t_0)\partial\tilde{\boldsymbol{D}}(t) = \boldsymbol{P}^A(t)\boldsymbol{G}_B(t,t_0)\tilde{\boldsymbol{D}}(t)\,. \tag{28}$$

and we return to the usual evolution equation

$$\partial\tilde{\boldsymbol{D}}(t) = \tilde{\boldsymbol{P}}^A(t)\tilde{\boldsymbol{D}}(t)\,, \qquad \tilde{\boldsymbol{P}}^A(t) \equiv \boldsymbol{G}_B^{-1}(t,t_0)\;\boldsymbol{P}^A(t)\boldsymbol{G}_B(t,t_0)\,, \tag{29}$$

with the usual solution

$$\boldsymbol{D}(t) = \boldsymbol{G}_B(t,t_0)\exp\left(\int_{t_0}^{t}\tilde{\boldsymbol{P}}^A(t')dt'\right)_T\boldsymbol{D}(t_0)\,. \tag{30}$$

The last step on the way to Eq. (2) is elimination of the operator $\boldsymbol{G}_B^{-1}(t,t_0)$ being part of $\tilde{\boldsymbol{P}}$. The reason for that is that $\boldsymbol{G}^{-1}$ is not well suited for any numerical evaluation, especially of the MC type, due to alternating sign in the exponential expansion, hence it is better to eliminate it from the final result. It is done with the help of the following identity

$$\begin{aligned}&\boldsymbol{G}_B(t,t_0)\exp\left(\int_{t_0}^{t}\tilde{\boldsymbol{P}}^A(t')dt'\right)_T\\ &= \boldsymbol{G}_B(t,t_0)+\sum_{n=1}^{\infty}\left[\prod_{i=1}^{n}\int_{t_0}^{t}dt_i\theta_{t_i>t_{i-1}}\boldsymbol{G}_B(t_{i+1},t_i)\boldsymbol{P}^A(t_i)\right]\boldsymbol{G}_B(t_1,t_0)\,,\end{aligned} \tag{31}$$

where $t_{n+1}\equiv t$. This identity is derived rather easily by inspecting each n-th term in the expansion of the time ordered exponent and applying the following relation[5] (analogous to Eq. (20))

[5] See Eqs. (12)–(13) and the accompanying discussion.

$$\boldsymbol{G}_B(t_{i+1},t_0)\boldsymbol{G}_B^{-1}(t_i,t_0)=\boldsymbol{G}_B(t_{i+1},t_i)\boldsymbol{G}_B(t_i,t_0)\boldsymbol{G}_B^{-1}(t_i,t_0)=\boldsymbol{G}_B(t_{i+1},t_i) \tag{32}$$

for each pair $\boldsymbol{G}_B\boldsymbol{G}_B^{-1}$ sandwiched between adjacent $\boldsymbol{P}^A$'s. The final solution reads

$$\begin{aligned}\boldsymbol{D}(t) \;=\; & \boldsymbol{G}_B(t,t_0)\;\boldsymbol{D}(t_0) \\ & +\sum_{n=1}^{\infty}\left[\prod_{i=1}^{n}\int_{t_0}^{t} dt_i\theta_{t_i>t_{i-1}}\boldsymbol{G}_B(t_{i+1},t_i)\boldsymbol{P}^A(t_i)\right]\boldsymbol{G}_B(t_1,t_0)\boldsymbol{D}(t_0)\,.\end{aligned} \tag{33}$$

When translated into the integro-tensorial notation, the above formula turns out to be identical with our target Eq. (2). In this way we have completed its derivation.

It is now obvious why Eq. (2) we call a *hierarchic* solution of the evolution equation. It is because its components $\boldsymbol{G}_B$ are solutions of another simpler evolution equation (gluonstrahlung) of its own. Higher level evolution embeds lower level simpler evolution as a building block.

2.3. Derivation by reorganizing time-ordered exponential

A disadvantage of the derivation presented above is that it exploits the inverse evolution operator $\boldsymbol{G}^{-1}$, which is in a general case difficult to define properly, while it drops out from the final result of Eqs. (2) or (33) anyway. The natural question is therefore whether we could derive Eq. (2) without introducing the operator $\boldsymbol{G}^{-1}$ in the intermediate stages of the proof.

Furthermore, going back to the modified evolution equation and solving it once again obscures the relation between variables (k_i,z_i) in the non-hierarchic solution of Eq. (19) on one hand and the hierarchic one of Eq. (2) on the other hand. Such a relation is relevant for parton shower applications; in the following we shall, therefore, present an alternative example of the derivation of Eq. (9) without explicit use of the inverse evolution operator $\boldsymbol{G}^{-1}$. In such a case, the relation between variables (k_i,z_i) in Eq. (19) and Eq. (2) can be traced back (recovered) more easily.

The following derivation will be strongly reminiscent to a derivation of identity $F(x,y)=\exp(x+y)=\exp(x)\exp(y)$ by means of the Taylor expansion[6] with respect y *i.e.* $F(x,y)=\sum_{n=0}^{\infty}(x^n/n!)\partial_x^n F(x,y)|_{x=0}$.

Let us introduce slightly modified evolution operator

$$\mathbf{G}'_{\boldsymbol{H}}(t,t_0)=\mathbf{G}'(\boldsymbol{H};t,t_0)=\boldsymbol{G}(\boldsymbol{H};t,t_0)\;\theta_{t\geq t_0}\,, \tag{34}$$

[6] Note that such a derivation is almost equivalent to a direct multiplication of the infinite sums for $\exp(x)$ and $\exp(y)$, but more transparent algebraically.

where $\boldsymbol{G}$ was already defined as the time-ordered exponential in Eq. (10). The additional θ-factor ensuring $t \geq t_0$ will make the following algebra more compact. We define $\boldsymbol{H} = \boldsymbol{H}_\lambda = \boldsymbol{B} + \lambda \boldsymbol{A}$ (we shall set $\lambda = 1$ at the very end of calculation). The whole derivation relies on the following identity

$$\partial_\lambda \mathbf{G}'_{\boldsymbol{H}}(t, t_0) = \int_{t_0}^{t} dt_1 \mathbf{G}'_{\boldsymbol{H}}(t, t_1) \boldsymbol{A}(t_1) \mathbf{G}'_{\boldsymbol{H}}(t_1, t_0)\,, \tag{35}$$

which can be derived using definition of Eq. (10), and reorganizing all integrations over t_i's. The second derivative follows trivially:

$$\begin{aligned}\partial_\lambda^2 \mathbf{G}'_{\boldsymbol{H}}(t, t_0) = & \int_{t_0}^{t} dt_1 dt_2 \mathbf{G}'_{\boldsymbol{H}}(t, t_2) \boldsymbol{A}(t_2) \mathbf{G}'_{\boldsymbol{H}}(t_2, t_1) \boldsymbol{A}(t_1) \mathbf{G}'_{\boldsymbol{H}}(t_1, t_0) \\ & + \int_{t_0}^{t} dt_1 dt_2 \mathbf{G}'_{\boldsymbol{H}}(t, t_1) \boldsymbol{A}(t_2) \mathbf{G}'_{\boldsymbol{H}}(t_1, t_2) \boldsymbol{A}(t_1) \mathbf{G}'_{\boldsymbol{H}}(t_2, t_0) \\ = & \, 2! \int_{t_0}^{t} dt_2 dt_1 \mathbf{G}'_{\boldsymbol{H}}(t, t_2) \boldsymbol{A}(t_2) \mathbf{G}'_{\boldsymbol{H}}(t_2, t_1) \boldsymbol{A}(t_1) \mathbf{G}'_{\boldsymbol{H}}(t_1, t_0)\,, \end{aligned} \tag{36}$$

and the n-th derivative is

$$\partial_\lambda^n \mathbf{G}'_{\boldsymbol{H}_\lambda}(t, t_0) = n! \prod_{i=1}^{n} \left(\int_{t_0}^{t} dt_i \mathbf{G}'_{\boldsymbol{H}_\lambda}(t_{i+1}, t_i) \boldsymbol{A}(t_i) \right) \mathbf{G}'_{\boldsymbol{H}_\lambda}(t_1, t_0)\,, \tag{37}$$

where $t_n \equiv t$. Now, let us use Taylor expansion

$$\mathbf{G}'_{\boldsymbol{H}_\lambda}(t, t_0) = \mathbf{G}'_{\boldsymbol{H}_{\lambda=0}}(t, t_0) + \sum_{0}^{\infty} \frac{\lambda^n}{n!} \partial_\lambda^n \mathbf{G}'_{\boldsymbol{H}_\lambda}(t, t_0) \Big|_{\lambda=0}\,. \tag{38}$$

Noticing that $\mathbf{G}'_{\boldsymbol{H}_\lambda}(t_{i+1}, t_i)|_{\lambda=0} = \mathbf{G}'_{\boldsymbol{B}}(t_{i+1}, t_i)$, we obtain

$$\mathbf{G}'_{\boldsymbol{H}_\lambda}(t, t_0) = \mathbf{G}'_{\boldsymbol{B}}(t, t_0) + \sum_{n=1}^{\infty} \lambda^n \prod_{i=1}^{n} \left(\int_{t_0}^{t} dt_i \mathbf{G}'_{\boldsymbol{B}}(t_{i+1}, t_i) \boldsymbol{A}(t_i) \right) \mathbf{G}'_{\boldsymbol{B}}(t_1, t_0)\,. \tag{39}$$

We may set $\lambda = 1$ at this point.

Identifying $\boldsymbol{A} = \boldsymbol{P}^A$, $\mathbf{G}'_{\boldsymbol{H}} = \mathbf{G}'_{P^A+P^B}$ and $\mathbf{G}'_{\boldsymbol{B}} = \mathbf{G}'_{P^B}$ we obtain more familiar identity

$$\mathbf{G}'_{P^A+P^B}(t,t_0) = \left\{ \boldsymbol{I} + \sum_{n=1}^{\infty} \prod_{i=1}^{n} \left(\int_{t_0}^{t} dt_i \mathbf{G}'_B(t_{i+1},t_i) \boldsymbol{P}^A(t_i) \right) \right\} \mathbf{G}'_B(t_1,t_0)\,, \tag{40}$$

where, as previously, we define $\mathbf{G}'_X(t_i,t_j) = \boldsymbol{G}_X(t_i,t_j)\theta_{t_i>t_j}$, which leads immediately to Eqs. (9) and (2). In this way we have completed the *second* proof of Eq. (2) — this time without any reference to backward evolution operator $\boldsymbol{G}^{-1}$.

2.4. Straightforward derivation

In addition to two elegant proofs of Eq. (2) presented in the previous Sections, we include in Appendix third proof, which relies on a rather straightforward method — it starts from Eq. (33) and through tedious reorganization of the sums over flavour indices (change of the summation order) and relabeling of the variables transforms it into Eq. (2). The advantage of this third proof is that relation between integration and summation variables in both formulas is exposed in a manifest way. This might be useful in the construction of the exclusive MC model of the parton shower type.

3. Discussion

We are fully aware, of course, that all three derivations of Eq. (2), shown in this work represent a well established mathematical formalism, very similar to that in use in the Quantum Mechanics, theory of Markovian processes and renormalization group in the Quantum Field Theory. We did not add much to the development of the corresponding area of mathematics. Rather, our main aim was to customize this known formalism to the specific needs of solving the QCD evolution (also numerically), such that solution of Eq. (2) and the other similar ones are obtained in an effortless and rigorous way. Having all this in mind, let us comment on certain selected aspects of the presented formalism, on their possible refinements, extensions and applications. We shall concentrate mainly on two points:

- Extension to beyond-DGLAP evolutions in QCD, like CCFM and others.

- Possible application in the Markovian MCs and the related question of the momentum sum rules and normalization of PDFs.

3.1. Extensions beyond DGLAP evolution

In our definitions of the evolution of PDFs Eqs. (1)–(2) and the rest of the paper we have restricted ourself to DGLAP type [7] evolution, leading-logarithmic (LL) version or its next-to-LL extensions. This restriction is however inessential and the validity of our derivations can be extended to a more general evolution equation

$$\partial_t D_k(t,x) = \sum_j \int_x^1 du \mathcal{K}_{kj}(t,x,u) D_j(t,u)\,, \tag{41}$$

in which the dependency of the generalized kernel $\mathcal{K}(t,x,u)$ is more general than only through the ratio $z = x/u$. The above more general evolution equation is used for instance in the CCFM-type models[7] of PDF [12]. The DGLAP case of Eq. (2) is obviously covered by Eq. (41), with the following identification

$$\mathcal{K}_{kj}(t,x,u) = \frac{1}{x}\mathcal{P}_{kj}\left(t,\frac{x}{u}\right) = \frac{\alpha(t)}{\pi}\frac{1}{x}P_{kj}\left(t,\frac{x}{u}\right)\,. \tag{42}$$

The compact matrix notation used in the time-ordered exponentials can easily accommodate multiplications of the kernels $\mathcal{K}(t,x,u)$ such that all relevant algebra in the previous sections remains unchanged. Let us only indicate how the product of two kernels gets redefined

$$(\boldsymbol{P}(t_2)\boldsymbol{P}(t_1))_{kj}(x,u) = \sum_{j'} \int_x^1 du' \mathcal{K}_{kj'}(t_2,x,u')\mathcal{K}_{j'j}(t_1,u',u)\,. \tag{43}$$

The reader can easily verify that the rest of the compact matrix algebra in our derivations remains unchanged.

3.2. Sum rules and Markovianization

As already mentioned, results of this work were instrumental in the modelling QCD evolution using *non-Markovian* type Monte Carlo techniques in Refs. [13] and [14]. The corresponding MC programs simulate DGLAP and CCFM class evolutions.

However, the solution Eq. (2) may be also used to construct an interesting example of the Markovian MC in which single step in the Markovian chain is a Markovian process of its own. Without going into fine details, let us

[7] It is also closer to the spirit of the parton shower MC and unintegrated PDFs.

indicate how this can be done. To this end we have to invoke momentum sum rule

$$\sum_k \int\limits_0^1 dx x D_k(t,x) = 0\,, \tag{44}$$

and reorganize slightly Eq. (2). Staying for simplicity with the DGLAP case (LL and beyond) the above sum rule determines virtual part of the kernel

$$\mathcal{P}^{\delta}_{jj}(t,\varepsilon) = \sum_k \int\limits_0^1 dz\; z\mathcal{P}^{\Theta}_{kj}(t,z)\,. \tag{45}$$

The above is used to set up properly Markovian MC and in particular to split Sudakov formfactor $\Phi_k(t)$ into bremsstrahlung part and the rest (flavour changing part)

$$\begin{aligned}
\Phi_k(t,t_0) &= \Phi^A_k(t,t_0) + \Phi^B_k(t,t_0)\,,\\
\Phi^B_k(t,t_0) &= \int\limits_{t_0}^{t} dt' \int\limits_0^1 dz z\mathcal{P}^{\Theta}_{kk}(t',z)\,,\\
\Phi^A_k(t,t_0) &= \int\limits_{t_0}^{t} dt' \sum_{j,j\neq k} \int\limits_0^1 dz\; z\mathcal{P}^{\Theta}_{jk}(t',z)\,.
\end{aligned} \tag{46}$$

By means of pulling out $\Phi^A_k(t)$ and multiplying both sides of Eq. (2) by x, we obtain the following formula suitable for a Markovian MC

$$\begin{aligned}
xD_k(t,x) &= \int\limits_0^1 dz' dx_0 \mathcal{U}^B_{kk}(t,t_0,z') x_0 D_k(t_0,x_0)\delta(x-z'x_0) + \sum_{n=1}^{\infty}\int\limits_0^1 dx_0\\
&\times \sum_{k_{n-1},\ldots,k_1,k_0} \left[\prod_{j=1}^{n}\int\limits_{t_0}^{t} dt_j \Theta(t_j - t_{j-1})\right] \int\limits_0^1 dz'_{n+1} \left[\prod_{i=1}^{n}\int\limits_0^1 dz'_i dz_i\right]\\
&\times \mathcal{U}^B_{kk}(t,t_n,z'_{n+1}) \left[\prod_{i=1}^{n} e^{-\Phi^A_{k_{i-1}}(t_i,t_{i-1})} z_i \mathcal{P}^A_{k_i,k_{i-1}}(t_i,z_i)\right.\\
&\left.\times\, \mathcal{U}^B_{k_{i-1}k_{i-1}}(t_i,t_{i-1},z'_i)\right] x_0 D_{k_0}(t_0,x_0)\\
&\times \delta\left(x - x_0 \prod_{i=1}^{n} z_i \prod_{i=1}^{n+1} z'_i\right), \qquad k_n = k\,,
\end{aligned} \tag{47}$$

where

$$\mathcal{U}^B_{kk}(t_1,t_0,z) \equiv e^{\Phi^A_k(t_1,t_0)} z G^B_{kk}(t_1,t_0,z)\,, \tag{48}$$

and G^B_{kk} is given by Eg. (7). The evolution operator $\mathcal{U}$ obeys nice "unitarity" rule

$$\int dz \mathcal{U}^B_{kk}(t,t_0,z) = 1 \tag{49}$$

for any t, $t \geq t_0$, in addition to the usual boundary condition $\mathcal{U}^A_{kk}(t_0,t_0,z) = \delta(1-z)$.

Eq. (47) can be now used to define hierarchic (nested) Markovian Monte Carlo algorithm. The normalized probability distribution of the forward Markovian step in the flavour-changing upper level Markovian process reads:

$$\begin{aligned}
&\omega(t_i,x_i,k_i|t_{i-1},x_{i-1},k_{i-1}) = \omega(t_i,z_iz'_ix_{i-1},k_i|t_{i-1},x_{i-1},k_{i-1}) \\
&= (1-\delta_{k_ik_{i-1}}) e^{-\Phi^A_{k_{i-1}}(t_i,t_{i-1})} z_i \mathcal{P}^A_{k_ik_{i-1}}(z_i) z'_i \mathcal{U}^B_{k_{i-1}k_{i-1}}(t_i,z'_i|t_{i-1})\,, \\
&\int\limits_{t_{i-1}}^{\infty} dt_i \sum_{k_i} \int\limits_0^1 dz_i \int\limits_0^1 dz'_i \omega(t_i,z_iz'_ix_{i-1},k_i|t_{i-1},x_{i-1},k_{i-1}) \equiv 1\,.
\end{aligned} \tag{50}$$

For the lower level bremsstrahlung process one may use standard Markovian MC technique of Ref. [1].

Let us discuss selected details of the above scenario. Here, all k_i and t_i, $i = 1,2,...n$ can be generated before generation of any z-variables in a separate Markovian algorithm with the stopping rule being the usual condition $t_{n+1} \geq t$. (See Ref. [1] for more details on the the Markovian class MC algorithms.) Variables z_i of the flavour-changing kernels can also be generated at this early stage.

The interesting question is: how and when do we generate z'_i according to gluonstrahlung operator $\mathcal{U}^B_{k_{i-1}k_{i-1}}(t_i,z'_i|t_{i-1})$? If we have known an analytical (even approximate) representation of this function, or its precise value from the look-up tables, then we could readily generate them before entering into MC simulation of the bremsstrahlung subprocess. That would lead us to the use of the constrained MC of Refs. [13–15] for the bremsstrahlung segments. Alternatively, z'_i may come out from a separate Markovian MC module simulating gluonstrahlung sub-process starting at t_{i-1} and stopping at t_i, with the normalized probability distribution of single Markovian step defined in Ref. [1]. In this latter case we would have simulated in the MC a hierarchic system of Markovian processes, with the master flavour-changing Markovian process and many Markovian subprocesses, each of them implementing pure bremsstrahlung, flavour conserving, emissions.

The above hierarchic Markovian MC scheme, although quite interesting, seems to have no immediate practical importance. However, it may find applications in some future works.

4. Summary

The basic aim of this paper is to provide solid technical foundation to other works in the area of the Monte Carlo simulation of the evolution of PDFs and parton shower in QCD. Our basic result is the solution of the evolution equation of Eq. (2), which was proved algebraically using three methods. Its primary application is construction of the constrained MC algorithms of Ref. [13]. In addition, we also describe application of such a solution in the Markovian MC algorithm. Although we are aware of many interesting relation of the discussed problems and solutions to other areas in physics, we did not attempt to elaborate on that too much, in order to keep the paper compact and transparent. Let us mention also, that our solution can be used many times leading to a nested structure with several levels of the hierarchy.

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Appendix A

Combinatorial proof

We are going to show how to transform non-hierarchic solution in Eq. (19) (with resummed virtual corrections) into hierarchic solution in Eq. (2) (with resummed gluonstrahlung) using straightforward method of changing summation order and relabeling integration variables.

The critical point in isolating two levels in the evolution, flavour-changing transitions and gluonstrahlung, will be the change of the summation order in Eq. (2), such that one is able to resum separately the pure bremsstrahlung segments obeying $k_i = k_{i-1}$. These segments will form (many) functions G^B_{kk}, as defined in Eq. (7). The corresponding transformation of the summation order (indexing) looks schematically as follows

$$\sum_{n=0}^{\infty} \sum_{k_{n-1}\ldots,k_1 k_0} t_{k_n k_{n-1}\ldots k_1 k_0} = \sum_{n=0}^{\infty} \sum_{\substack{k_{n-1}\ldots,k_1 k_0 \\ k_n \neq k_{n-1} \neq \ldots \neq k_1 \neq k_0}} \sum_{j_n, j_{n-1}\ldots j_0=1}^{\infty} t_{k_n^{(j_n)}\ldots k_n^{(2)} k_n^{(1)} k_{n-1}^{(j_{n-1})}\ldots k_{n-1}^{(2)} k_{n-1}^{(1)} \ldots\ldots k_1^{(j_1)}\ldots k_1^{(2)} k_1^{(1)} k_0^{(j_0)}\ldots k_0^{(2)} k_0^{(1)}}, \quad \text{(A.1)}$$

where we have $k_r^{(j_r)} = \ldots = k_r^{(2)} = k_r^{(1)}$ and the purpose of the upper index in this context is simply to show that the same index k is repeated j_r times. On the other hand variables $z_r^{(m)}$ and $\tau_r^{(m)},\ r = 1, 2, \ldots, n,\ m = 1, 2, \ldots, j_r$ are truly different (independent), with the upper index truly differentiating them.

The aim is now to show that one can factorize out the functions G^B_{kk} and identify precisely the remaining functions and integrations. Employing the above index transformation in the product of the $\mathcal{P}$-functions we obtain

$$\begin{aligned}
\{\mathcal{P}_{k_n k_n}(t^{(n)}_{j_n}, z^{(n)}_{j_n}) \ &\ldots\ \mathcal{P}_{k_n k_n}(t^{(n)}_2, z^{(n)}_2)\}\mathcal{P}_{k_n k_{n-1}}(t^{(n)}_1, z^{(n)}_1) \\
&\ldots \\
\ldots\ &\ldots\ \mathcal{P}_{k_1 k_1}(t^{(2)}_2, z^{(2)}_2)\}\mathcal{P}_{k_2 k_1}(t^{(2)}_1, z^{(2)}_1) \\
\{\mathcal{P}_{k_1 k_1}(t^{(1)}_{j_1}, z^{(1)}_{j_1}) \ &\ldots\ \mathcal{P}_{k_1 k_1}(t^{(1)}_2, z^{(1)}_2)\}\mathcal{P}_{k_1 k_0}(t^{(1)}_1, z^{(1)}_1) \\
\{\mathcal{P}_{k_0 k_0}(t^{(0)}_{j_0}, z^{(0)}_{j_0}) \ &\ldots\ \mathcal{P}_{k_0 k_0}(t^{(0)}_2, z^{(0)}_2)\mathcal{P}_{k_0 k_0}(t^{(0)}_1, z^{(0)}_1)\}\,,
\end{aligned} \tag{A.2}$$

where curly bracket embrace the diagonal elements $\mathcal{P}_{kk}$, to be collected into the G^B_{kk}-functions; the remaining, nondiagonal ones, are now clearly isolated.

Each $\mathcal{P}_{k_i,k_{i-1}}$, $k_i \neq k_{i-1}$ in Eq. (19) is accompanied by an exponential factors. All of them (including the first one which does not belong to any $\mathcal{P}$) are now reorganized as follows:

$$\begin{aligned}
& e^{\Phi_{k_n}(t,t^{(n)}_n)} \\
e^{\Phi_{k_n}(t^{(n)}_n,t^{(n)}_{j_n-1})} \ &\ldots\ e^{\Phi_{k_n}(t^{(n)}_2,t^{(n)}_1)}e^{\Phi_{k_{n-1}}(t^{(n)}_1,t^{(n-1)}_{j_{n-1}})} \\
&\ldots \\
e^{\Phi_{k_1}(t^{(1)}_{j_1},t^{(1)}_{j_1-1})} \ &\ldots\ e^{\Phi_{k_1}(t^{(1)}_2,t^{(1)}_1)}e^{\Phi_{k_0}(t^{(1)}_1,t^{(0)}_{j_1})} \\
e^{\Phi_{k_0}(t^{(0)}_{j_1},t^{(0)}_{j_1-1})} \ &\ldots\ e^{\Phi_{k_0}(t^{(0)}_2,t^{(0)}_1)}e^{\Phi_{k_0}(t^{(0)}_1,t_0)} \\
= e^{\Phi_{k_n}(t,t^{(n)}_1)}e^{\Phi_{k_{n-1}}(t^{(n)}_1,t^{(n-1)}_1)} \ &\ldots\ e^{\Phi_{k_1}(t^{(2)}_1,t^{(1)}_1)}e^{\Phi_{k_0}(t^{(1)}_1,t_0)}\,,
\end{aligned} \tag{A.3}$$

where all factors entering into products in G^B_{kk}-functions are shown inside the curly brackets in Eq. (A.2). Together with the flavour-changing $\mathcal{P}$'s, the above exponential form-factors look as follows:

$$\begin{aligned}
& e^{\Phi_{k_n}(t,t^{(n)}_1)} \quad \mathcal{P}_{k_n k_{n-1}}(z^{(n)}_1)e^{\Phi_{k_{n-1}}(t^{(n)}_1,t^{(n-1)}_1)} \\
& \ldots \mathcal{P}_{k_2 k_1}(z^{(2)}_1)e^{\Phi_{k_1}(t^{(2)}_1,t^{(1)}_1)}\mathcal{P}_{k_1 k_0}(z^{(1)}_1)e^{\Phi_{k_0}(t^{(1)}_1,t_0)}\,.
\end{aligned} \tag{A.4}$$

The other diagonal $\mathcal{P}$'s will enter into G^B_{kk}-functions.

In this rather sketchy way we have shown that indeed Eq. (19) can be transformed into Eq. (2) by means of the straightforward reorganization of multiple sums and integrals. (More systematic proof would require completing mathematical induction with respect to n.)

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