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On the recursive properties of Dawson's integral

Erno Sajo
Nuclear Science Centre, Louisiana State University, Baton Rouge, LA 70803, USA

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Abstract. The generalized Dawson integral $F(p, x)$ is considered. Closed formulae are given for the nth derivatives with respect to the arguments x and p in terms of the function itself. A recursion relation is developed which may be regarded as the $(n+1)$st-order differential equation satisfied by $F(p, x)$. It is shown that known results concerning Dawson's function are merely specific cases of the generalized Dawson equation. The application of the successive derivatives of $F(2, x)$ in the context of the Voigt spectrum line profiles is demonstrated.

1. Introduction

The motivation of this study of Dawson's integral is provided by the analysis of certain non-linear, time-dependent atmospheric source–receptor relationships involving partial differential equations by hypergeometric series solution.

Dawson's integral [1],

$$F(x) = \int_0^x e^{t^2-x^2}\,dt \qquad x \geqslant 0 \tag{1.1}$$

frequently arises in various physical problems, such as spectroscopy, electrical oscillations and heat conduction. The integral is closely related to the modified and complex error functions as:

$$\mathrm{Erf\,i}(z) = -\mathrm{i}\,\mathrm{Erf}(\mathrm{i}z) = e^{z^2} F(z) \tag{1.2}$$

and

$$w(z) = e^{-z^2}\mathrm{Erfc}(-\mathrm{i}z) = e^{-z^2} + \frac{2\mathrm{i}}{\sqrt{\pi}}F(z) \tag{1.3}$$

respectively. For all complex values z the function satisfies the differential equations

$$F'(z) + 2zF(z) = 1 \tag{1.4}$$

and for $k \geqslant 1$

$$F^{[k+1]}(z) + 2z\,F^{[k]}(z) + 2k\,F^{[k-1]}(z) = 0 \tag{1.5}$$

where the conventional notation $F^{[k]}$ is used to indicate the kth derivative of the function $F(z)$. Note that due to (1.3), the complex error function $w(z)$ is also a solution to the latter equation as may be verified by direct differentiation. If one expands $F(z)$ about a point

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x on the real axis, it can be shown that the coefficients d_n of the Taylor series satisfy the recurrence relation [2]:

$$
\begin{aligned}
d_0 &= F(x) \\
d_1 &= 1 - 2x\, d_0 \\
d_n &= -\frac{2}{n}(x d_{n-1} + d_{n-2}) \qquad n \geqslant 2.
\end{aligned}
\tag{1.6}
$$

A sequence of rational approximations to Dawson's integral have appeared in the works of Cody *et al* [3] and McCabe [4] in the forms of Chebyshev polynomials and continued fraction expansions, respectively. Earlier work concerning the tabulation of $F(x)$ is described by those authors.

The generalization of Dawson's integral entails introducing the arbitrary positive parameter p in place of the second-order power appearing in the exponent of (1.1):

$$F(p, x) = \int_0^x \mathrm{e}^{t^p - x^p}\, \mathrm{d}t. \tag{1.7}$$

For $p \geqslant 2$, $F(p, x)$ has regular poles, while for $1 < p < 2$, $F(p, x)$ has regular singular poles.

The importance of this generalization is indicated in numerous problems of practical interest. The function $F(3, x)$ has application in viscous fluid flow while, $F(p, qx)$ plays an important role in the inverse analysis of transient source–receptor problems, where it is distinguished as the 'universal-source' term [5]. The various derivatives of Dawson's integral arise in the problems of time-dependent atmospheric dispersion involving transient sources and radiative transfer in the upper atmosphere. The integral also frequently appears in other branches of physics where kernel methods are used to describe transient transport phenomena in various media.

An important property of $F(p, x)$ is that it gives an exact representation of the remainder in the truncated Taylor series for e^{-z}:

$$\mathrm{e}^{-z} = \sum_{k=0}^{N-1} \frac{(-z)^k}{k!} + \frac{(-1)^N}{N!} F\left(\frac{1}{N}, z^N\right) \qquad N = 1, 2, 3, \ldots. \tag{1.8}$$

In many physical and engineering applications this characteristic is used to model sums of exponentially decaying functions. To illustrate its close connections to higher transcendental functions, it is worthwhile to point out that the integral (1.7) can also be expressed in terms of the incomplete gamma function:

$$F(p, x) = \mathrm{e}^{-x^p} \frac{x}{p} \Gamma\left(\frac{1}{p}\right) \gamma^*\left(\frac{1}{p}, -x^p\right) \tag{1.9}$$

or, with the aid of Kummer's transformation, in terms of the confluent hypergeometric function M:

$$F(p, x) = x\, M\left(1; \frac{1}{p} + 1; -x^p\right). \tag{1.10}$$

The latter equation forms the basis of the development by Dijkstra [6], who gives a rapidly convergent continued fraction expansion for $F(p, x)$.

In the present paper the differential equation (1.5), listed by Cody *et al* [3] and McCabe [4], and the recurrence relation (1.6) derived by Faddeyeva and Terent'ev [2] will be generalized for $F(p, x)$ $(p > 1)$. Further, the nth derivatives of the generalized Dawson integral with respect to x and p will be given in closed forms and in terms of the function $F(p, x)$ itself. An application for the repeated derivatives of $F(x)$ will be demonstrated through the expansion of the Voigt function occurring in astrophysical problems.

2. The generalized Dawson differential equation

The first derivative of the generalized Dawson integral (1.7) gives rise to the differential equation

$$F'(p,x) + p\,F(p,x)\,x^{p-1} = 1. \tag{2.1}$$

The nth derivative of $F(p,x)$ can be obtained by using the Leibniz rule, as

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}F(p,x) = \sum_{i=0}^{n}\binom{n}{i}\frac{\mathrm{d}^i}{\mathrm{d}x^i}\int_0^x \mathrm{e}^{t^p}\,\mathrm{d}t\,\frac{\mathrm{d}^{n-i}}{\mathrm{d}x^{n-i}}\mathrm{e}^{-x^p}. \tag{2.2}$$

By a suitable substitution, this equation may be reduced in complexity, however, it will be still rather cumbersome to handle. In particular, it can be seen that the ith derivative of the integral in (2.2) is irreducible, while reduction of derivatives of the type $\mathrm{d}^k(\mathrm{e}^{-z^p})/\mathrm{d}z^k$ will entail a sum of the same type of derivatives. For the specific case of $p = 2$, it is readily seen that the last term on the right-hand side will entail Hermite polynomials due to Rodrigues' formula. The connection between Dawson's integral and Hermite polynomials will be further emphasized later in this section.

In deriving a closed form for $\mathrm{d}^nF(p,x)/\mathrm{d}x^n$ one may recognize that all derivatives of $F(p,x)$ involve the sum of the lower-order derivatives of the same function. This way, it is possible to formulate a practical recursion-like identity as follows:

Theorem 1. For $n \geqslant 2$ and for $p > 1$, $x \geqslant 0$, the nth derivative of $F(p,x)$ becomes expressible in terms of the sum of the first $n-1$ derivatives of $F(p,x)$ and may be written as

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}F(p,x) = F^{[n]} = -\sum_{i=0}^{n-1}\binom{n-1}{i}p^{(n-i)}x^{p-n+i}F^{[i]} \tag{2.3}$$

where $p^{(k)}$ denotes the Stirling factorial polynomial of order k.

The proof may be substantiated by induction but omitted here since the steps are routine, being similar to the proof of the Leibniz formula.

This theorem together with the relation $p^{(n-i)}x^{p-n+i} = (x^p)^{[n-i]}$ enables us to generalize McCabe's result [4] and express it as the $(n+1)$st-order Dawson differential equation:

$$F^{[n+1]} + \sum_{i=0}^{n}\binom{n}{i}(x^p)^{[n+1-i]}F^{[i]} = 0 \qquad n = 1,2,3\ldots. \tag{2.4}$$

It can be clearly seen that (1.5) is a special case of (2.4) corresponding to $p = 2$. In the particular case of $p = 2$, $n = 1$, (2.4) becomes a diffusion-type equation which may be satisfied by various other functions, for example e^{-x^2}.

The relation between Dawson's integral and various orthogonal polynomials (Hermite and Laguerre, in particular) can be explored without difficulties by realizing that (2.4) may be regarded as a generalization of the Hermitian equation

$$f''(x) + 2x\,f'(x) + 2n\,f = 0 \tag{2.5}$$

which is satisfied by

$$f(x) = H_{n-1}(x)\frac{\mathrm{e}^{-x^2}}{\Gamma(n)\mathrm{i}^n}\left[\mathrm{i}C_1\Gamma\left(\frac{n+1}{2}\right) - C_2x\Gamma\left(\frac{n}{2}\right)\right] \tag{2.6}$$

establishing thereby a relation between the derivatives of $F(2, x)$ and the Hermite polynomials:

$$F^{[k]}(2, x) = H_k(x) \frac{\mathrm{e}^{-x^2}}{\Gamma(k+1)\mathrm{i}^k} \left[C_1 \Gamma \left(\frac{k+2}{2} \right) + \mathrm{i} C_2 x \Gamma \left(\frac{k+1}{2} \right) \right]. \tag{2.7}$$

The latter identity has important implications in the expansion of the Voigt function to be discussed in section 4.

3. The higher derivatives of $F(p, x)$

3.1. Derivatives with respect to x

From (1.10) it is easily perceived that the recurrent derivatives of $F(p, x)$ may be expressed in terms of Kummer's functions

$$M\left(1; \frac{1}{p} + 1; -x^p\right) \qquad \text{and} \qquad M\left(n; \frac{1}{p} + n; -x^p\right).$$

The disadvantage of this representation lies in the fact that $M(a; b; z)$ is an infinite sum and the terminating hypergeometric series $M(n; 1/p + n; -x^p)$ is irreducible for all but some n. Thus, it may be rather difficult to obtain accurate function values for all arguments. On the ground of theorem 1, however, it is possible to construct the nth derivatives of $F(p, x)$ in closed form, in terms of the function itself:

Theorem 2. For $p > 1$ and $n \geqslant 2$

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n} F(p, x) = F^{[n]} = \sum_{k=1}^{n} (-1)^{n+k-1} p^{n-k+1} x^{p(n-k+1)-n} [F(p, x) B_k^{(n)} + x\, D_{k-1}^{(n)}]. \tag{3.1}$$

The coefficients $B_k^{(n)}$ $(k = 1, 2, 3, \ldots, n)$ and $D_k^{(n)}$ $(k = 0, 1, 2, 3, \ldots, n-1)$ are defined as follows.

$$B_1^{(n)} = 1 \qquad B_2^{(n)} = (p-1)\binom{n}{2}.$$

For $3 \leqslant k \leqslant n$

$$\begin{aligned} B_k^{(n)} = (p-1) \sum_{i=3}^{n-k+3} \binom{i-1}{2} [(i-2)p - (i-1)] \sum_{j=i}^{(n-k+3)\vartheta_{k,4}} [(j-2)p - j] \\ \times \sum_{l=j}^{(n-k+3)\vartheta_{k,5}} [(l-2)p - (l+1)] \ldots \sum_{m}^{(n-k+3)\vartheta_{k,n}} [(m-2)p - (m+n-4)] \end{aligned} \tag{3.2}$$

$$D_0^{(n)} = 0 \qquad D_1^{(n)} = 1 \qquad D_2^{(n)} = (p-1)\left[\binom{n}{2} - 1\right].$$

For $3 \leqslant k \leqslant n-1$

$$D_k^{(n)} = \sum_{i=1}^{(k-2)\eth_{n-2,k}} \prod_{j=1}^{i-1}[(n-k)p-(n-1-j)]\left\{B_{k-i+1}^{(n-i)} - (p-1)\binom{n-k+1}{2}\right.$$
$$\left. \times \prod_{j=1}^{k-1-i}[(n-k)p-(n-k+j)]\right\} + (p-1)\left[(k-1)\binom{n-k+1}{2} + (n-k)\right]$$
$$\times \prod_{j=1}^{k-2}[(n-k)p-(n-k+j)]. \tag{3.3}$$

Here $\eth_{i,j}$ is defined as

$$\eth_{i,j} = \begin{cases} 0 & \text{if } i < j \\ 1 & \text{if } i \geqslant j \end{cases} \tag{3.4}$$

and in particular, one may note that

$$\binom{i-1}{2} = \mathfrak{S}_{i-1}^{(i-2)}$$

i.e. Stirling numbers of the second kind. The notations $B_k^{(n)}$ and $D_k^{(n)}$ are used to signify the fact that these coefficients depend on the order of the derivative in addition to the index k. They are not to be confused either with Stirling's numbers or with the Stirling factorial polynomial.

Simple examination of (3.2) and (3.3) shows that $B_k^{(n)}$ and $D_k^{(n)}$ are closely related. The proof of theorem 2 along with the derivation of various recursion relations for $B_k^{(n)}$ and $D_k^{(n)}$ are presented in the appendix.

Apart from its analytical significance, theorem 2 has important implications in the field of numerical computations. For example, by virtue of the efficient continued fraction expansion given by Dijkstra [6], it becomes possible to calculate $F^{[n]}(p,x)$ accurately for both small and large values of x without the use of exponential functions.

3.2. Derivatives with respect to p

For the sake of completeness and since the method of proof has the merit of being simple, though lengthy, one may construct the nth derivative of $F(p,x)$ with respect to p. This time, however, the higher derivatives will not be expressible in terms of $F(p,x)$.

Theorem 3.

$$\frac{\mathrm{d}^n}{\mathrm{d}p^n}F(p,x) = (-1)^n \mathrm{e}^{-x^p} \sum_{k=0}^{n} \mathcal{Z}_{k,n} \ln^{n-k}(x)(x^p)^{1-\delta_{k,n}} \qquad n = 1,2,3\ldots \tag{3.5}$$

where $\delta_{k,n}$ is the Kronecker symbol and $\mathcal{Z}_{k,n}$ is defined as

$$\mathcal{Z}_{0,n} = \mathrm{e}^{x^p} F(p,x) \sum_{i=0}^{n-1} \mathfrak{S}_{n-i}^{(i+1)} x^{ip} \tag{3.6}$$

$$\mathcal{Z}_{k,n} = (-1)^k \binom{n}{k} \int_0^x t^p \mathrm{e}^{t^p} \ln^k(t) \sum_{j=0}^{k-1} \mathfrak{S}_{k-j}^{(j+1)} t^{jp}\, \mathrm{d}t \sum_{i=0}^{n-k-1} \mathfrak{S}_{n-k-i}^{(i+1)} x^{ip} \qquad k = 1,2,3,\ldots. \tag{3.7}$$

Here the parameters $\mathfrak{S}_n^{(m)}$ are the Stirling numbers of the second kind.

The proof of theorem 3 may be substantiated by mathematical induction, where once again the identity

$$\frac{\mathrm{d}}{\mathrm{d}p}F^{[n]}(p,x) = F^{[n+1]}(p,x)$$

can be shown by expanding $\mathrm{d}(F^{[n]}(p,x))/\mathrm{d}p$ and, subsequently, collecting the coefficients of the same powers. The development of the proof is not given here due to the rather lengthy derivation and because the procedure is analogous to the one shown in the case of the previous theorem. One may, however, note that with little effort, a similar form to (2.2) can also be found for $\mathrm{d}^n(F(p,x))/\mathrm{d}p^n$. Unfortunately, as was the case for $\mathrm{d}^n(F(p,x))/\mathrm{d}x^n$, this form is of little practical use, therefore it is omitted from the discussion.

4. Application

As was indicated in the introduction, higher derivatives of the generalized Dawson integral occur in the inverse or adjoint formulation of atmospheric source–receptor relations with transient source term. There, the nature of the inverse problem necessitates the evaluation of a resolvent kernel entailing Dawson's integral.

Moreover, in many physical problems dealing with radiative transfer in the upper atmosphere, or in astrophysics, the spectrum line shape resulting from a superposition of independent Lorentz and Doppler broadenings (known as Voigt profile) is described by the following function:

$$K(x,y) = \frac{y}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{e}^{-t^2}}{y^2+(x-t)^2}\,\mathrm{d}t. \tag{4.1}$$

For $y > 0$, the Voigt function (4.1) and the function

$$L(x,y) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{(x-t)\mathrm{e}^{-t^2}}{y^2+(x-t)^2}\,\mathrm{d}t \tag{4.2}$$

make up the real and imaginary terms, respectively, in the integral representation of the complex error function $w(z)$ [2].

In the general expansion of $K(x,y)$ in powers of y, the coefficients of even powers entail Hermite polynomials, while those of odd powers comprise successively higher derivatives of Dawson's integral $F(2,x)$ [7].

$$K(x,y) = \sum_{n=0}^{\infty}\left(\mathrm{e}^{-x^2}H_n(x)\frac{y^n}{n!}\cos\left(\frac{n\pi}{2}\right) - \frac{2}{\sqrt{\pi}}F^{[n]}(2,x)\sin\left(\frac{n\pi}{2}\right)\frac{y^n}{n!}\right). \tag{4.3}$$

By employing the relation between Hermite polynomials and Dawson's integral (2.7), the series representation of the Voigt function (4.3) may be brought to a form that will only entail either Hermite polynomials or Dawson's integral.

In the computer implementation of $K(x,y)$ involving $F^{[n]}(2,x)$ the recurrence relation (1.6) is generally used. In doing so, considerable care must be taken since this recurrence relation successively differentiates $F(2,x)$ *numerically*, thus, very high precision of $F(2,x)$

is needed [7]. Although accurate continued fraction representation of the generalized Dawson integral is available [6], this method is limited to small y and x to avoid excessive error due to the repeated differentiation, thereby severely impairing applications in atmospheric sciences where a wide range of y is encountered.

Theorem 2 of this paper, on the other hand, allows us to express $F^{[n]}(p,x)$ solely in terms of $F(p,x)$ without successive differentiations. This significantly improves the accuracy and computational efficiency of the Voigt function.

In addition to the example discussed above, the developments presented in sections 2 and 3 have applications in many other fields of physics such as acoustics, plasma wave propagation and in non-linear atmospheric source–receptor relations.

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Appendix. Recurrence relations and proof of theorem 2

Apart from the obvious connection between $D_k^{(n)}$ and a series of $B_{k-i}^{(n-i)}$ given by (3.3) there are further important relations to be explored. Let us therefore, first try to establish some recursion relations involving $B_k^{(n)}$ and $D_k^{(n)}$. The formulae derived in the following will be instrumental in proving theorem 2.

A1. Recursion for $B_k^{(n)}$

Alternative expansions of (3.2) for $B_k^{(n+1)}$ and $B_{k-1}^{(n)}$ provide a relatively easy way to obtain the desired recursion formula. For $k \geqslant 3$ we have:

$$B_k^{(n+1)} = (p-1)\sum_{i=3}^{n-k+4}\binom{i-1}{2}[(i-2)p-(i-1)]\ldots\sum_{l}^{(n-k+4)\mathfrak{d}_{k,n}}[(l-2)p-(l+k-5)]$$
$$\times\sum_{m=l}^{(n-k+4)\mathfrak{d}_{k,n+1}}[(m-2)p-(m+k-4)]. \tag{A1}$$

Here, we used the fact that

$$[(m-2)p-(m+n-3)] = [(m-2)p-(m+k-4)]$$

since when k reaches the last term of the expansion then $k = n+1$. Moreover, since in (3.2)

$$B_k^{(n)}|_{k-1} \text{ terminates at } \sum^{(n-k+3)\mathfrak{d}_{k,n-1}}|_{k-1} = \sum^{(n-k+4)\mathfrak{d}_{k-1,n-1}}$$

we find that

$$B_{k-1}^{(n)} = (p-1)\sum_{i=3}^{n-k+4}\binom{i-1}{2}[(i-2)p-(i-1)]\cdots\sum_{m}^{(n-k+4)\mathfrak{d}_{k-1,n-1}}[(m-2)p-(m+k-5)]. \tag{A2}$$

Subtracting (3.2) from (A1) we have

$$B_k^{(n+1)} - B_k^{(n)} = [(m-2)p-(m+k-4)]|_{m=n-k+4}(p-1) \sum_{i=3}^{(n-k+4)\vartheta_{k,3}} \binom{i-1}{2} [(i-2)p-(i-1)]$$
$$\times \sum_{j=i}^{(n-k+4)\vartheta_{k,4}} [(j-2)p-j)] \ldots \sum_{i=3}^{(n-k+4)\vartheta_{k-1,n-1}} [(m-2)p-(m+k-5)] \quad \text{(A3)}$$

where the first factor on the right-hand side is none other than the last term in the expansion of the last sum in (A1). Comparison of the above equation with (A2) yields the recurrence relation

$$B_k^{(n)} = B_k^{(n+1)} - B_{k-1}^{(n)}[(n-k+2)p-n)]. \quad \text{(A4)}$$

Furthermore, upon comparing the definition for $B_k^{(n)}$ with the above equation, we find that the restriction $k \geqslant 4$ can be removed and (A4) is valid for all $k \geqslant 1$ with the proviso of $B_0^{(n)} = 0$.

A2. Recursion for $D_k^{(n)}$

In seeking an expression for $D_k^{(n)}$ similar to (A4) we may rewrite (3.3) for $k \geqslant 3$ as follows

$$D_k^{(n+1)} = B_k^{(n)} + Q_k^{(n+1)} + R_k^{(n+1)} \quad \text{(A5)}$$

where

$$R_k^{(n+1)} = (p-1)\left[(k-2)\binom{n-k+2}{2} + (n-k+1)\right] \prod_{j=1}^{k-2} [(n-k+1)p-(n-k+j+1)] \quad \text{(A6)}$$

$$Q_k^{(n+1)} = \sum_{i=1}^{(k-3)\vartheta_{n-1,k}} \left\{ B_{k-i}^{(n-i)} - (p-1)\binom{n-k+2}{2} \prod_{j=1}^{k-2-i} [(n-k+1)p-(n-k+j+1)] \right\}$$
$$\times \prod_{j=1}^{i} [(n-k+1)p-(n-j)]. \quad \text{(A7)}$$

Notice that

$$Q_{k=3}^{(n+1)} = Q_{k=n}^{(n+1)} = 0$$

due to the upper limit $(k-3)\vartheta_{n-1,k}$ of the summation. If we now further expand (A7) employing the definition of $B_k^{(n)}$, we have:

$$Q_k^{(n+1)} = (p-1) \sum_{i=3}^{(n-k+2)\vartheta_{k,4}} \binom{i-1}{2} [(i-2)p-(i-1)] \left\{ \prod_{s=1}^{k-3} [(n-k+1)p-(n-s)] \right.$$
$$+ \prod_{s=1}^{k-4} [(n-k+1)p-(n-s)] \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] + \prod_{s=1}^{k-5} [(n-k+1)p-(n-s)]$$

$$
\begin{aligned}
&\times \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] \sum_{l=j}^{(n-k+3)\vartheta_{k,6}} [(l-2)p-(l+1)]+\cdots+[(n-k+1)p-(n-1)] \\
&\times \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] \sum_{l=j}^{(n-k+3)\vartheta_{k,6}} [(l-2)p-(l+1)] \ldots \\
&\times \sum_{m}^{(n-k+3)\vartheta_{k,n-1}} [(m-2)p-(m+k-5)] \Bigg\} = [(n-k+1)p-(n-1)] \Bigg\{ (p-1) \\
&\times \sum_{i=3}^{(n-k+2)\vartheta_{k,4}} \binom{i-1}{2} [(i-2)p-(i-1)] \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] \ldots \\
&\times \sum_{m}^{(n-k+3)\vartheta_{k,n-1}} [(m-2)p-(m+k-5)] + (p-1) \\
&\times \sum_{i=3}^{(n-k+2)\vartheta_{k,4}} \binom{i-1}{2} [(i-2)p-(i-1)] \\
&\times \left(\prod_{s=1}^{k-4} [(n-k+1)p-(n-1-s)] + \prod_{s=1}^{k-5} [(n-k+1)p-(n-1-s)] \right. \\
&\times \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] + \cdots + [(n-k+1)p-(n-2)] \\
&\times \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] \sum_{l=j}^{(n-k+3)\vartheta_{k,6}} [(l-2)p-(l+1)] \ldots \\
&\times \left. \sum_{m}^{(n-k+3)\vartheta_{k,n-2}} [(m-2)p-(m+k-6)] \right) \Bigg\}. \qquad \text{(A8)}
\end{aligned}
$$

Here, we may recognize that the last sum with respect to i, complete with the nested terms in the parentheses, is actually $Q_{k-1}^{(n)}$. Hence, the recursion for $Q_k^{(n+1)}$:

$$
\begin{aligned}
Q_k^{(n+1)} = [(n-k+1)p-(n-1)] \Bigg\{ & Q_{k-1}^{(n)} + (p-1) \sum_{i=3}^{(n-k+2)\vartheta_{k,4}} \binom{i-1}{2} [(i-2)p-(i-1)] \\
&\times \sum_{j=i}^{(n-k+3)\vartheta_{k,5}} [(j-2)p-j] \ldots \sum_{m}^{(n-k+3)\vartheta_{k,n-1}} [(m-2)p-(m+k-5)] \Bigg\}. \qquad \text{(A9)}
\end{aligned}
$$

The multiple sums in the above equation can be written in terms of $B_{k-1}^{(n-1)}$ as follows

$$
\begin{aligned}
Q_k^{(n+1)} = [(n-k+1)p-(n-1)] \Bigg\{ & B_{k-1}^{(n-1)} - (p-1) \binom{n-k+2}{2} \\
&\times \prod_{i=1}^{k-3} [(n-k+1)p-(n-k+i+1)] + Q_{k-1}^{(n)} \Bigg\} \qquad \text{(A10)}
\end{aligned}
$$

with the caveat that $n-1 \geqslant k \geqslant 4$. It can be further observed that the product in the curly brackets in (A10) can be expressed as

$$(p-1)[(n-k+1)p-(n-1)]\binom{n-k+2}{2}\prod_{i=1}^{k-3}[(n-k+1)p-(n-k+i+1)]$$
$$= [(n-k+1)p-(n-1)]R_{k-1}^{(n)} - R_k^{(n+1)}. \tag{A11}$$

Hence,

$$Q_k^{(n+1)} = [(n-k+1)p-(n-1)](B_{k-1}^{(n-1)} + Q_{k-1}^{(n)} + R_{k-1}^{(n)}) - R_k^{(n+1)}. \tag{A12}$$

Employing the relation given by (A5) where $n+1$ and k are replaced by n and $k-1$, respectively, we find that

$$Q_k^{(n+1)} = [(n-k+1)p-(n-1)]D_{k-1}^{(n)} - R_k^{(n+1)} \tag{A13}$$

which finally yields

$$D_k^{(n+1)} = B_k^{(n)} + [(n-k+1)p-(n-1)]D_{k-1}^{(n)}. \tag{A14}$$

As in case of the recursion relation for $B_k^{(n)}$, here too, upon comparing the definition of $D_k^{(n)}$ with the above equation the condition $k \geqslant 4$ can be relaxed. Thus, (A14) is valid for $k \geqslant 1$.

Proof of theorem 2. In substantiating the proof we may use mathematical induction where we assume that $\mathrm{d}(F^{[n]})/\mathrm{d}x = F^{[n+1]}$ and deduce that it holds as it stands. The $(n+1)$st derivative of $F(p,x)$ can be written as follows:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x}F^{[n]}(p,x) &= \sum_{k=1}^{n}(-1)^{n+k-1}p^{n-k+1}B_k^{(n)}\Big\{[(n-k+1)p-n]x^{p(n-k+1)-n-1}F(p,x) \\
&\quad + [1-px^{p-1}F(p,x)]x^{p(n-k+1)-n}\Big\} \\
&\quad + \sum_{k=1}^{n-1}(-1)^{n+k}D_k^{(n)}p^{n-k}[(n-k)p-n+1]x^{p(n-k)-n} \\
&= \sum_{k=1}^{n}(-1)^{n+k-1}p^{n-k+1}B_k^{(n)}\Big\{[(n-k+1)p-n]x^{p(n-k+1)-n-1} \\
&\quad - px^{p(n-k+2)-n-1}\Big\}F(p,x) + \sum_{k=1}^{n}(-1)^{n+k-1}p^{n-k+1}B_k^{(n)}x^{p(n-k+1)-n} \\
&\quad + \sum_{k=1}^{n-1}(-1)^{n+k}D_k^{(n)}p^{n-k}[(n-k)p-n+1]x^{p(n-k)-n}.
\end{aligned} \tag{A15}$$

Making use of the recursion relations (A4) and (A14), the above expression simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}x}F^{[n]}(p,x) = F(p,x)\sum_{k=1}^{n}(-1)^{n+k-1}p^{n-k+1}[B_{k+1}^{(n+1)} - B_{k+1}^{(n)}]x^{p(n-k+1)-n-1} - F(p,x)$$
$$\times \sum_{k=1}^{n}(-1)^{n+k-1}p^{n-k+2}B_k^{(n)}x^{p(n-k+2)-n-1}$$
$$+ \sum_{k=1}^{n}(-1)^{n+k-1}p^{n-k+1}B_k^{(n)}x^{p(n-k+1)-n} + \sum_{k=1}^{n-1}(-1)^{n+k}p^{n-k}$$
$$\times [D_{k+1}^{(n+1)} - B_{k+1}^{(n)}]x^{p(n-k)-n}. \tag{A16}$$

Upon expanding the sums and collecting the coefficients of the same powers of x, one finds that

$$\frac{\mathrm{d}}{\mathrm{d}x}F^{[n]}(p,x) = (-1)^{n+1}p^{n+1}B_1^{(n)}x^{p(n+1)-n-1}F(p,x) + (-1)^{n+2}p^nB_2^{(n+1)}x^{np-n-1}F(p,x)$$
$$+\cdots+(-1)^{2n+1}pB_{n+1}^{(n+1)}x^{p-n-1}F(p,x) + (-1)^n p^n B_1^{(n)}x^{np-n} + (-1)^{n+1}p^{n-1}$$
$$\times D_2^{(n+1)}x^{p(n-1)-n} + \cdots + (-1)^{2n-1}pD_n^{(n+1)}x^{p-n}$$
$$= \sum_{k=1}^{n+1}(-1)^{n+k}B_k^{(n+1)}p^{n-k+2}x^{p(n-k+2)-n-1}F(p,x)$$
$$+ \sum_{k=1}^{n}(-1)^{n+k-1}D_k^{(n+1)}p^{n-k+1}x^{p(n-k+1)-n}$$
$$= \sum_{k=1}^{n+1}(-1)^{n+k}p^{n-k+2}x^{p(n-k+2)-n-1}[F(p,x)B_k^{(n+1)} + xD_{k-1}^{(n+1)}] = F^{[n+1]}(p,x). \tag{A17}$$

That is, the resulting expression (A17) is the same as (3.1) with $n+1$ substituted for n, therefore the induction is complete.

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