A note on harmonic numbers, umbral calculus and generating functions

G. Dattoli\textsuperscript{a}, H.M. Srivastava\textsuperscript{b,∗}

\textsuperscript{a} Gruppo Fisica Teoria e Matematica (Unità Tecnico), Scientifica Tecnologie Fisiche Avanzate, ENEA - Centro Richerche Frascati, Via Enrico Fermi 45, I-00044 Frascati, Rome, Italy

\textsuperscript{b} Department of Mathematics and Statistics, University of Victoria, Victoria, British Columbia V8W 3P4, Canada

Received 11 May 2007; accepted 13 July 2007

Abstract

We use methods of umbral calculus and algebraic nature to make some progress in the theory of generating functions involving harmonic numbers. We derive old and new results on generating functions in a fairly simple way and show that the method can be applied to find a common bridge with the theory of well-known (rather classical) generating functions.

© 2007 Elsevier Ltd. All rights reserved.

Keywords: Umbral calculus; Operational identities; Generating functions; Monomiality principle; Harmonic numbers; Laguerre polynomials; Kampé de Fériet polynomials; Bessel function; Gaussian identity

1. Introduction

The familiar harmonic numbers (which are denoted here, for convenience, by \(h_n\) instead of the standard notation \(H_n\)) are defined as follows:

\[
h_n := \sum_{k=1}^{n} \frac{1}{k} = h_{n-1} + \frac{1}{n} \quad (n \in \mathbb{N} := \{1, 2, 3, \cdots\}; \ h_0 := 0)
\]

(1)
or, equivalently, by

\[
h_n = \gamma + \psi(n + 1) \quad (n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\})
\]
in terms of the Euler–Mascheroni constant \(\gamma\) and the Digamma function \(\psi(z)\) (see [1]). For a detailed account of their properties and of recent advances in this well-understood subject, the interested reader should refer to the Web Site mentioned in [6].

∗ Corresponding author.

E-mail addresses: dattoli@frascati.enea.it (G. Dattoli), harimsri@math.uvic.ca (H.M. Srivastava).

0893-9659/S - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.aml.2007.07.021
In this note we discuss some aspects relevant to the associated generating functions and to the use of an umbral-calculus formalism, which can be proved to be quite useful for making further progress in the field.

The following generating function for the harmonic numbers $h_n$ is attributed to Gosper (see, e.g., [6, Eqs. (25) and (26))):

$$F_1(z) := \sum_{n=1}^{\infty} \frac{z^n}{n!} h_n = e^z [\ln z + \Gamma(0, z) + \gamma] = -e^z \Phi(z), \quad (2)$$

where $\Phi(z)$ denotes the entire exponential integral given by

$$\Phi(z) := \sum_{n=1}^{\infty} \frac{(-z)^n}{n \cdot n!} = -[E_1(z) + \gamma + \ln z] \quad (3)$$

and, as usual, $\Gamma(0, z)$ denotes the complementary incomplete Gamma function defined by

$$\Gamma(0, z) := \int_z^{\infty} e^{-t} \frac{dt}{t} =: E_1(z), \quad (4)$$

$E_1(z)$ being the relatively more familiar exponential integral (see, for details, [4]; see also the references cited therein).

By means of a suitable umbral-calculus formalism (see [5]), we make use of (2) in order to derive new and old identities which are relevant to the harmonic numbers $h_n$. First of all, we find it to be convenient to rewrite (2) in a more compact form by using the following notation:

$$[h]_n = h_n \quad (n \in \mathbb{N}) \quad (5)$$

and defining a function $F(z)$ by

$$F(z) := e^{[h]} - 1. \quad (6)$$

Even though it seems to be naïve, the above restyling allows the possibility of getting new results. We note indeed that, according to this notation, we can deduce the following sum:

$$\sum_{n=1}^{\infty} \frac{z^n}{n!} h_{n+\ell} = [h]^{\ell} \left( e^{[h]} - 1 \right) = \frac{d^\ell}{dz^\ell} \{ F_1(z) \} - [h]^{\ell} \quad (\ell \in \mathbb{N}_0). \quad (7)$$

Consequently, we have readily found that

$$\sum_{n=1}^{\infty} \frac{z^n}{n!} h_{n+\ell} = -z^{\ell} \sum_{k=0}^{\ell} \binom{\ell}{k} \Phi^{(k)}(z) - h_{\ell} \quad (\ell \in \mathbb{N}_0), \quad (8)$$

which, for $\ell = 0$, reduces immediately to the known generating function (2). Here, as usual, the superscript in $\Phi^{(k)}(z)$ denotes the derivative of $\Phi(z)$ of order $k$ with respect to $z$.

2. Harmonic numbers and special functions

The rather simple technique (which we have already illustrated in Section 1) allows the derivation of other interesting results. First of all, since

$$[h]^{2n} = h_{2n} \quad (n \in \mathbb{N}), \quad (9)$$

we can write

$$F_2(z) := \sum_{n=1}^{\infty} \frac{z^{2n}}{n!} h_{2n} = e^{z^2 [h]^2} - 1. \quad (10)$$
Thus, by making use of the Gaussian identity:
\[ \exp \left( b^2 \right) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp \left( -\xi^2 + 2b\xi \right) \, d\xi, \] (11)
we find from (10) that
\[ F_2(z) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp \left( -\xi^2 \right) F_1(2\xi z) \, d\xi. \] (12)
This last integral in (12) can be evaluated fairly easily. We finally obtain
\[ F_2(z) = \sum_{n=1}^{\infty} \frac{z^{2n}}{n!} h_{2n} = -\exp \left( z^2 \right) \Psi(z), \] (13)
where, for convenience,
\[ \Psi(z) := \sum_{n=1}^{\infty} \frac{z^n}{n \cdot n!} H_n(-2z, 1) \] (14)
and \( H_n(x, y) \) denotes the two-variable Kampé de Fériet polynomials defined by (see [3])
\[ H_n(x, y) := n! \sum_{k=0}^{[n/2]} \frac{x^{n-2k} y^k}{k!(n-2k)!} = (-i)^n y^{n/2} H_n \left( \frac{ix}{2\sqrt{y}} \right), \] (15)
\( H_n(z) \) being the classical Hermite polynomials.
Furthermore, since (see [6, Eq. (12)])
\[ h'_{2n} := \sum_{k=1}^{2n} \frac{(-1)^{k-1}}{k} = h_{2n} - h_n, \] (16)
we can easily deduce from the generating functions (2) and (13) that
\[ \sum_{n=1}^{\infty} \frac{z^n}{n!} h'_{2n} = -e^z \left( \Psi \left( \sqrt{z} \right) - \Phi(z) \right), \] (17)
where the functions \( \Phi(z) \) and \( \Psi(z) \) are defined by (3) and (14), respectively.

The results which we have obtained so far are based upon the assumption that the umbral-calculus formalism applies to harmonic numbers \( h_n \), too. We have used a numerical procedure to test the validity of such an assumption at least within the framework of the above two examples. In fact, in each case, we first calculated the sum directly and then we compared the result with the analytical expression. We have thus found a complete agreement for an arbitrary number of digits. In the case of the generating function (10), we found that, with both procedures, the sum is
\[ 3.09270185396793 \text{ for } z = 1, \]
while it equals
\[ 140.645877250313 \text{ for } z = 2. \]

The use of the umbral-calculus method yields yet another interesting rule as follows:
\[ \sum_{n=1}^{\infty} \frac{h_n}{n!} H_n(x, y) = e^{x+y} \Theta(x, y), \] (18)
where
\[ \Theta(x, y) := \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n \cdot n!} H_n(x + 2y, y). \] (19)
With a view to sketching a proof of the generating function (18), we recall that (see [3])

\[ H_n(x, y) = \exp \left( y \frac{\partial^2}{\partial x^2} \right) \{x^n\}, \]  

(20)

so that, in terms of the function \( F_1(z) \) defined by (2), we have

\[
\sum_{n=1}^{\infty} \frac{h_n}{n!} H_n(x, y) = \exp \left( y \frac{\partial^2}{\partial x^2} \right) \{F_1(x)\}
= - \left[ \exp \left( y \frac{\partial^2}{\partial x^2} \right) \cdot e^x \cdot \exp \left( -y \frac{\partial^2}{\partial x^2} \right) \right] \cdot \left\{ \exp \left( y \frac{\partial^2}{\partial x^2} \right) \{\Phi(x)\} \right\}.
\]  

(21)

The generating function (18) would now result from (21) in light of (2), (20), and the following operational identity:

\[
\exp \left( y \frac{\partial^2}{\partial x^2} \right) \cdot e^x \cdot \exp \left( -y \frac{\partial^2}{\partial x^2} \right) = e^x + y \cdot \exp \left( \frac{\partial}{\partial x} \right).
\]  

(22)

Even though they still are at a preliminary stage, these results are fairly interesting and suggest the possibility of extending the method in a number of other useful ways.

In the same spirit as before, therefore, we take the freedom of defining the following polynomials:

\[
L_n(x, [h]) = n! \sum_{k=0}^{n} \frac{(-x)^k [h]^{n-k}}{(n-k)! (k)!} \quad (h_0 := 0),
\]  

(23)

which can be viewed as the umbral-calculus version of the two-variable Laguerre polynomials \( L_n(x, y) \) whose generating function is given by (see [3])

\[
\sum_{n=0}^{\infty} \frac{z^n}{n!} L_n(x, y) = e^{yz} J_0(2\sqrt{xz}),
\]  

(24)

\( J_\nu(z) \) being the Bessel function of order \( \nu \) of the first kind. Now, by setting \( y \mapsto [h] \) in (24) and by applying Gosper’s generating function (2), we get the following identity:

\[
\sum_{n=0}^{\infty} \frac{z^n}{n!} L_n(x, [h]) = (e^{[h]z} - 1) J_0(2\sqrt{xz}) = -e^{z} \Phi(z) J_0(2\sqrt{xz}),
\]  

(25)

where \( \Phi(z) \) is given, as before, by (3).

The validity of the generating function (25) has also been checked in accordance with the above-mentioned prescription. We reiterate the fact that the generating functions (7), (13) and (25) should be framed within the context of Experimental Mathematics (see [2]) and should, therefore, be considered as hypotheses, which have passed a severe numerical check.

3. Concluding remarks and further observations

Using once more the spirit of umbral calculus, we introduce a harmonic number derivative \( \hat{\Delta}_{[h]} \) and a multiplicative operator \( \hat{M}_h \) such that, by analogy with the recurrence relation in (1) for the harmonic numbers \( h_n \), we have

\[
\hat{\Delta}_{[h]} [h]^n = n [h]^{n-1} = n \left( h_n - \frac{1}{n} \right) \quad (n \in \mathbb{N})
\]  

(26)

and

\[
\hat{M}_h [h]^n = [h]^{n+1} \quad (n \in \mathbb{N}).
\]  

(27)
Now, recalling that the following identity:
\[
\frac{\partial}{\partial y} \{ H_n(x, y) \} = \frac{\partial^2}{\partial x^2} \{ H_n(x, y) \}
\]  
(28)
holds true for the ordinary Kampé de Fériet polynomials \( H_n(x, y) \) defined by (15), it can easily be checked that the umbral-calculus versions of the Kampé de Fériet polynomials satisfy the following equation:
\[
\Delta_{[h]} H_n(x, [h]) = \frac{\partial^2}{\partial x^2} \{ H_n(x, [h]) \},
\]  
(29)
which can be viewed as a kind of heat equation for which the time derivative is replaced by the harmonic number derivative \( \Delta_{[h]} \).

In general, we can consider the following Cauchy problem:
\[
\Delta_{[h]} F(x, [h]) = \frac{\partial^2}{\partial x^2} \{ F(x, [h]) \}
\]  
(30)
under the initial condition:
\[
F(x, 0) = f(x).
\]  
(31)
The solution to this Cauchy problem can be written as follows:
\[
F(x, [h]) = \left[ \exp \left( [h] \frac{\partial^2}{\partial x^2} \right) - 1 \right] f(x)
\]  
\[= - \exp \left( \frac{\partial^2}{\partial x^2} \right) \Phi \left( \frac{\partial^2}{\partial x^2} \right) f(x), \]  
(32)
where \( \Phi(z) \) is given by (3).

In view of
\[
H_n(x, 0) = x^n \quad (n \in \mathbb{N}_0)
\]  
(33)
and the operational representation (20) above, in the case of the Kampé de Fériet polynomials \( H_n(x, y) \), we can use the operational identity (29) to obtain the following explicit form of the \( H_n(x, [h]) \):
\[
H_n(x, [h]) = \sum_{k=1}^{[n/2]} \frac{(-1)^{k-1}}{k} \cdot \frac{n!}{k!(n-2k)!} H_{n-2k}(x, 1).
\]  
(34)

Such operators as
\[
\exp \left( [h] \frac{\partial^2}{\partial x^2} \right) \quad \text{and} \quad \exp \left( [h] \frac{\partial}{\partial x} \frac{\partial}{\partial x} \right)
\]
can be viewed as kinds of evolution operators. Their mathematical foundations deserve to be studied carefully and systematically.

An analogous result holds true for the harmonic Laguerre polynomials (16), which can be written explicitly as follows:
\[
L_n(x, [h]) = \sum_{k=1}^{n} \frac{(-1)^{k-1}}{k} \binom{n}{k} L_{n-k}(x, 1),
\]  
(35)
since
\[
L_n(x, y) = \exp \left( -y \frac{\partial}{\partial x} x \frac{\partial}{\partial x} \right) \left\{ \frac{(-x)^n}{n!} \right\}
\]  
(36)
for the two-variable Laguerre polynomials \( L_n(x, y) \) generated by (24), so that, analogously, we have

\[
L_n(x, [h]) = \left[ \exp \left( [h] \frac{\partial}{\partial x} \frac{\partial}{\partial x} \right) - 1 \right] \left\{ \frac{(-x)^n}{n!} \right\}
\]

for its umbral-calculus version given by (24).

Before concluding this note, we consider a further example by evaluating the following sum:

\[
A(z) := \sum_{n=1}^{\infty} z^n h_n.
\]

This can easily be deduced from (2) by using the Borel transform, which yields the following already known result (see, for example, [6, Eq. (34) with \( r = 1 \)):

\[
A(z) = \int_{0}^{\infty} e^{-t} F_1(zt) dt = -(1 - z)^{-1} \ln(1 - z) \quad (|z| < 1).
\]

For a direct evaluation of in (38) without using (2), we observe that

\[
A(z) = \sum_{n=1}^{\infty} \sum_{k=1}^{n} \frac{1}{k} = \sum_{k=1}^{\infty} \frac{z^k}{k} \sum_{n=0}^{\infty} z^n
\]

\[
= -(1 - z)^{-1} \ln(1 - z) \quad (|z| < 1),
\]

which is precisely the same as the summation formula (39).

Alternatively, since

\[
\frac{\partial}{\partial \lambda} \left\{ (\lambda)_\mu \right\} := \frac{\partial}{\partial \lambda} \left\{ \Gamma(\lambda + \mu) \right\} = (\lambda)_\mu \left[ \psi(\lambda + \mu) - \psi(\lambda) \right],
\]

by differentiating both sides of the following binomial expansion:

\[
(1 - z)^{-\lambda} = \sum_{n=0}^{\infty} \frac{(\lambda)_n}{n!} z^n \quad (|z| < 1)
\]

partially with respect to the parameter \( \lambda \), we have

\[
\sum_{n=0}^{\infty} \frac{(\lambda)_n}{n!} [\psi(\lambda + n) - \psi(\lambda)] z^n = -(1 - z)^{-\lambda} \ln(1 - z) \quad (|z| < 1),
\]

which, in the special case when \( \lambda = 1 \), immediately yields the summation formula (39) once again.

It may be of interest to observe that, in view of Hankel’s contour integral representation for the Gamma function in its equivalent form:

\[
\frac{1}{\Gamma(z)} = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} e^s s^{-z} ds \quad (\sigma > 0; \Re(z) > 0),
\]

we can easily derive the following interesting generalization of Gosper’s result (2):

\[
\sum_{n=0}^{\infty} \frac{z^n}{n!} [\psi(\lambda + n) - \psi(\lambda)] = -e^z \Phi(z; \lambda),
\]

where

\[
\Phi(z; \lambda) := \sum_{n=1}^{\infty} \frac{(-z)^n}{n \cdot (\lambda)_n} \quad \text{and} \quad \Phi(z; 1) \equiv \Phi(z),
\]

\( \Phi(z) \) being given, as before, by (3).
We choose to outline our derivation of the general formula (43) as follows. Indeed, upon replacing \( z \) in (41) by \( z/s \), if we multiply both sides of the resulting equation by \( e^{s-z} \) and apply Hankel’s contour integral (42), we have

\[
\sum_{n=0}^{\infty} \frac{z^n}{n!} \left[ \psi(\lambda + n) - \psi(\lambda) \right] = \sum_{m=1}^{\infty} \frac{z^m}{m \cdot (\lambda)_m} \ {} _1 F _1 (\lambda; \lambda + m; z)
\]

\[
= e^s \sum_{m=1}^{\infty} \frac{z^m}{m \cdot (\lambda)_m} \ {} _1 F _1 (m; \lambda + m; -z)
\]

\[
= e^s \sum_{\ell=0}^{\infty} \sum_{m=1}^{\infty} \frac{(\ell + m - 1)! (-z)^\ell z^m}{(\lambda)_{\ell+m} \cdot \ell! m!}
\]

\[
= e^s \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell+1}}{\ell + 1 \cdot (\lambda)_{\ell+1}} \cdot \left( \sum_{m=0}^{\ell+1} (-1)^m \binom{\ell+1}{m} \right)
\]

\[
= -e^s \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell+1}}{\ell + 1 \cdot (\lambda)_{\ell+1}} = -e^s \sum_{n=1}^{\infty} \frac{(-z)^n}{n \cdot (\lambda)_n},
\]

where we have also made use of Kummer’s First Formula for the confluent hypergeometric function \( {} _1 F _1 \).

Incidentally, in the umbral-calculus formalism, (39) or (40) can be written as follows:

\[
A(z) := \sum_{n=1}^{\infty} z^n h_n = \frac{z [h]}{1 - z [h]}.
\] (45)

More generally, if we set

\[
A_\ell(z) := \sum_{n=1}^{\infty} z^n h_{n+\ell},
\] (46)

then, in the umbral-calculus formalism, we get

\[
A_\ell(z) := \sum_{n=1}^{\infty} z^n [h]^{n+\ell} = \frac{z [h]^{\ell+1}}{1 - z [h]},
\] (47)

which leads us to the following result:

\[
A_\ell(z) = -(1 - z)^{-1} \left[ \sum_{k=1}^{\ell} \binom{\ell}{k} \varphi_k(z) + \ln(1 - z) \right] \quad (|z| < 1),
\] (48)

where

\[
\varphi_k(z) := \sum_{j=k}^{\infty} (-1)^j \frac{z^j}{j!} \left( \frac{z}{1-z} \right)^{j-k}.
\] (49)

Before closing this section, we note that many of the identities (which we have dealt with in this investigation) can be extended to hold true for the generalized harmonic numbers \( h_{n,v} \) (instead of the standard notation \( H_{n,v} \)) defined by [6, Eq. (30)]

\[
h_{n,v} := \sum_{k=1}^{n} \frac{1}{k^v} \quad (n \in \mathbb{N}; \ v \in \mathbb{C}) \quad \text{and} \quad h_{n,1} \equiv h_n.
\] (50)

for which it is easily seen that [6, Eq. (34)]

\[
A(z; v) := \sum_{n=1}^{\infty} z^n h_{n,v} = \sum_{n=1}^{\infty} z^n \sum_{k=1}^{n} \frac{1}{k^v}
\]
\[ = \sum_{k=1}^{\infty} \frac{1}{k^\nu} \sum_{n=k}^{\infty} z^n \]
\[ = (1 - z)^{-1} \text{Li}_\nu(z) \quad (|z| < 1; \ \nu \in \mathbb{C}) \]  
\hspace{1cm} (51)

in terms of the Polylogarithm \( \text{Li}_\nu(z) \) defined by

\[ \text{Li}_\nu(z) := \sum_{n=1}^{\infty} \frac{z^n}{n^\nu} \quad (|z| < 1; \ \nu \in \mathbb{C}). \]  
\hspace{1cm} (52)

Clearly, since

\[ \text{Li}_1(z) = -\ln(1 - z) \quad (|z| < 1), \]  
\hspace{1cm} (53)

the generating function (51) would reduce immediately to (39) when we set \( \nu = 1 \). Moreover, we have the following relationship of the Polylogarithm \( \text{Li}_s(z) \) with the Riemann Zeta function \( \zeta(s) \):

\[ \text{Li}_s(1) = \sum_{n=1}^{\infty} \frac{1}{n^s} =: \zeta(s) \quad (\Re(s) > 1). \]  
\hspace{1cm} (54)

A more systematic treatment of the problems touched upon in this note and a further discussion of some useful consequences of such results as (40) and (48) would seem to be a worthwhile future investigation.

Acknowledgements

It is a pleasure for us to recognize several useful and enlightening discussions on the methods of umbral calculus with Professor D. Levi. The present investigation was supported, in part, by the Natural Sciences and Engineering Research Council of Canada under Grant OGP0007353.

References