Formulas for Higher Derivatives of the Riemann Zeta Function

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Abstract. The functional equation for $\zeta(s)$ is used to obtain formulas for all derivatives $\zeta^{(k)}(s)$. A closed form evaluation of $\zeta^{(k)}(0)$ is given, and numerical values are computed to 15D for k = 0(1)18.

The functional equation for the Riemann zeta function states that

(1)
$$\zeta(1-s) = 2(2\pi)^{-s} \cos \frac{\pi s}{2} \Gamma(s) \zeta(s)$$

(see [3, Theorem 12.7]). If this is differentiated k times we obtain a formula which, as noted by Spira [11], can be put in the form

$$(-1)^{k} \zeta^{(k)}(1-s) = 2(2\pi)^{-s} \sum_{j=0}^{k} \sum_{m=0}^{k} \left(a_{jkm} \cos \frac{\pi s}{2} + b_{jkm} \sin \frac{\pi s}{2} \right) \Gamma^{(j)}(s) \zeta^{(m)}(s),$$

where the coefficients a_{jkm} and b_{jkm} are independent of s. This formula was used by Spira [11], [12] to determine zero-free regions for $\zeta^{(k)}(s)$, and by Berndt [5], to determine the asymptotic number of zeros of $\zeta^{(k)}(s)$ with 0 < t < T, where $s = \sigma + it$.

This paper gives a variant of this formula (Theorem 1) which enables us to determine the coefficients a_{jkm} and b_{jkm} explicitly (Theorem 2). Our version also leads to a closed form evaluation of $\zeta^{(k)}(0)$ (Theorem 3) which contains the well-known values $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\frac{1}{2} \log(2\pi)$ as well as a formula for $\zeta''(0)$ obtained by Ramanujan. The results for $k \ge 3$ appear to be new. Alternate formulas expressing $\zeta^{(k)}(s)$ in terms of integrals are also given (Theorem 4). The values of $\zeta^{(k)}(0)$ are computed to 16S for k = 0(1)18 (Table 2).

Notation. Throughout this paper, z denotes the fixed complex number x + iy with $x = -\log 2\pi$, $y = -\pi/2$, and z^* denotes the complex conjugate of z.

THEOREM 1. For each integer $k \ge 1$ and all complex s we have

(2)
$$(-1)^{k}\zeta^{(k)}(1-s) = \sum_{m=0}^{k} {k \choose m} \{e^{sz}z^{k-m} + e^{sz^{*}}(z^{*})^{k-m}\} \{\Gamma(s)\zeta(s)\}^{(m)}.$$

Received January 3, 1984.

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¹⁹⁸⁰ Mathematics Subject Classification. Primary 10H05.

Key words and phrases. Riemann zeta function.

Proof. First we put the functional equation in a form which is more convenient for repeated differentiation. Since $(2\pi)^{-s} = e^{-s\log(2\pi)}$ and $2\cos \pi s/2 = e^{\pi i s/2} + e^{-\pi i s/2}$ we can rewrite (1) as follows:

(3)
$$\zeta(1-s) = \varphi(s; z) + \varphi(s; z^*),$$

where

$$\varphi(s;z)=\Gamma(s)\zeta(s)e^{sz}.$$

Differentiation of (3) gives us

(4)
$$(-1)^{k} \zeta^{(k)}(1-s) = \varphi^{(k)}(s;z) + \varphi^{(k)}(s;z^{*}).$$

Using Leibniz's rule to calculate $\varphi^{(k)}(s; z)$ we find

$$\varphi^{(k)}(s;z) = e^{sz} \sum_{m=0}^{k} {k \choose m} z^{k-m} \{ \Gamma(s)\zeta(s) \}^{(m)}$$

which, together with (4), proves (2).

THEOREM 2. For each integer $k \ge 1$ and all complex s we have

(5)
$$(-1)^{k} \zeta^{(k)}(1-s) = 2(2\pi)^{-s} \sum_{m=0}^{k} {k \choose m} \Big\langle \operatorname{Re}(z^{k-m}) \cos \frac{\pi s}{2} + \operatorname{Im}(z^{k-m}) \sin \frac{\pi s}{2} \Big\rangle \{\Gamma(s) \zeta(s)\}^{(m)}$$

(6)
$$= 2(2\pi)^{-s} \sum_{m=0}^{k} \sum_{r=0}^{m} {k \choose m} {m \choose r} \Big\langle \operatorname{Re}(z^{k-m}) \cos \frac{\pi s}{2} + \operatorname{Im}(z^{k-m}) \sin \frac{\pi s}{2} \Big\rangle \Gamma^{(r)}(s) \zeta^{(m-r)}(s).$$

Proof. To deduce (5) from (2) we note that

$$e^{sz}z^{k-m} + e^{sz^*}(z^*)^{k-m} = 2(2\pi)^{-s} \Big\langle \operatorname{Re}(z^{k-m})\cos\frac{\pi s}{2} + \operatorname{Im}(z^{k-m})\sin\frac{\pi s}{2} \Big\rangle,$$

and to deduce (6) from (5) we use Leibniz's rule for the *m*th derivative $\{\Gamma(s)\zeta(s)\}^{(m)}$. Examples. If z = x + iy we have

$$Re(z^{2}) = x^{2} - y^{2}, \qquad Im(z^{2}) = 2xy, Re(z^{3}) = x^{3} - 3xy^{2}, \qquad Im(z^{3}) = 3x^{2}y - y^{3}.$$

When $x = -\log 2\pi$ and $y = -\pi/2$ we find, by taking k = 1, 2, 3 in (5),

$$-\zeta'(1-s) = 2(2\pi)^{-s} \left\{ x \cos \frac{\pi s}{2} + y \sin \frac{\pi s}{2} \right\} \Gamma(s)\zeta(s) + 2(2\pi)^{-s} \cos \frac{\pi s}{2} \left\{ \Gamma(s)\zeta(s) \right\}', \zeta''(1-s) = 2(2\pi)^{-s} \left\{ (x^2 - y^2) \cos \frac{\pi s}{2} + 2xy \sin \frac{\pi s}{2} \right\} \Gamma(s)\zeta(s) + 2(2\pi)^{-s} \left\{ 2x \cos \frac{\pi s}{2} + 2y \sin \frac{\pi s}{2} \right\} \left\{ \Gamma(s)\zeta(s) \right\}' + 2(2\pi)^{-s} \cos \frac{\pi s}{2} \left\{ \Gamma(s)\zeta(s) \right\}'',$$

$$-\zeta'''(1-s) = 2(2\pi)^{-s} \left\{ (x^3 - 3xy^2) \cos \frac{\pi s}{2} + (3x^2y - y^3) \sin \frac{\pi s}{2} \right\} \Gamma(s)\zeta(s) + 2(2\pi)^{-s} \left\{ 3(x^2 - y^2) \cos \frac{\pi s}{2} + 6xy \sin \frac{\pi s}{2} \right\} \left\{ \Gamma(s)\zeta(s) \right\}'' + 2(2\pi)^{-s} \left\{ 3x \cos \frac{\pi s}{2} + 3y \sin \frac{\pi s}{2} \right\} \left\{ \Gamma(s)\zeta(s) \right\}'' + 2(2\pi)^{-s} \cos \frac{\pi s}{2} \left\{ \Gamma(s)\zeta(s) \right\}'''.$$

It should be noted that when s is an integer one of the factors $\cos \pi s/2$ or $\sin \pi s/2$ vanishes, and Eqs. (5) and (6) simplify further. For example, if s = 2n + 1, where n = 1, 2, 3, ..., we have $\cos \pi s/2 = 0$ and $\sin \pi s/2 = (-1)^n$ and (6) becomes

$$(-1)^{k} \zeta^{(k)}(-2n) = \frac{2(-1)^{n}}{(2\pi)^{2n+1}} \sum_{m=0}^{k} \sum_{r=0}^{m} {k \choose m} {m \choose r} \operatorname{Im}(z^{k-m}) \Gamma^{(r)}(2n+1) \zeta^{(m-r)}(2n+1).$$

Thus, $\zeta^{(k)}(-2n)$ is a linear combination of $\zeta(2n + 1), \zeta'(2n + 1), \ldots, \zeta^{(k)}(2n + 1)$. Similarly, when s = 2n the sine terms vanish and we get

$$(-1)^{k} \zeta^{(k)}(1-2n) = \frac{2(-1)^{n}}{(2\pi)^{2n}} \sum_{m=0}^{k} \sum_{r=0}^{m} {k \choose m} {m \choose r} \operatorname{Re}(z^{k-m}) \Gamma^{(r)}(2n) \zeta^{(m-r)}(2n),$$

a linear combination of $\zeta(2n), \zeta'(2n), \ldots, \zeta^{(k)}(2n)$.

If we put s = 1 in (2), we get $(-1)^{k} \zeta^{(k)}(0)$ on the left, but on the right we have an indeterminate form. By expanding each of the functions e^{sz} , e^{sz^*} and $\{\Gamma(s)\zeta(s)\}^{(m)}$ in powers of s - 1 and letting $s \to 1$ we can obtain a closed form for $(-1)^k \zeta^{(k)}(0)$. A simpler method which gives the same result is based on the functional equation in (1).

Since the left member of (1) is analytic at s = 1 it has a power series expansion

$$\zeta(1-s) = \sum_{n=0}^{\infty} \frac{(-1)^n \zeta^{(n)}(0)}{n!} (s-1)^n.$$

Now we expand the right member of (1) in powers of s - 1 and equate coefficients. Again we use Eq. (3) which served us so well in proving Theorem 1, and first find the expansion of $\varphi(s; z)$ in powers of s - 1.

The product $\Gamma(s)\zeta(s)$ has a Laurent expansion of the form

(7)
$$\Gamma(s)\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} a_n(s-1)^n,$$

and for the exponential factor e^{sz} we write

$$e^{sz} = e^{z}e^{(s-1)z} = \sum_{n=0}^{\infty} e_n(z)(s-1)^n,$$

where

$$e_n(z)=\frac{e^z z^n}{n!}.$$

Therefore the product $\varphi(s; z) = \Gamma(s)\zeta(s)e^{sz}$ has the expansion

$$\varphi(s;z) = \left(\frac{1}{s-1} + \sum_{n=0}^{\infty} a_n (s-1)^n\right) \left(\sum_{n=0}^{\infty} e_n (z) (s-1)^n\right)$$
$$= \frac{e^z}{s-1} + \sum_{n=0}^{\infty} \left(e_{n+1}(z) + \sum_{k=0}^n a_k e_{n-k}(z)\right) (s-1)^n$$

Equating coefficients of $(s-1)^n$ in the functional equation (3) we find, for $n \ge 0$,

(8)
$$(-1)^n \frac{\zeta^{(n)}(0)}{n!} = e_{n+1}(z) + e_{n+1}(z^*) + \sum_{k=0}^n a_k(e_{n-k}(z) + e_{n-k}(z^*)).$$

But $e^{z} = -i/(2\pi)$ and $e^{z^{*}} = i/(2\pi)$, so

$$e_n(z) + e_n(z^*) = \frac{iz^n - i(z^*)^n}{2\pi n!} = \frac{1}{\pi} \frac{\operatorname{Im}(z^n)}{n!}$$

Hence (8) becomes

$$(-1)^{n} \frac{\zeta^{(n)}(0)}{n!} = \frac{1}{\pi} \frac{\mathrm{Im}(z^{n+1})}{(n+1)!} + \frac{1}{\pi} \sum_{k=0}^{n} a_{k} \frac{\mathrm{Im}(z^{n-k})}{(n-k)!}$$

Since $\text{Im}(z^0) = 0$ and $a_0 = 0$ (as we will show later), the first and last terms of the sum can be deleted and we obtain the following theorem.

THEOREM 3. If $z = -\log(2\pi) - i\pi/2$ and $n \ge 0$, we have

(9)
$$(-1)^{n} \frac{\zeta^{(n)}(0)}{n!} = \frac{1}{\pi} \frac{\mathrm{Im}(z^{n+1})}{(n+1)!} + \frac{1}{\pi} \sum_{k=1}^{n-1} a_{k} \frac{\mathrm{Im}(z^{n-k})}{(n-k)!},$$

where the coefficients a_k are determined by (7).

Examples. For $0 \le n \le 4$, we find that (9) gives us

$$\begin{split} \zeta(0) &= -\frac{1}{2}, \\ \zeta'(0) &= -\frac{1}{2\pi} \operatorname{Im}(z^2) = -\frac{xy}{\pi} = -\frac{1}{2} \log(2\pi), \\ \zeta''(0) &= \frac{1}{3\pi} \operatorname{Im}(z^3) + \frac{2}{\pi} a_1 \operatorname{Im}(z) = \frac{1}{3\pi} (3x^2y - y^3) + \frac{2}{\pi} a_1 y \\ &= -\frac{1}{2} \log^2(2\pi) + \frac{\pi^2}{24} - a_1, \\ \zeta'''(0) &= -\frac{1}{4\pi} \operatorname{Im}(z^4) - \frac{3!}{\pi} \sum_{k=1}^2 a_k \frac{\operatorname{Im}(z^{3-k})}{(3-k)!} \\ &= -\frac{1}{2} \log^3(2\pi) + \frac{\pi^2}{8} \log(2\pi) - 3a_1 \log(2\pi) + 3a_2, \\ \zeta^{(4)}(0) &= \frac{1}{5\pi} \operatorname{Im}(z^5) + \frac{4!}{\pi} \sum_{k=1}^3 a_k \frac{\operatorname{Im}(z^{4-k})}{(4-k)!} \\ &= -\frac{1}{2} \log^4(2\pi) + \frac{\pi^2}{4} \log^2(2\pi) - \frac{\pi^4}{160} - 6a_1 \log^2(2\pi)) \\ &+ \frac{\pi^2}{2} a_1 + 12a_2 \log(2\pi) - 12a_3. \end{split}$$

The formulas for $\zeta(0)$ and $\zeta'(0)$ are well-known [13, p. 20], and the formula for $\zeta''(0)$ was obtained by Ramanujan [6, p. 25]. Numerical values are given below in Table 2.

The coefficients a_k which appear in (9) and are defined by (7) can be calculated. They are related to the coefficients in the Laurent expansion

(10)
$$\zeta(s+1) = \frac{1}{s} + \sum_{n=0}^{\infty} A_n s^n$$

and those in the power series expansion

(11)
$$\Gamma(s+1) = \sum_{n=0}^{\infty} c_n s^n$$

The A_n are named after Stieltjes who showed [4, p. 155] that

$$(-1)^{n} n! A_{n} = \lim_{N \to \infty} \left(\sum_{k=1}^{N} \frac{\log^{n} k}{k} - \frac{\log^{n+1} N}{n+1} \right).$$

In particular, A_0 is Euler's constant γ . The first 20 Stieltjes constants have been calculated by Liang and Todd [9].

The numbers c_n in (11) are, of course, $\Gamma^{(n)}(1)/n!$. The derivatives $\Gamma^{(n)}(1)$ can be expressed in terms of Euler's constant and the values of $\zeta(s)$ at positive integers. This property of the c_n is easily derived as follows. Start with the power series expansion for $\psi(x + 1) = \Gamma'(x + 1)/\Gamma(x + 1)$, [1, p. 259],

(12)
$$\psi(x+1) = \sum_{n=0}^{\infty} (-1)^{n+1} s_{n+1} x^n,$$

where $s_1 = \gamma$ and $s_n = \zeta(n)$ for $n \ge 2$. Equating coefficients of x^n in the identity $\Gamma'(x+1) = \psi(x+1)\Gamma(x+1)$, using (11) and (12), we obtain the recursion formula

(13)
$$(n+1)c_{n+1} = \sum_{k=0}^{n} (-1)^{k+1} s_{k+1} c_{n-k}$$

with $c_0 = 1$. (See Nielsen [10, p. 40].)

Equation (13) also leads to a closed form evaluation of the derivatives $\Gamma^{(n)}(1)$ in terms of Euler's constant γ and $\zeta(2), \zeta(3), \ldots$ For example,

$$\begin{split} \Gamma'(1) &= -\gamma, \quad \Gamma''(1) = \zeta(2) + \gamma^2, \quad \Gamma'''(1) = -2\zeta(3) - 3\gamma\zeta(2) - \gamma^3, \\ \Gamma^{(4)}(1) &= 6\zeta(4) + 3\zeta^2(2) + 8\gamma\zeta(3) + 6\gamma^2\zeta(2) + \gamma^4, \\ \Gamma^{(5)}(1) &= -24\zeta(5) - 20\zeta(2)\zeta(3) - 15\gamma\zeta^2(2) - 30\gamma\zeta(4) \\ &- 20\gamma^2\zeta(3) - 10\gamma^3\zeta(2) - \gamma^5. \end{split}$$

Jeffery [8] has calculated the first 20 coefficients c_n to 12 decimals. Bourguet [7] later calculated to 16 decimals the first 18 coefficients b_n in the expansion

$$(x+1)\Gamma(x+1) = \sum_{n=0}^{\infty} b_n x^n.$$

This relation implies $b_0 = c_0 = 1$ and

$$b_n = c_n + c_{n-1}$$
 for $n \ge 1$,

n	Stieltjes constants A_n	$c_n = \Gamma^{(n)}(1)/n!$
0	0.5772156649015329	1.0000000000000000000000000000000000000
1	0.7281584548367672 (-01)	-0.5772156649015329
2	-0.4845181596436160 (-02)	0.9890559953279726
3	-0.3423057367172240 (-03)	-0.9074790760808863
4	0.9689041939447080 (-04)	0.9817280868344002
5	-0.6611031810842190 (-05)	-0.9819950689031452
6	0.3316240908752770 (-06)	0.9931491146212762
7	0.1046209458447920 (-06)	-0.9960017604424315
8	-0.8733218100273800 (-08)	0.9981056937831289
9	0.9478277782762000 (-10)	-0.9990252676219549
10	0.5658421927608700 (-10)	0.9995156560727774
11	-0.6768689863514000 (-11)	-0.9997565975086013
12	0.3492115936670000 (-12)	0.9998782713151333
13	0.4410424742000000 (-14)	-0.9999390642064443
14	-0.2399786222000000 (-14)	0.9999695177634821
15	0.2167731220000000 (-15)	-0.9999847526993770
16	-0.954446600000000 (-17)	0.9999923744790732
17	-0.738770000000000 (-19)	-0.9999961865894733
18	0.480090000000000 (-19)	0.9999980930811309
		-0.999999046469

TABLE 1

TABLE 2

n	<i>a_n</i>	$\zeta^{(n)}(0)$	$\zeta^{(n)}(0)/n!$
0	0.0000000000000000000000000000000000000	-0.5000000000000000	-0.5000000000000000
1	0.7286939170039305	-0.9189385332046727	-0.9189385332046727
2	-0.3834560903754670	-2.006356455908585	-1.003178227954292
3	0.5323903060606865	-6.004711166862254	-1.000785194477042
4	-0.4859027759456871	-23.99710318801370	-0.9998792995005709
5	0.5018073423500181	-120.0002329075584	-1.000001940896320
6	-0.4985920362510443	-720.0009368251297	-1.000001301146014
7	0.4998425924690323	-5039.999150176233	-0.9999998313841731
8	-0.4998028591976903	-40320.00023243172	-1.00000005764676
9	0.4999251541081416	-362880.0003305895	-1.00000000911016
10	-0.4999581497598492	-3628799.999456764	-0.999999998502988
11	0.4999798488252394	-39916800.00037562	-1.0000000009410
12	-0.4999897969263561	-479001600.0000220	-1.00000000000046
13	0.4999949183147713	-6227020799.999629	-0.99999999999999405
14	-0.4999974562188593	-87178291200.00114	-1.0000000000013
15	0.4999987285230217	-1307674368000.008	-1.00000000000006
16	-0.4999993642057035	-20922789888000.15	-1.00000000000007
17	0.4999996821100205	-355687428096002.6	-1.00000000000007
18	-0.49999984106	-6402373705728048.	-1.000000000000008

so we have a simple way of calculating the c_n in (11) recursively from the b_n . The numerical values of the c_n in Table 1 were obtained in this way from Bourguet's values. When rounded off to 12 decimals they agree with Jeffery's results except for c_{10} where Jeffery lists the 12th decimal place as 4 instead of 2.

To relate a_n to the A_n and c_n we write (7) as

$$\Gamma(s+1)\zeta(s+1) = \frac{1}{s} + \sum_{n=0}^{\infty} a_n s^n,$$

then multiply (10) and (11), and equate coefficients to get

(14)
$$a_n = c_{n+1} + \sum_{k=0}^n A_k c_{n-k}$$

This gives a closed form evaluation of the a_n in terms of the Stieltjes constants and values of the zeta function at positive integers. The first few values are

$$\begin{aligned} a_0 &= c_1 + A_0 = 0, \\ a_1 &= \frac{1}{2}\zeta(2) - \frac{1}{2}\gamma^2 + A_1, \\ a_2 &= -\frac{1}{3}\zeta(3) + \frac{1}{3}\gamma^3 - \gamma A_1 + A_2, \\ a_3 &= \frac{1}{4}\zeta(4) + \frac{1}{8}\zeta^2(2) - \frac{1}{4}\gamma^2\zeta(2) - \frac{1}{8}\gamma^4 + \frac{1}{2}\zeta(2)A_1 + \frac{1}{2}\gamma^2A_1 - \gamma A_2 + A_3. \end{aligned}$$

Numerical values for the a_n are given in Table 2. The calculations were based on (14) using the values for the A_n given by Liang and Todd [9] and the values of c_n listed in Table 1. These values, in turn, were used together with (9) to calculate the derivatives $\zeta^{(n)}(0)$ in Table 2. The numbers in Table 2 reveal that $(-1)^n a_n$ converges to $-\frac{1}{2}$ and that $\zeta^{(n)}(0)/n!$ converges to -1. These facts are easily proved by observing that we have the power series expansions

$$\zeta(1-s) + \frac{1}{s} = \sum_{n=0}^{\infty} \left(\frac{\zeta^{(n)}(0)}{n!} + 1 \right) (1-s)^n$$

and

$$\Gamma(s)\zeta(s) + \frac{1}{2s} = \sum_{n=0}^{\infty} \left((-1)^n a_n + \frac{1}{2} \right) (1-s)^n,$$

each of which converges for s = 0; so when s = 0 the general term of each series tends to 0.

Alternate formulas for $\zeta^{(k)}(s)$ can be obtained from the representation [1, p. 807]

(15)
$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} + \sum_{r=1}^{n} \frac{B_{2r}}{2r} \left(\frac{s+2r-2}{2r-1} \right) - \left(\frac{s+2n}{2n+1} \right) \int_{1}^{\infty} \frac{P_{2n+1}(x)}{x^{s+2n+1}} dx$$

which is a consequence of Euler's summation formula. The B_{2r} are Bernoulli numbers and the integral involves the periodic Bernoulli function

(16)
$$P_{2n+1}(x) = (-1)^{n+1} \frac{2(2n+1)!}{(2\pi)^{2n+1}} \sum_{k=1}^{\infty} \frac{\sin 2k\pi x}{k^{2n+1}}$$

The representation for $\zeta(s)$ in (15) is valid in the half-plane $\sigma > -2n$, n = 1, 2, 3, ..., and can be rewritten as follows:

(17)
$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} + \sum_{r=1}^{n} \frac{B_{2r}}{2r} Q_{2r-1}(s) - Q_{2n+1}(s) I_{2n+1}(s),$$

where $Q_m(s)$ is the binomial coefficient (a polynomial in s of degree m),

(18)
$$Q_m(s) = {\binom{s+m-1}{m}} = \frac{s(s+1)(s+2)\cdots(s+m-1)}{m!}$$

and

$$I_m(s) = \int_1^\infty \frac{P_m(x)}{x^{s+m}} dx.$$

The k th derivative of this integral is simply

(19)
$$I_m^{(k)}(s) = (-1)^k \int_1^\infty \frac{P_m(x)(\log x)^k}{x^{s+m}} dx,$$

and the k th derivative of $Q_m(s)$ vanishes identically if k > m.

By differentiating (17) repeatedly we obtain the following theorem.

THEOREM 4. In the half-plane $\sigma > -2n$, $n = 1, 2, 3, \ldots$, we have

(20)
$$\zeta^{(k)}(s) = \frac{(-1)^{k}k!}{(s-1)^{k+1}} + \sum_{r=1}^{n} \frac{B_{2r}}{2r} Q_{2r-1}^{(k)}(s) - \sum_{\nu=0}^{k} {k \choose \nu} Q_{2n+1}^{(\nu)}(s) I_{2n+1}^{(k-\nu)}(s).$$

For the special case n = 1 the sum on r vanishes identically if $k \ge 2$, and the sum on ν contains at most four terms since $Q_3^{(\nu)}(s)$ vanishes identically for $\nu > 3$. Thus, for $\sigma > -2$ we have

(21)
$$\zeta'(s) = \frac{-1}{(s-1)^2} + \frac{1}{12} - \frac{s(s+1)(s+2)}{6}I'_3(s) - \frac{3s^2+6s+2}{6}I_3(s),$$

and, for $k \ge 2$,

$$(22) \quad \zeta^{(k)}(s) = \frac{(-1)^{k} k!}{(s-1)^{k+1}} - \frac{s(s+1)(s+2)}{6} I_{3}^{(k)}(s) \\ - \frac{k}{6} (3s^{2} + 6s + 2) I_{3}^{(k-1)}(s) - \frac{k(k-1)}{2} (s+1) I_{3}^{(k-2)}(s) \\ - k(k-1)(k-2) I_{3}^{(k-3)}(s).$$

(If k = 2 the last term on the right of (22) is understood to be zero.)

When s = 0 the formulas are even simpler. From (21) we get

(23)
$$\zeta'(0) = -1 + \frac{1}{12} - \frac{1}{3}I_3(0),$$

and for $k \ge 2$, we have

(24)
$$\zeta^{(k)}(0) = -k! - \frac{k}{3}I_3^{(k-1)}(0) - \frac{k(k-1)}{2}I_3^{(k-2)}(0) - k(k-1)(k-2)I_3^{(k-3)}(0).$$

These formulas, used in conjunction with Theorem 3, lead to successive closed form evaluations of the integrals $I_3(0)$, $I'_3(0)$, $I''_3(0)$,.... For example, using the formulas derived earlier for $\zeta'(0)$ and $\zeta''(0)$, we find

$$I_3(0) = \int_1^\infty \frac{P_3(x)}{x^3} dx = -\frac{11}{4} + \frac{3}{2}\log(2\pi) = 0.006815599614018225$$

and

$$I'_{3}(0) = \int_{1}^{\infty} \frac{P_{3}(x)(-\log x)}{x^{3}} dx$$

= $\frac{9}{8} - \frac{9}{4} \log(2\pi) + \frac{3}{4} \log^{2}(2\pi) - \frac{\pi^{2}}{16} + \frac{3}{2}a_{1} = -0.000688715558150.$

The same type of analysis can be applied to the Hurwitz zeta function $\zeta(s, a)$, the analytic continuation of the series

$$\zeta(s,a)=\sum_{n=0}^{\infty}\frac{1}{(n+a)^s},$$

where a > 0 and $\sigma > 1$. For $\sigma > -1$, Euler's summation formula gives the representation

(25)
$$\zeta(s,a) = a^{-s} \left(\frac{1}{2} + \frac{a}{s-1} \right) - s(s+1) \int_0^\infty \frac{\varphi_2(x)}{(x+a)^{s+2}} dx,$$

where $\varphi_2(x) = \int_0^x (t - [t] - \frac{1}{2}) dt$ is periodic with period 1 and satisfies $\varphi_2(x) = \frac{1}{2}x(x - 1)$ if $0 \le x \le 1$.

Differentiating (25) k times we obtain the formula

$$(-1)^{k} \zeta^{(k)}(s, a) = (\log^{k} a) a^{-s} \left(\frac{1}{2} + \frac{a}{s-1}\right) + k! a^{1-s} \sum_{r=0}^{k-1} \frac{\log^{r} a}{r! (s-1)^{k-r+1}}$$
$$-s(s+1) \int_{0}^{\infty} \frac{\varphi_{2}(x) \log^{k}(x+a)}{(x+a)^{s+2}} dx$$
$$+k(2s+1) \int_{0}^{\infty} \frac{\varphi_{2}(x) \log^{k-1}(x+a)}{(x+a)^{s+2}} dx$$
$$-k(k-1) \int_{0}^{\infty} \frac{\varphi_{2}(x) \log^{k-2}(x+a)}{(x+a)^{s+2}} dx.$$

For s = 0 this simplifies to

(26)
$$\zeta^{(k)}(0, a) = \left(\log^{k} \frac{1}{a}\right) \left(\frac{1}{2} - a\right) - k! + k! a \sum_{r=k}^{\infty} \frac{\log^{r} 1/a}{r!} + (-1)^{k} k \int_{0}^{\infty} \frac{\varphi_{2}(x) \log^{k-1}(x+a)}{(x+a)^{2}} dx - (-1)^{k} k (k-1) \int_{0}^{\infty} \frac{\varphi_{2}(x) \log^{k-2}(x+a)}{(x+a)^{2}} dx.$$

When a = 1 this can be transformed to (24) using integration by parts.

When a = 1 and k = 1, Eq. (26) reduces to

$$\zeta'(0) = -1 - \int_0^\infty \frac{\varphi_2(x)}{(x+1)^2} dx = -1 - \int_1^\infty \frac{\varphi_2(x)}{x^2} dx.$$

But, from [2, p. 616], we see that

$$1 + \int_{1}^{\infty} \frac{\varphi_2(x)}{x^2} dx = \frac{1}{2} \log(2\pi),$$

so we have another derivation of the formula

$$\zeta'(0)=-\tfrac{1}{2}\log(2\pi).$$

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