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Expansions of the Exponential Integral in Incomplete Gamma Functions

W. GAUTSCHI
Department of Computer Sciences, Purdue University
West Lafayette, IN 47907-1398, U.S.A.

F. E. HARRIS
Quantum Theory Project, University of Florida
P.O. Box 118435, Gainesville, FL 32611, U.S.A.

N. M. TEMME
Center for Mathematics and Computer Science (CWI)
P.O. Box 94079, 1090 GB Amsterdam, The Netherlands

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Abstract—An apparently new expansion of the exponential integral E_1 in incomplete gamma functions is presented and shown to be a limiting case of a more general expansion given by Tricomi in 1950 without proof. This latter expansion is proved here by interpreting it as a "multiplication theorem". A companion result, not mentioned by Tricomi, holds for the complementary incomplete gamma function and can be applied to yield an expansion connecting E_1 of different arguments. A general method is described for converting a power series into an expansion in incomplete gamma functions. In a special case, this provides an alternative derivation of Tricomi's expansion. Numerical properties of the new expansion for E_1 are discussed.

1. INTRODUCTION

The exponential integral

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t}\,dt \tag{1.1}$$

occurs widely in applications, most notably in quantum-mechanical electronic structure calculations. In view of the extremely large number of evaluations that are often required, there is a continuing interest in improving the efficiency of its calculation. In a search for better methods of evaluating E_1, one of us (F.E.H.) discovered the expansion

$$E_1(z) = -\gamma - \ln z + \sum_{n=1}^{\infty} \frac{\gamma(n,z)}{n!}, \tag{1.2}$$

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where

$$\gamma(a,z) = \int_0^z e^{-t} t^{a-1}\, dt$$

is the incomplete gamma function (cf. [1, Section 6.5]). Another of us (W.G,) observed the relevance of an expansion given in 1950 by Tricomi, of which (1.2) is a limiting case.

2. AN EXPANSION OF TRICOMI

In 1950, Tricomi [2, equation (45)] stated without proof the expansion

$$\gamma(a,\lambda z) = \lambda^a \sum_{n=0}^{\infty} \frac{\gamma(a+n,z)}{n!} (1-\lambda)^n. \tag{2.1}$$

For any fixed complex $a \neq 0, -1, -2, \dots$, the left-hand side is analytic in the domain $\lambda z \in \mathbb{C} \backslash \mathbb{R}_-$, where $\mathbb{R}_-$ is the negative real axis; it is an entire function if a is a positive integer. For fixed a and z, the series in (2.1) converges for arbitrary complex λ.

An interesting proof derives from the observation that (2.1) is a "multiplication theorem" (see [3, Volume 1, Section 6.14]). Such theorems can usually be obtained when all derivatives of the function to be expanded can be expressed in terms of the same family of functions [3, Volume 1, Section 6.14]. In the present instance, we have the relation

$$\gamma(a+n,z) = (-1)^n z^{a+n} \frac{d^n}{dz^n} \left(z^{-a}\gamma(a,z)\right), \tag{2.2}$$

which follows readily from the integral representation

$$z^{-a}\gamma(a,z) = \int_0^1 e^{-zt} t^{a-1}\, dt.$$

When using (2.2) in the right-hand side of (2.1), one obtains

$$\lambda^a z^a \sum_{n=0}^{\infty} \frac{h^n}{n!} \frac{d^n}{dz^n} \left(z^{-a}\gamma(a,z)\right), \qquad h = (\lambda - 1)z. \tag{2.3}$$

The series can be seen to be the Taylor expansion of $(z+h)^{-a}\gamma(a,z+h)$. Since $z+h = \lambda z$, expression (2.3) becomes

$$\lambda^a z^a (z+h)^{-a} \gamma(a, z+h) = \gamma(a,\lambda z).$$

This completes the proof of (2.1).

Multiplication theorems (and related addition theorems) are available for many other special functions, such as Bessel functions [4, Chapter 11; 1, p. 363; 5, Section 4.10; 6, Chapter 5, Section 5, Chapter 8, Section 6] and orthogonal polynomials [5, Section 9.8; 7, Section 4.10(7)]. Equation (2.1) is a special case of a multiplication theorem for confluent hypergeometric functions [3, Section 6.14].

3. DERIVATION OF (1.2) FROM TRICOMI'S EXPANSION

Separating out the first term on the right of (2.1) and bringing it to the left, we write Tricomi's result in the form

$$\frac{\gamma(a,\lambda z) - \lambda^a \gamma(a,z)}{\lambda^a} = \sum_{n=1}^{\infty} \frac{\gamma(a+n,z)}{n!} (1-\lambda)^n. \tag{3.1}$$

From the power series of $\gamma(a,\lambda z)$ (cf. [1, equation 6.5.29]) one gets

$$\frac{\gamma(a,\lambda z) - \lambda^a \gamma(a,z)}{\lambda^a} = \frac{z^a}{a} \left[1 - \frac{a}{a+1}\lambda z + \frac{a}{2a+4}(\lambda z)^2 + \cdots \right] - \gamma(a,z),$$

which, as $\lambda \downarrow 0$, has the limit $z^a/a - \gamma(a,z)$. Thus, by (3.1),

$$\frac{z^a}{a} - \gamma(a,z) = \sum_{n=1}^{\infty} \frac{\gamma(a+n,z)}{n!}. \tag{3.2}$$

If $\gamma(a,z)$ on the left is replaced by $\Gamma(a) - \Gamma(a,z)$ and $\Gamma(a)$ written as $\Gamma(a+1)/a$, equation (3.2) takes the form

$$\frac{z^a - \Gamma(a+1)}{a} + \Gamma(a,z) = \sum_{n=1}^{\infty} \frac{\gamma(a+n,z)}{n!}.$$

Now take the limit $a \downarrow 0$. Applying Bernoulli-l'Hospital's rule to the first term on the left and noting that $\Gamma'(1) = -\gamma$ and $\Gamma(0,z) = E_1(z)$, one gets

$$\ln z + \gamma + E_1(z) = \sum_{n=1}^{\infty} \frac{\gamma(n,z)}{n!},$$

which proves (1.2).

4. A COMPANION TO TRICOMI'S EXPANSION WITH AN APPLICATION TO THE EXPONENTIAL INTEGRAL

There is a companion result to (2.1), not mentioned by Tricomi, for the complementary incomplete gamma function,

$$\Gamma(a,\lambda z) = \lambda^a \sum_{n=0}^{\infty} \frac{\Gamma(a+n,z)}{n!} (1-\lambda)^n, \qquad |\lambda - 1| < 1. \tag{4.1}$$

This follows from (2.1) by inserting the definition $\gamma(a,z) = \Gamma(a) - \Gamma(a,z)$ in both sides of the expansion and noting that, by Taylor's series for λ^{-a} at $\lambda = 1$, one has

$$\sum_{n=0}^{\infty} \frac{\Gamma(a+n)(1-\lambda)^n}{n!} = \lambda^{-a}\Gamma(a), \qquad |\lambda - 1| < 1. \tag{4.2}$$

Equation (4.1) holds also for $a = 0$, by analytic continuation, and yields

$$E_1(\lambda z) = E_1(z) + \sum_{n=1}^{\infty} \frac{\Gamma(n,z)}{n!} (1-\lambda)^n, \qquad |\lambda - 1| < 1. \tag{4.3}$$

Here, the coefficients are elementary functions

$$\frac{\Gamma(n,z)}{n!} = \frac{1}{n} e^{-z} e_{n-1}(z), \qquad n \geq 1,$$

where $e_m(z) = 1 + z + z^2/2! + \cdots + z^m/m!$ are the partial sums of the exponential series. These can be generated by recursion in a stable fashion, at least when z is real (cf. [8]). If $\lambda = 1/2$, for example, then

$$E_1\left(\frac{z}{2}\right) = E_1(z) + \sum_{n=1}^{\infty} \frac{\Gamma(n,z)}{2^n n!}.$$

For positive z, the sum converges more rapidly than that of $(2^n n)^{-1}$.

5. OTHER EXPANSIONS IN INCOMPLETE GAMMA FUNCTIONS

We return to (3.2) and write it as

$$\frac{z^{a+k}}{a+k} = \sum_{n=k}^{\infty} \frac{\gamma(a+n,z)}{(n-k)!}, \qquad k \geq 0. \tag{5.1}$$

We next form the following series, with arbitrary d_k (subject to convergence), and insert (5.1) in it,

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{d_k z^{a+k}}{k!(a+k)} &= \sum_{k=0}^{\infty} d_k \sum_{n=k}^{\infty} \binom{n}{k} \frac{\gamma(a+n,z)}{n!} \\ &= \sum_{n=0}^{\infty} \frac{\gamma(a+n,z)}{n!} \sum_{k=0}^{n} \binom{n}{k} d_k \\ &= \sum_{n=0}^{\infty} c_n \frac{\gamma(a+n,z)}{n!}, \end{aligned} \tag{5.2}$$

where

$$c_n = \sum_{k=0}^{n} \binom{n}{k} d_k. \tag{5.3}$$

Any power series that can be cast in the form given in the left-hand side of (5.2) can therefore be written as a series in incomplete gamma functions.

We illustrate the procedure by applying (5.2) to $\gamma(a, \lambda z)$, which has the power series expansion

$$\gamma(a, \lambda z) = \sum_{k=0}^{\infty} \frac{(-1)^k \lambda^{a+k} z^{a+k}}{k!(a+k)}.$$

In this example, $d_k = (-1)^k \lambda^{a+k}$, and from (5.3) we obtain $c_n = \lambda^a (1-\lambda)^n$, thereby recovering (2.1).

6. NUMERICAL PROPERTIES OF (1.2)

Tricomi [2, p. 148] expressed the thought that some of the series expansions he listed without proof, including (2.1), might prove useful also for computational purposes. We discuss here the computational merits of the series (1.2), which, as has been shown, is a limiting case of (2.1).

Compared with the power series in

$$E_1(z) = -\gamma - \ln z + \sum_{n=1}^{\infty} \frac{(-1)^{n-1} z^n}{n n!}, \tag{6.1}$$

the series in (1.2) has some definite drawbacks. In (6.1), the terms of the series can be generated recursively in forward direction, $n = 1, 2, 3, \ldots$, until they no longer contribute to the sum within the desired accuracy. This is not possible with (1.2). Although it is true that the terms in (1.2) also satisfy a forward recursion,

$$\begin{aligned} \gamma(n+1, z) &= n\gamma(n,z) - z^n e^{-z}, \qquad n = 1, 2, 3, \ldots, \\ \gamma(1, z) &= 1 - e^{-z}, \end{aligned} \tag{6.2}$$

the recursion becomes severely unstable as n exceeds $|z|$. (This can be shown by an analysis similar to the one in [9, Section 2.4].) To preserve numerical stability when $n > |z|$, one must generate $\gamma(\nu, z), \gamma(\nu-1, z), \ldots, \gamma(n, z)$ backwards with ν chosen sufficiently large, whereby $\gamma(\nu+1, z)$ may be replaced by zero. The choice of ν depends on the number of terms in (1.2) required for given accuracy, which has to be estimated *a priori*. Thus, summing the series to a prescribed accuracy is considerably more involved for the series in (1.2) than it is for the one in (6.1).

Another important consideration is internal cancellation of terms in a series. In this regard, the series in (1.2) and (6.1) complement each other. There is no significant cancellation of terms in either series if $|z|$ is relatively small, say $|z| \leq 5$. For larger values of $|z|$, the severity of cancellation increases with increasing $\arg z$ for the series in (1.2) and decreases with increasing $\arg z$ for the series in (6.1). Near the positive real axis ($\arg z \approx 0$) the series (1.2) is practically free of cancellation but subject to severe cancellation near the negative real axis ($\arg z \approx \pi$), more so the larger $|z|$. For the series (6.1), it is just the other way around.

With regard to speed of convergence, the two series are comparable, since for bounded z, as $n \to \infty$, one has $\gamma(n, z)/n! \sim z^n e^{-z}/(nn!)$ (cf. [10, Section 4.3, equation (3)]).

Another source of impaired accuracy is the cancellation that may occur when the series in (1.2), respectively, (6.1) is added to $-\gamma - \ln z$. This can be quite pronounced if $|z|$ is large and z near the positive real axis. The severity of the problem diminishes as $\arg z$ increases and becomes negligible near the negative real axis.

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