

On the Evaluation of Generalized Exponential Integrals $E_\nu(x)$

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In a previous paper we presented a method for evaluating the generalized exponential integral function, $E_\nu(x)$, which is valid whenever $x > 0$ and $\nu > 0$. Here we extend the evaluation of $E_\nu(x)$ to the whole domain ($x > 0, \nu \in R$). In the case $x \geq 1$, we start from an initial value in the region of asymptotic calculation and then reach the required $E_\nu(x)$, making use of a suitable combination of Taylor expansions and recurrences, whenever $\nu \neq 0, -1, -2, \dots$. Otherwise, the evaluation method for $E_\nu(x)$ is mainly based on recursive calculations starting from a suitable initial element calculated by means of proper analytical expressions. Computational accuracy has been tested and some results of interest for applications are given. © 1988 Academic Press, Inc.

1. INTRODUCTION

In applied sciences the problem of evaluating the following generalized exponential integral function [1] arises

$$E_\nu(x) = \int_1^\infty e^{-tx} t^{-\nu} dt \quad (x > 0, \nu \in R) \quad (1)$$

which, for positive integer values n of the order ν , reduces to the usual exponential integral $E_n(x)$ (see Ref. [2] for a recent review, Ref. [3] for alternative notation, and Ref. [4] for physical accounts). Exponential integrals, (1), for $\nu = -n$ correspond to the so-called molecular integrals $A_n(x) \equiv E_{-n}(x)$ of quantum chemistry [5].

In physical applications, function $E_\nu(x)$ is related to angular asymmetries in

transport theory [1] applied, for instance, to reactor physics and radiative transfer, and in flow dynamics. Moreover, evaluation of the exponential integral is needed for a theoretical estimate of the energy spectra of prompt neutrons emitted in the fission reaction [6]; the generalized exponential integral of half-integer order appears when a thermal $(1/v)$ energy dependence of the compound-nucleus cross section is considered [7] instead of an approximate constant value.

In addition to Eq. (1), the generalized exponential integral function can be defined [1] in terms of the incomplete gamma function, $\Gamma(a, x)$, as

$$E_\nu(x) = x^{\nu-1} \Gamma(1-\nu, x). \quad (2)$$

For later use, it is advantageous to rewrite the relevant expression in Eq. (2) as

$$E_\nu(x) = \Gamma(1-\nu) [x^{\nu-1} - e^{-x} \Phi^*(1, 2-\nu; x)], \quad (3)$$

where $\Gamma(a)$ is the usual gamma function, and $\Phi^*(a, b; x) \equiv \Phi(a, b; x)/\Gamma(b)$ the Tricomi version [8] of the Kummer function $\Phi(a, b; x)$.

Equation (3) has been derived from Eq. (2) making use of the following relations [8]

$$\Gamma(a, x) = \Gamma(a) [1 - x^a \gamma^*(a, x)] \quad (a \neq 0, -1, -2, \dots) \quad (4)$$

$$\gamma^*(a, x) = e^{-x} \Phi^*(1, a+1; x), \quad (5)$$

where $\gamma^*(a, x) \equiv x^{-a} \gamma(a, x)/\Gamma(a)$, is the modified version of the incomplete gamma function $\gamma(a, x)$, which is an entire function of both a and x .

Owing to the numerous applications mentioned above, the development of computational methods for $E_\nu(x)$ deserves some interest. To this end, in Ref. [9] we have presented a numerical method for $E_\nu(x)$, valid for $x > 0$ and $\nu > 0$, which has been tested with the algorithm [10, 11] for incomplete gamma functions, which resulted as the only procedure generally available for calculating generalized exponential integrals.

In this paper, we extend the above method in order to obtain an algorithm for evaluating $E_\nu(x)$, valid whenever $x > 0$ and $\nu \in R$. Basic formulation for calculating generalized exponential integrals in the region $x \geq 1$ is shown in Section 2, together with the relevant computational scheme, while the background of the method for the case $x < 1$ is described in Section 3. The efficiency of the present algorithm is confirmed by the accuracy of the results reported in Section 4, where the numerical features of the whole procedure are discussed.

2. OUTLINE OF THE METHOD IN THE REGION $x \geq 1$

In the case $x \geq 1$, the present method for evaluating $E_\nu(x)$ makes use of a suitable asymptotic formula, Taylor series expansions, and proper recurrences.

The relevant asymptotic expansion is that used in Ref. [9] for large positive values s of the order ν and reads [12]

$$E_s(x) = \frac{e^{-x}}{x+s} \left[\sum_{l=0}^{k-1} s^{-l} (1+x/s)^{-2l} h_l(x/s) + R_k(x, s) \right], \quad (6)$$

where $\{h_l(u)\}$ are polynomials defined recursively by

$$h_{l+1}(u) = (1-2lu)h_l(u) + u(1+u)h'_l(u) \quad (l=0, 1, 2, \dots) \quad (7)$$

with $h_0(u) = 1$, while $h'_l(u)$ is the usual notation for the first derivative of polynomial $h_l(u)$.

In practice, the $h_l(u)$ are generated according to the scheme described in Ref. [9] (see also Ref. [13]). Furthermore, the functions, $R_k(x, s)$, satisfy suitable conditions (see Refs. [9, 12] for the explicit expressions), ensuring that Eq. (6) is well grounded for sufficiently large values of s .

As regards the Taylor series expansion, the following expression is used

$$E_\nu(x-y) = \sum_{k=0}^{\infty} \frac{y^k}{k!} E_{\nu-k}(x) \quad (x > 0, \nu \in R) \quad (8)$$

which has been obtained from the Taylor series

$$E_\nu(x-y) = \sum_{k=0}^{\infty} \frac{(-y)^k}{k!} \frac{d^k}{dx^k} E_\nu(x), \quad (9)$$

taking into account the following differential formula [1]

$$\frac{d^k}{dx^k} E_\nu(x) = (-1)^k E_{\nu-k}(x). \quad (10)$$

Function $E_{\nu-k}(x)$ in Eq. (8) can be generated recursively by means of the relation [1]

$$E_r(x) = \frac{1}{x} [e^{-x} - rE_{r+1}(x)], \quad (11)$$

whatever the index $r \in R$.

In the present method, recurrence (11) (which, for $r=0$, reduces to the known expression $E_0(x) = e^{-x}/x$) is also used for evaluation of $E_\nu(x)$ ($\nu=0, -1, -2, -3, \dots; x > 0$) using $E_0(x)$ as starting element.

Furthermore, the proposed algorithm for $E_\nu(x)$ involves the use of the forward recursion

$$E_{r+1}(x) = \frac{1}{r} [e^{-x} - xE_r(x)] \quad (r \neq 0). \quad (12)$$

The above expressions are properly inserted into a suitable computational procedure in order to evaluate $E_\nu(x)$ in the region ($x \geq 1$). More precisely, apart from the case $E_{-\nu}(x)$ ($\nu = 0, 1, 2, \dots$), considered above, the sought-for evaluation of $E_\nu(x)$ when $x \geq 1$ is performed according to the following procedure.

First, we are involved in determining a suitable key element, $E_{\nu^*}(x^*)$, which is evaluated asymptotically, via Eq. (6) and used as starting point of the procedure to find $E_\nu(x)$ ($\nu \neq 0, -1, -2, \dots; x \geq 1$). The corresponding order, ν^* , and argument, x^* , are positive values related to the required ν and x by

$$\nu^* = x^* = \bar{\nu} + k, \tag{13}$$

where $k = 0$ or $k = [x_a] - [\bar{\nu}]$ according as $x \geq x_a$ (x_a being the lower bound of the "asymptotic" region) or otherwise, and $\bar{\nu}$ reads

$$\bar{\nu} = [x] + D + 1 - H(\nu) + \nu - [\nu]. \tag{14}$$

Here $[w]$ denotes the truncated part of w , $H(\nu)$ is the Heaviside step function, and the constant $D = 1$ when $(1 - H(\nu) + \nu - [\nu]) < (x - [x])$, and $D = 0$ otherwise.

At this point, if $\nu^* \neq \bar{\nu}$, i.e., $k \neq 0$, we apply p -times (with $p = 0, 1, \dots, k - 1$) to the following procedure (also sketched in Fig. 1a), in order to obtain $E_{\bar{\nu}}(\bar{\nu})$:

(I) Compute $E_{\nu^* - p - 1}(\nu^* - p)$ by a single step of backward recursion, Eq. (11), using $E_{\nu^* - p}(\nu^* - p)$ as the initial value.

(II) Starting from the previously calculated value of $E_{\nu^* - p - 1}(\nu^* - p)$, iterate (for $q = 0, 1, \dots, l - 1$) the Taylor series expansion of $E_{\nu^* - p - 1}(\tilde{\nu} - \bar{y})$ (with $\tilde{\nu} = \nu^* - p - q\bar{y}$ and $\bar{y} = 1/l$), until $E_{\nu^* - p - 1}(\nu^* - p - 1)$ is reached.

Once the value of $E_{\bar{\nu}}(\bar{\nu})$ has been obtained, we make use of different computational steps, depending on whether $\nu \geq \bar{\nu}$ or $\nu < \bar{\nu}$.

In the former case, one proceeds as follows:

(a) Starting from $E_{\bar{\nu}}(\bar{\nu})$, $E_{\bar{\nu}}(x)$ is evaluated by means of Taylor series of $E_{\bar{\nu}}(\bar{\nu} - y)$ (with $y = \bar{\nu} - x$).

(b) Calculate $E_\nu(x)$ by forward recursion for $\nu > \bar{\nu}$, using $E_{\bar{\nu}}(x)$ as initial value.

Otherwise, i.e., when $\nu < \bar{\nu}$, we apply the following computing steps:

(a') Compute $E_{\bar{\nu} - 1}(\bar{\nu})$ by a single step of backward recursion, using $E_{\bar{\nu}}(\bar{\nu})$ as the initial value.

(b') Starting from $E_{\bar{\nu} - 1}(\bar{\nu})$, evaluate $E_{\bar{\nu} - 1}(x)$ by means of the Taylor series of $E_{\bar{\nu} - 1}(\bar{\nu} - y)$.

(c') Compute $E_\nu(x)$ by backward recursion for $\nu < \bar{\nu} - 1$, using $E_{\bar{\nu} - 1}(x)$ as the initial value.

Figure 1b illustrates the above procedure from $E_{\bar{\nu}}(\bar{\nu})$ to $E_\nu(x)$, which is the only one needed when the required x lies in the "asymptotic" region ($x \geq x_a$). In actual computations $x_a \simeq 20$.

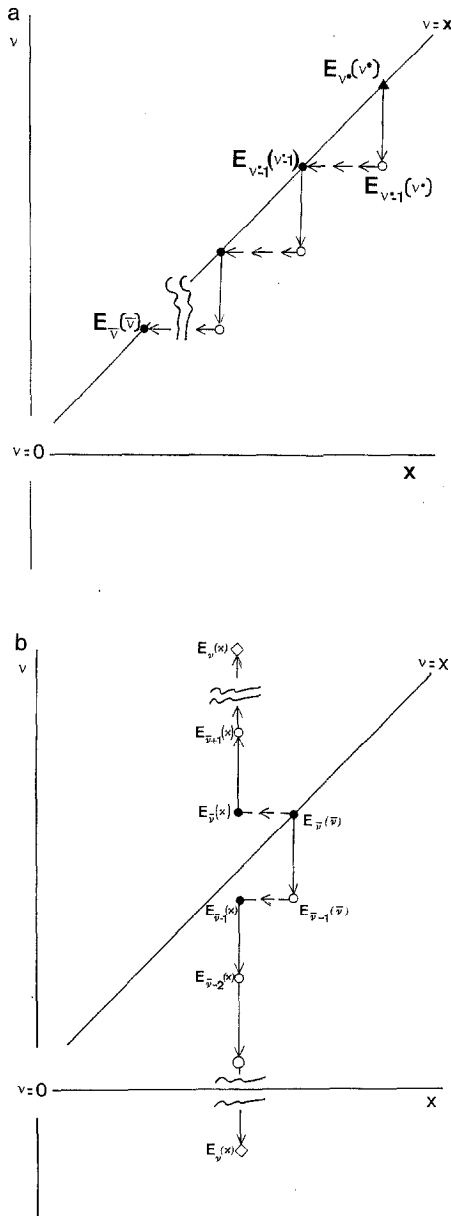


FIG. 1. (a) Scheme of the preliminary computational procedure (from $E_{v^*}(v^*)$ to $E_{\bar{v}}(\bar{v})$) for evaluating $E_v(x)$, required when $v^* \neq \bar{v}$: \blacktriangle : starting asymptotic value, Eq. (6); \circ : computed by backward recursion, Eq. (11); \bullet : computed by Taylor expansions, Eq. (8). (b) Schematic representation of the basic computational procedure for $E_v(x)$, starting from $E_{\bar{v}}(\bar{v})$ (see Eq. (14)); \bullet : computed by Taylor expansions, Eq. (8); \circ : computed by backward or forward recursions, Eqs. (11), (12); \diamond : searched value.

3. BACKGROUND OF THE PROCEDURE IN THE REGION $x < 1$

In the case $x < 1$, the generalized exponential integral, $E_\nu(x)$, is evaluated recursively. Apart from the case $E_{-\nu}(x)$ ($\nu = 0, 1, 2, 3, \dots$), considered above, we start from an initial element, $E_{\nu_0}(x)$ ($\nu_0 = 1 - H(\nu) + \nu - [\nu]$ for $\nu \neq [\nu]$ and $\nu_0 = 1$ otherwise), obtained by means of different series expansions according as $0 < \nu_0 \leq d$ ($d = 0.9$), or otherwise.

In the former case, the adopted series representation is the same as in Ref. [9] and reads

$$E_\nu(x) = \Gamma(1 - \nu) \left[x^{\nu-1} - e^{-x/2} \sum_{m=0}^{\infty} a_m (x/2)^m \xi_{m+1-\nu}(-\nu x/2) \right], \tag{15}$$

where the coefficients a_m can be generated recursively by

$$(n + 1) a_{n+1} = (n - \nu + 1) a_{n-1} + \nu a_{n-2} \quad (n = 2, 3, \dots) \tag{16}$$

with $a_0 = 1$, $a_1 = 0$, and $a_2 = 1 - \nu/2$.

The Tricomi functions [8], $\xi_g(t)$, are defined by

$$\xi_g(t) = \sum_{k=0}^{\infty} \frac{(-1)^k t^k}{\Gamma(g + k + 1) k!}, \tag{17}$$

or in terms of the Bessel functions, $J_g(z)$, by

$$\xi_g(t) = t^{-g/2} J_g(2\sqrt{t}), \tag{18}$$

and are entire for every value $g \in R$.

By introducing expansion (17) into Eq. (15) one gets the more explicit expressions

$$\begin{aligned} E_\nu(x) &= x^{\nu-1} \Gamma(1 - \nu) - e^{-x/2} \sum_{m,k=0}^{\infty} a_m (x/2)^{m+k} \frac{\nu^k}{k! (1 - \nu)_{m+1+k}} \\ &= \frac{1}{(1 - \nu)} \left[\frac{\Gamma(2 - \nu)}{x^{1-\nu}} - e^{-x/2} \sum_{i=0}^{\infty} \frac{(x/2)^i \nu^i}{i! (2 - \nu)_i} \sum_{m=0}^i \frac{a_m}{\nu^m} (i - m + 1)_m \right], \end{aligned} \tag{19}$$

where $i = m + k$, and $(\mu)_n$ is Pochhammer's symbol defined as

$$(\mu)_n = \mu(\mu + 1) \dots (\mu + n - 1).$$

The representation (15) has been obtained by means of the expansion [8]

$$\Phi^*(1, 2 - \nu; x) = e^{x/2} \sum_{m=0}^{\infty} a_m (x/2)^m \xi_{m+1-\nu}(-\nu x/2), \tag{20}$$

which, introduced into Eq. (3), gives the sought-for series representations of formulae (15)–(19).

Otherwise, i.e., when $d < \nu_0 \leq 1$, we adopt for the starting element, $E_{\nu_0}(x)$, the series representation used in Ref. [9], which has been obtained from the expansion

$$E_{\nu}(x) = -x^{\nu-1} \left[\frac{g(1-\nu)}{1 + (1-\nu)g(1-\nu)} + \frac{x^{1-\nu} - 1}{1-\nu} \right] - \sum_{m=1}^{\infty} \frac{(-1)^m x^m}{(1-\nu+m)m!}, \quad (21)$$

where

$$g(z) = \left[\frac{1}{z\Gamma(z)} - 1 \right] / z = \gamma + \sum_{m=1}^{\infty} b_{m+2} z^m, \quad |z| < 1. \quad (22)$$

γ is Euler's constant and b_j are the coefficients of the power series for $1/\Gamma(z)$, which have been tabulated in Ref. [14].

From expansion (21) we easily obtain the sought-for representation of $E_{\nu}(x)$ on ($d < \nu_0 \leq 1$) by making use of the relations [10, 11]

$$\begin{aligned} \frac{x^{1-\nu} - 1}{1-\nu} &= \frac{e^{(1-\nu)\ln x} - 1}{(1-\nu)\ln x} \ln x \\ &= \left\{ 1 + \sum_{m=1}^{\infty} \frac{[(1-\nu)\ln x]^m}{(m+1)!} \right\} \ln x, \end{aligned} \quad (23)$$

to be inserted into Eq. (21), respectively, when $|(1-\nu)\ln x| \geq 1$ or otherwise. Once $E_{\nu_0}(x)$ has been so calculated, if $\nu \neq \nu_0$, the use of forward recurrence, Eq. (12), when $\nu > 0$ (backward recursion, Eq. (11), when $\nu < 0$), finally leads to the required $E_{\nu}(x)$. By also taking into account the results of Section 2, the generalized exponential integral, $E_{\nu}(x)$, can be evaluated in the whole region ($x > 0$, $\nu \in R$) by means of the proposed numerical method.

4. NUMERICAL RESULTS AND DISCUSSION

In the case $\nu > 0$, the present algorithm is essentially similar to the one of Ref. [9], and the results of the related numerical analysis are still valid for the present procedure when $\nu > 0$.

In particular, the adopted series representations have been properly used in the computational process in conditions ensuring stable recursive computations of $E_{\nu}(x)$, according to Gautschi's results [15, 16].

Moreover, the relevant series in Eq. (8) (for $\nu > 0$ as in Section 2) and Eq. (19) (for $0 < \nu < 1$) are positive, so that achievement of convergence and error checks are easily determined.

In particular, coefficients $E_{\nu-k}(x)$ in Eq. (8) are positive functions for negative

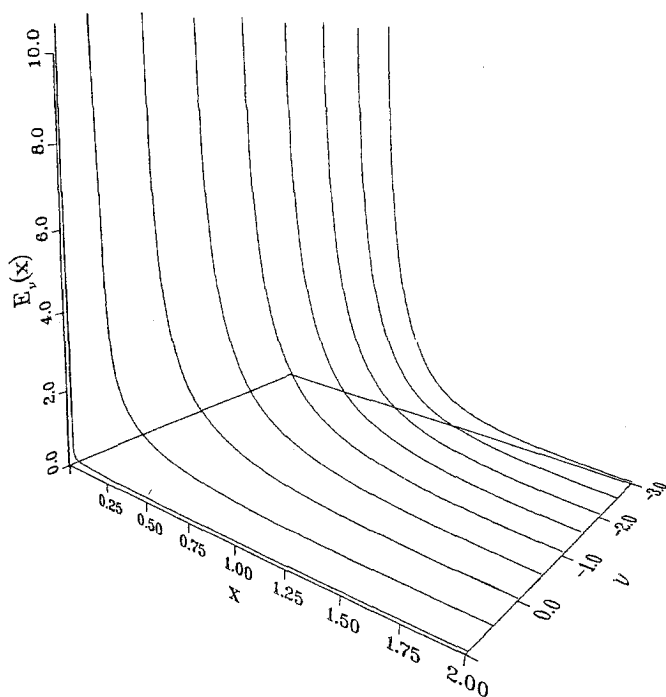


FIG. 2. Function $E_\nu(x)$ versus x ($0 \leq x \leq 2$) and ν ($= 1, \frac{1}{2}, 0, -\frac{1}{2}, -1, -\frac{3}{2}, -2, -\frac{5}{2}, -3$).

values of the index too, as deduced from Eq. (11), whose stability is well established.¹

As regards the procedure in the case $\nu < 0$, we note that its analytical background and related computational steps are similar to those in the case $\nu > 0$.

Furthermore, we have it that, apart from the stages inherent in backward recursions, Eq. (11), the computing process still works on the range ($x > 0, \nu > 0$). It follows that the numerical considerations made for the case $\nu > 0$ are valid for the region ($\nu \leq 0$) too.

Once basic aspects concerning the stability of the procedure have been so proved, its accuracy has to be tested.

To this end, the efficiency of the algorithm in case $\nu > 0$ is proved by the results of the numerical checks presented in Ref. [9]. As for the accuracy of the method when $\nu < 0$, comparisons have been made between the results of our procedure and the GAMMA algorithm of Refs. [10, 11].

More precisely, computed values of $E_\nu(x)$, obtained within the present approach for very many values of ν in the interval $(-100, 0)$ and x in $(0, 100)$, have been

¹ Recursions (11), for negative values of the index, are stable since the involved recurrence is positive.

compared with the corresponding ones calculated by means of the GAMMA routine [11]. Results are in overall agreement.

Numerical values for a significant set of $E_\nu(x)$ functions are illustrated in Fig. 2. Moreover, results of interest for applications [7], concerning values of $E_{-n/2}(x)$ (for $0 < x \leq 200$; $n = 1, 3, 5, 7, 9$), are presented² in Table I for the sake of comparison with other algorithms. They have been obtained on an IBM 370/168 computer, working in double-precision, and are significant up to fifteen digits.

In conclusion, the present method allows reliable evaluation of the generalized exponential integral function, $E_\nu(x)$, in the region ($x > 0, \nu \in R$).

Note. A FORTRAN version of the code, ERA, is available upon request from the authors.

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² The limit values as x approaches zero for fixed ν are $E_\nu(0) = \infty$, for $-\infty < \nu \leq 1$; and $1/(\nu - 1)$, for $\nu > 1$.