

Note

A General Method for an Accurate Evaluation of Exponential Integrals $E_1(x)$, $x > 0^*$

The generalized exponential integrals occur very frequently as auxiliary functions in many branches of theoretical physics, such as in the molecular, solid state, and surface physics for studying the electronic structure and physical properties of a variety of systems, in nuclear physics for the theoretical analysis of neutron diffusion and in radiative transfer in astrophysics. Their accurate numerical evaluation is extremely important and, consequently, many numerical tables have been published in the past for various ranges of the relevant parameters with a limited accuracy [1-4].

The generalized exponential integrals are defined by

$$E_n(\alpha) = \int_1^\infty (e^{-\alpha t}/t^n) dt. \quad (1)$$

For $n = 1$, $E_n(\alpha)$ becomes a well-known exponential integral of negative argument, $-Ei(-\alpha)$, which has also been the subject of tabulation by various authors [3, 4]. Because of their importance the analytic properties of $E_n(\alpha)$ have been discussed extensively in the literature [1, 2, 5]. Some of these properties have been employed in calculating and tabulating $E_n(\alpha)$. However, for the needs of the quantum chemists and molecular and solid state physicists [7] the accuracy and range of the available tables are often not adequate. We have also faced the same difficulty in developing a method for analytic evaluation of multicenter integrals using the expansion [7] of Slater orbitals from one center on to the other where one needs to evaluate the functions $E_n(\alpha)$ very accurately. Besides this, since a single expression is not applicable for the calculation of $E_n(\alpha)$ for all ranges of n and α , one is forced to use different expressions [1] in different ranges which creates a major difficulty in large-scale calculations of molecules and solids. To the knowledge of authors a simple method which can be employed for all ranges of n and α straightforwardly for the "machine" calculations is not yet known. The aim of this article is to point out a method suitable for the evaluation of $E_1(\alpha)$ for any value of α with a desired high accuracy.

The expression connecting $E_n(\alpha)$ ($n > 1$) and $E_1(\alpha)$ is given by

$$E_n(\alpha) = e^{-\alpha} \sum_{k=1}^{n-1} (-\alpha)^{k-1} \frac{(n-k-1)!}{(n-1)!} + \frac{(-\alpha)^{n-1}}{(n-1)!} E_1(\alpha) \quad (2)$$

which is easily obtained by means of the recurrence formula

$$E_{n+1}(\alpha) = (1/n)[e^{-\alpha} - \alpha E_n(\alpha)], \quad n \geq 1.$$

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TABLE I

Comparison of the Values (up to Nine Significant Figures) of $(\alpha + n) \exp(\alpha) E_n(\alpha)$ (Calculated from Eq. (2) for $\alpha = 50$) and the Corresponding Correct Values (Refs. [1, 4])^a

n	$(\alpha + n) \exp(\alpha) E_n(\alpha)$	
	From Eq. (2)	Correct value ^b
2	1.000 714 18	1.000 714 18
3	1.001 032 87	1.001 032 87
4	1.001 328 62	1.001 328 62
5	1.001 603 <u>20</u>	1.001 603 21
6	1.001 858 <u>28</u>	1.001 858 25
7	1.002 094 <u>88</u>	1.002 095 22
8	1.002 317 <u>84</u>	1.002 315 46
9	1.002 505 <u>02</u>	1.002 520 22
10	1.002 796 <u>55</u>	1.002 710 62
11	1.002 452 <u>01</u>	1.002 887 69
12	1.005 059 <u>20</u>	1.003 052 39
13	<u>0.994 699 40</u>	1.003 205 60
14	<u>1.036 874 99</u>	1.003 348 10
15	<u>0.882 958 98</u>	1.003 480 66
16	<u>1.407 656 24</u>	1.003 603 94
17	<u>-0.293 124 99</u>	1.003 718 57
18	<u>4.871 562 49</u>	1.003 825 15
19	<u>-9.918 749 99</u>	1.003 924 21
20	<u>30.0 124 99</u>	1.004 016 23

^a The starting value of $E_1(50)$ in Eq. (2) is taken to be $E_1(50) = 0.378\ 326\ 403 \times 10^{-23}$. The table demonstrates how the significant figure accuracy is lost in using Eq. (2) as n increases. The underlined figures are in error and for $n = 17$ and 19 even the sign comes out to be wrong in using Eq. (2).

^b From Refs. [1, 4].

Though Eq. (2) appears to be useful for computing $E_n(\alpha)$ if one knows $E_1(\alpha)$ accurately, it turns out that there occurs cancellation errors in numerical evaluation of the right-hand side of Eq. (2). This is clear from Table I where we have listed values of $E_n(\alpha)$ for $\alpha = 50$ and n ranging from 2 to 20. In Table I the results obtained by using Eq. (2) with the starting value of $E_1(50) = 0.378\ 326\ 402\ 955\ 04 \times 10^{-23}$ are compared with the correct results [1, 4]. The underlined figures show where the errors have occurred. In fact the error builds up so fast that the results for $n = 17$ and 19 are wrong even in sign. This point has been discussed extensively by Gautschi [9]. Our aim in this paper is to point out a method for evaluating $E_1(\alpha)$ correctly to the desired accuracy applicable for all values of α . However, what one would really like to have is a similar expression for $E_n(\alpha)$ for $n > 1$ so that the use of Eq. (2) would be obviated.

For the calculation of $E_1(\alpha)$ there exists a series expansion which is adequate [6, 8] only for small values of the argument α ($0 \leq \alpha \leq 4$). For large α there remains a problem of calculating $E_1(\alpha)$ accurately. Several authors [1, 4, 10-12] have suggested methods for evaluating $E_1(\alpha)$ (and $E_n(\alpha)$ in general) for large arguments. However, these methods involve different expressions in different ranges and require complicated calculational procedures.

In order to obtain a general expression adequate for all values of α we first recall that if $\alpha \rightarrow \infty$, $E_1(\alpha) \rightarrow 0$. Accordingly, we assume α_{\max} to be a (particular) large value of α and divide the region between α and α_{\max} into m parts of widths $\alpha_1, \alpha_2 \dots \alpha_m$ such that

$$\alpha_{\max} = \alpha + \alpha_1 + \alpha_2 + \alpha_3 \dots + \alpha_m. \tag{3}$$

As a first step in obtaining the final expression we substitute Eq. (3) for α in Eq. (1) and expand the exponential $e^{-\alpha_1 t}$. We have for $E_1(\alpha)$,

$$E_1(\alpha) = \int_1^\infty \frac{dt}{t} \exp\{-(\alpha_{\max} - \alpha_2 - \alpha_3 - \dots - \alpha_m)t\} + \sum_{n=0}^\infty \frac{\alpha_1^{n+1}}{(n+1)!} \int_1^\infty dt t^n \exp\{-(\alpha_{\max} - \alpha_2 - \dots - \alpha_m)t\}.$$

Next we use in the above expression, in general,

$$\int_1^\infty t^n e^{-\beta t} dt = e^{-\beta} \sum_{p=0}^n \frac{n!}{(n-p)!} \frac{1}{\beta^{p+1}}$$

to obtain

$$E_1(\alpha) = \int_1^\infty \frac{dt}{t} \exp\{-(\alpha_{\max} - \alpha_2 - \alpha_3 - \dots - \alpha_m)t\} + \sum_{n=0}^\infty \frac{\alpha_1^{n+1}}{(n+1)!} \sum_{p=0}^n \frac{e^{-(\alpha_{\max} - \alpha_2 - \dots - \alpha_m)}}{(\alpha_{\max} - \alpha_2 - \dots - \alpha_m)^{p+1}} \frac{1}{(n-p)!} = \int_1^\infty \frac{dt}{t} \exp\{-(\alpha_{\max} - \alpha_2 - \alpha_3 - \dots - \alpha_m)t\} + \sum_{n=0}^\infty \frac{\alpha_1^{n+1}}{(n+1)!} \sum_{p=0}^n \frac{e^{-(\alpha + \alpha_1)}}{(\alpha + \alpha_1)^{p+1}} \frac{1}{(n-p)!}. \tag{4}$$

Expanding $\exp(-\alpha_2 t)$ in Eq. (4) and integrating in the above manner and repeating the process, one obtains

$$E_1(\alpha) = E_1(\alpha_{\max}) + \sum_{n=0}^{\infty} \frac{1}{(n+1)} \sum_{t=0}^n \frac{1}{(n-t)!} \left\{ \frac{\alpha_1^{n+1} e^{-(\alpha+\alpha_1)}}{(\alpha+\alpha_1)^{t+1}} + \frac{\alpha_2^{n+1} e^{-(\alpha+\alpha_1+\alpha_2)}}{(\alpha+\alpha_1+\alpha_2)^{t+1}} \right. \\ \left. + \dots + \frac{\alpha_m^{n+1} e^{-(\alpha+\alpha_1+\alpha_2+\dots+\alpha_m)}}{(\alpha+\alpha_1+\alpha_2+\dots+\alpha_m)^{t+1}} \right\}. \quad (5)$$

For simplicity we take equal intervals, $\alpha_1 = \alpha_2 = \dots = \alpha_m = h$ which reduces Eq. (5) to

$$E_1(\alpha) = E_1(\alpha_{\max}) + h e^{-\alpha} \sum_{n=0}^{\infty} \frac{h^n}{(n+1)} \sum_{t=0}^n \frac{1}{(n-t)!} \sum_{p=1}^m \frac{e^{-ph}}{(\alpha+ph)^{t+1}}. \quad (6)$$

There are many advantages associated with the above expression. First, its convergence is in one's control. One needs to take only $h < \alpha$. Also, the smaller the h , the more convergent the expression becomes. Second, the terms in the expression are all positive which completely avoids the cancellation problems and hence the loss of significant figures. Third, the terms in Eq. (6) decrease fast with n and the series can be cut off at a low value of n . Moreover, $h e^{-\alpha}$ appears as a factor outside the series which is very desirable since it generates the required order of magnitude of $E_1(\alpha)$ leaving behind the summation as a correction part. Fourth, with the required significant figure accuracy of $E_1(\alpha)$, α_{\max} can be chosen such that $E_1(\alpha_{\max}) \ll E_1(\alpha)$ making $E_1(\alpha_{\max})$ negligible compared with $E_1(\alpha)$. This point is clear if one notes that $E_1(10) \simeq 10^{-6}$, $E_1(50) \simeq 10^{-24}$, and $E_1(100) \simeq 10^{-45}$. An alternate and better way is to calculate $E_1(\alpha_{\max})$ (using Eq. (6) or otherwise) once and for all, and use it in Eq. (6) to calculate $E_1(\alpha)$ for any value of α .

In molecular physics one usually requires $E_1(\alpha)$ for $\alpha \leq 60$. For actual calculations, assuming that the accuracy required is about 17 significant figures, one may take $\alpha_{\max} = 100$ and very well neglect $E_1(100)$ in Eq. (6) to calculate $E_1(60)$. This value of $E_1(60)$ may then be fixed as $E_1(\alpha_{\max})$ in Eq. (6) to make it versatile for the calculation of $E_1(\alpha)$ for any α in molecular problems. For the required accuracy of the significant figures the summation over n in Eq. (6) can be cut off at a suitable value depending on the value of h taken. In our calculations (for 24 figure significant accuracy) we have taken $n_{\max} \leq 30$ and h close to $\alpha/10$. In this case one does not require completion of the t and p summations for all their values since the terms decrease very fast due to the decreasing effect of the exponential factor and increasing effect of the denominator. The cutoff for the t and p summations can be made such that the product of all the factors in a term has the value less than 10^{-8} where s is the number of figure accuracy required. The cutoff on the t and p summation makes expression (6) very efficient for calculations.

Our calculations using Eq. (6) yield $E_1(0.5) = 0.559\ 773\ 594\ 776\ 16$, $E_1(1) = 0.219\ 383\ 934\ 395\ 52$, $E_1(10) = 0.415\ 696\ 892\ 968\ 53 \times 10^{-5}$, $E_1(20) = 0.983\ 552\ 529\ 064\ 98 \times 10^{-10}$, $E_1(50) = 0.378\ 326\ 402\ 955\ 04 \times 10^{-23}$, $E_1(60) = 0.143\ 586\ 756\ 568\ 12 \times 10^{-27}$.

For large-scale calculations Eq. (6) may be made very efficient and fast by first calculating accurately $E_1(\alpha)$ by the above method for some judiciously selected values of α (as, for example, $\alpha = 0.5, 1, 10, 20, 30, 40, 50,$ and 60). Now having these results readily available as $E_1(\alpha_{\max})$ one calculates $E_1(\alpha)$ for any value of α by employing the value of $E_1(\alpha_{\max})$ corresponding to the α_{\max} closest to α . As for example, in order to calculate $E_1(\alpha)$ for $1 < \alpha < 10$ one may use $E_1(10)$ as $E_1(\alpha_{\max})$ in Eq. (6). This procedure will further reduce the number of terms in n summation in Eq. (6) and hence reduce the calculational time.

In summary, we have developed a formula for $E_1(\alpha)$ (Eq. (6)) applicable for all values of α which, in conjunction with Eq. (2) is useful for theorists and particularly the molecular physicists and quantum chemists for accurate machine calculations of multicenter integrals in molecular problems.

As mentioned before what one likes to have is a single expression for $E_n(\alpha)$ similar to $E_1(\alpha)$ applicable for all ranges of n and α . This will eliminate the use of Eq. (2) which suffers from the drawback of cancellation of significant figures and hence loss of accuracy. The research in this regard is in progress.

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