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Use of analytical relations in evaluation of exponential integral functions

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Analytical formulas through the initial values suitable for numerical computation are developed for the exponential integral functions $E_n(x)$. The relationships obtained are numerically stable for all values of n and for $x < 1$. Numerical results are also given.

KEY WORDS: exponential integral functions, slater type orbitals, multicenter integrals

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1. Introduction

It is well known that the exponential integral (EI) functions occur in many physical problems, including, for example, the evaluation of multicenter integrals over Slater type orbitals arising when Hartree–Fock–Roothaan and explicitly correlated methods are employed [1–7]. In the literature, the EI functions have already been investigated by numerous authors with different algorithms [8–24]. It is the purpose of this communication to obtain the analytical formulas for the evaluation of EI functions. These relations are useful in the fast and efficient evaluation of multicenter molecular integrals with Slater type orbitals.

2. Definition and recurrence relation for EI functions

The exponential integral functions are defined by

$$E_n(x) = \int_1^\infty t^{-n} \mathrm{e}^{-xt} \mathrm{d}t, \tag{1}$$

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where $n = 1, 2, 3, \ldots$ and x is a real variable. These functions satisfy the following recursive relation:

$$(n-1)E_n(x) = \mathrm{e}^{-x} - xE_{n-1}(x), \tag{2}$$

where the starting term is given by

$$E_1(x) = \int_1^{\infty} t^{-1}\mathrm{e}^{-xt}\mathrm{d}t. \tag{3}$$

Recent works in this area discuss the efficient evaluation of the function $E_1(x)$ (see Refs. [15–20] and references therein).

3. Analytical relations for EI functions

In order to establish the analytical formulas for EI functions in terms of starting values, equation (3), we take into account the recurrence relation (2) and use the method set out in our previous work [25]. Then, it is easy to obtain the desired analytical relations of EI functions:

$$E_n(x) = \frac{(-x)^k(n-k-1)!}{(n-1)!}E_{n-k}(x) + \mathrm{e}^{-x}\sum_{i=0}^{k-1}\frac{(-x)^i(n-i-2)!}{(n-1)!}, \tag{4}$$

where $1 \leqslant k \leqslant n-1$.

In special case of equation (4) for $k = n-1$, we obtain for the EI functions the following analytical relation in terms of initial values:

$$E_n(x) = \frac{(-x)^{n-1}}{(n-1)!}E_1(x) + \mathrm{e}^{-x}\sum_{i=0}^{n-2}\frac{(-x)^i(n-i-2)!}{(n-1)!}. \tag{5}$$

4. Numerical results and discussion

New analytical formulas are presented to fast and accurately calculate the EI functions that arise in many physical problems. These relations can be used for arbitrary values of parameters n and for $x < 1$.

On the basis of formulas (Equations (4) and (5)) established in this paper we constructed a program for computation of EI functions in the Turbo Pascal language using personal computer Pentium III 800 MHz. The examples of computer calculation are shown in table 1. The accuracy of the computer results can be determined with the help of equation (4) for different values of indices k. The numbers of correct decimal figures a_n curring in $\Delta f_n = 10^{-a_n}$ are also presented in table 1, where $\Delta f_n = |\Delta f_{nk} - \Delta f_{nk-1}|$. Here, the values Δf_{nk} and Δf_{nk-1} are determined from equation (4) for $k = n-1$. Our calculation results of EI functions are in excellent agreement with literature [9].

Table 1
Numbers of correct decimal figures for exponential integral function $E_n(x)$.

n	x	k	Equation (5) a_n	Maple 8.0 a_n	Mathematica 5 a_n
5	0.0004	4	∞	∞	∞
18	0.8	17	21	30	29
25	0.003	24	∞	∞	∞
30	0.0001	29	∞	∞	∞
48	0.3	47	∞	∞	∞
56	0.07	55	∞	∞	∞
65	0.006	64	∞	∞	∞
78	0.4	77	∞	∞	∞
86	0.005	85	∞	∞	∞
94	0.07	93	∞	∞	∞
125	0.01	124	∞	∞	∞
40	0.006	39	∞	∞	∞

As can be seen from the table, our results are in excellent agreement with the results Maple 8.0 and Mathematica 5 international mathematical software. Hopefully, this simplification will persist at higher orders. We have tested the program by comparing with much available data Maple 8.0 and Mathematica 5 international mathematical software.

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