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Incomplete Gamma $F_m(x)$ Functions for Real Negative and Complex Arguments

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Incomplete gamma functions $F_m(x)$, originally defined and used in the electronic structure theory, have been examined from the viewpoint of electron–molecule scattering theory for their possible use in calculation of two-electron integrals in a mixed Gaussian and plane-wave basis set. Effective calculation of $F_m(z)$ functions with a complex argument is discussed.

Key Words: complex incomplete Gamma function; two-electron integrals.

I. INTRODUCTION

The family of functions defined as

$$F_m(t) = \int_0^1 u^{2m} \exp(-tu^2)\, du \qquad (t > 0; m = 0, 1, 2 \ldots) \tag{1}$$

are of crucial importance in the electronic structure theory for the evaluation of two-electron integrals over Gaussian basis set functions [1, 2]. Two-electron integrals of that type are also met in the electron–molecule scattering theory [3], though their evaluation requires complex arguments to be used [4] in F_m functions. For a complex argument z we have [1]

$$F_0(z) = \frac{1}{2}\sqrt{\frac{\pi}{z}}\mathrm{erf}(\sqrt{z}) \tag{2}$$

and

$$F_{m+1}(z) = -\frac{d}{dz}F_m(z). \tag{3}$$

The complex error function is related to the $w(z)$ function [5]

$$\mathrm{erf}(z) = 1 - w(iz)e^{-z^2} \tag{4}$$

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and for the evaluation of $w(z)$ the algorithm proposed by Gautschi [6] has been advocated [7]. However, this way of calculation of two-electron integrals in the electron scattering theory has not been used much in practice. Instead, Watson and McKoy [8] developed a method based on a partial wave expansion of plane wave functions.

Our interest in use of F_m functions in electron scattering calculations arose from our intention to keep close similarity between electronic structure and electron scattering calculations. Such a similarity is very beneficial. It permits us to modify and extend highly effective codes developed for *ab initio* molecular orbital calculations for purposes of electron scattering. Also, it permits us to apply merits of the electronic structure theory such as the Rys numerical quadrature for the evaluation of two-electron integrals [9] and gradient techniques [10, 11] for calculation of cross sections of vibrational excitation of polyatomic molecules by electron impact. We considered it therefore expedient to inspect the properties of F_m functions in greater detail and to use our knowledge thus obtained for evaluation of integrals in a mixed plane-wave and Gaussian basis set [12].

II. ASYMPTOTES OF F_m FOR LARGE NEGATIVE REAL ARGUMENTS

Upon first looking at Eq. (2), it appears that real functions $F_m(x)$ cannot accommodate negative real arguments x. However, the error function may be expanded in polynomial series [5] and then $F_0(x)$ may be expressed in the form

$$F_0(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!(2n+1)}, \tag{5}$$

which enables analytical continuation of the $F_0(x)$ function defined originally [1] for positive arguments only. The alternative expansion [1]

$$F_0(x) = e^{-x} \sum_{i=0}^{\infty} \frac{(2x)^i}{(2i+1)!!} \tag{6}$$

also permits us to use negative arguments. However, as the absolute value of negative x is increased, the two expansions (5) and (6) become poorly convergent; a computer cannot maintain the required numerical precision, and, in any case, the value of $F_0(x)$ goes to infinity.

Another expansion for F_0 in the asymptotic region is obtained from Eqs. (2) and (4), and from the asymptotic expansion [6] for $w(z)$ as

$$F_0(x) = e^{-x} \left(-\frac{1}{2x} + \sum_{i=2} (-1)^i \frac{(2i-3)!!}{(2x)^i} \right), \tag{7}$$

from which we obtain for very large negative x,

$$F_0(x) \sim \frac{e^{-x}}{-2x}. \tag{8}$$

By differentiation of $F_0(x)$ in the form of Eq. (7) and from Eq. (3) we obtain

$$\lim_{x \to -\infty} F_m(x) = \lim_{x \to -\infty} F_0(x), \qquad m > 0. \tag{9}$$

III. F_0 FUNCTION FOR COMPLEX ARGUMENTS

We systematically tested four different ways of calculation of F_0 in order to find the most economical calculation for a particular region of complex arguments z. These four ways of calculation are described briefly as follows:

1. We closely followed the usual procedure for computation of real $F_m(x)$ functions [1]. As in the routine FMTGEN from the Gaussian 94 package [13], we employed the usual formulas for two different series, but we coded them in complex arithmetics with some modifications. Hence, for $|z| \leq 11$ the expansion

$$F_m(z) = e^{-z} \sum_{i=0} \frac{(2z)^i}{(2m+2i+1)!!} \tag{10}$$

is used and for $|z| > 11$ the asymptotic expansion [1]

$$F_m(z) \approx \frac{\Gamma(m+1/2)}{2z^{m+1/2}} - \frac{\Gamma(m+1/2)}{2z} e^{-z} \sum_{i=0} \frac{1}{\Gamma(m-i+1/2) z^i}. \tag{11}$$

2. As the second way of calculation we used the routine WOFZ [14] for the evaluation of $w(z)$. If z, $z = x + iy$, lies inside the ellipse

$$\left(\frac{|x|}{6.3}\right)^2 + \left(\frac{|y|}{4.4}\right)^2 = 0.085264, \tag{12}$$

$w(z)$ is obtained from Eq. (4) and the following expansion of the error function [5]

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \sum_{n=0} \frac{(-1)^n z^{2n+1}}{n!(2n+1)}. \tag{13}$$

For z outside this ellipse the $w(z)$ function is calculated by two different variants of the Laplace continued fraction.

3. We have coded our own routine based on the algorithm by Gautschi [6]. It evaluates $w(z)$ by a simple algorithm related to the Laplace continued fraction for any $|z|$. Specifically, we have used Eqs. (3.8) and (3.11)–(3.13) from Gautschi's paper [6].

4. The last mode of calculation of $F_0(z)$ is suitable only for arguments with a large negative $\operatorname{Re} z$. To protect the calculation against overflow we calculate $F_0(z)$ in its asymptotic form (7) as

$$\frac{F_0(z)}{e^{-z}} = -\frac{1}{2z} + \sum_{i=2} (-1)^i \frac{(2i-3)!!}{(2z)^i}. \tag{14}$$

Four terms in (14) secure precision to 10 significant digits for $\operatorname{Re} z < -500$. By differentiation of Eq. (14) and from Eq. (3), we obtain the higher $F_m(z)$ functions.

The method of the choice for a particular z is shown in Fig. 1. For each method we tested the number of terms to be evaluated in the expansion series and we checked that both real and imaginary parts of $F_0(z)$ are calculated at least with the precision to nine significant digits. We have coded Fig. 1 as a table internally stored in a program, so that the selection of the method for a pair (x, y) is simple and fast.

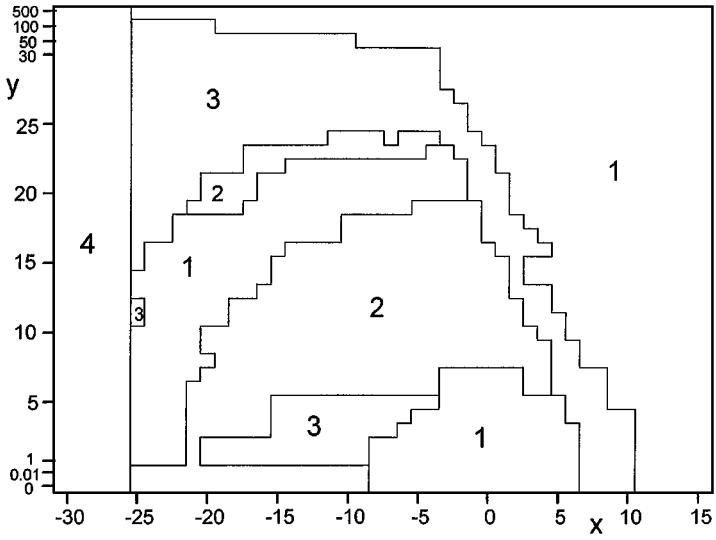

FIG. 1. Recommended method of calculation for complex $F_m(z)$ functions with $0 \le \arg z \le \pi$. 1. Standard routine for the evaluation of $F_n(x)$ (as for example routine FMTGEN from Gaussian 94) rewritten in complex arithmetics. 2. WOFZ routine. 3. algorithm by Gautschi. 4. Three-term asymptote given by Eq. (14). Note that $F_m(x+iy) = \overline{F_m(x-iy)}$.

The referee of this paper made us aware of another possibility of obtaining the complex error function. It may be obtained from a special routine coded for the evaluation of the Dawson's integral [15]. However the accuracy of the real version of this rourtine is only 2.10^{-7} and we estimate that the evaluation of the complex error function would not be faster than by the procedures noted above.

IV. HIGHER FUNCTIONS $F_m(z)$

For higher real $F_m(x)$ functions with positive x the following recursion formula [1] is commonly used:

$$(2m-1)F_{m-1}(x) = 2xF_m(x) + e^{-x}. \tag{15}$$

To secure the computational stability, the downward recursion formula must be used. In fact, the accuracy of F_m functions increases as we go to lower orders. In contrast, for the asymptotic region with large negative x, the upward recursion formula must be used,

$$\frac{F_m(z)}{e^{-z}} = \left[(2m-1)\frac{F_{m-1}(z)}{e^{-z}} - 1\right] \Big/ 2z. \tag{16}$$

Alternatively, by differentiation of Eq. (14) and from Eq. (3), we obtain the higher $F_m(z)$ functions as

$$\frac{F_m(z)}{e^{-z}} = -\frac{1}{2z}\left[1 + \frac{2m-1}{2z} + \frac{(2m-1)(2m-3)}{(2z)^2} + \cdots + \frac{(2m-1)\cdots(2m-2l+3)}{(2z)^{l-1}}\right]. \tag{17}$$

Higher $F_m(z)$ functions may also be obtained by differentiation of the $w(z)$ function as described below.

Define

$$t = i\sqrt{z}, \tag{18}$$

$$W_0(t) = -\frac{1}{it}\left[1 - w(t)e^{t^2}\right], \tag{19}$$

and

$$b(t) = 1 - w(t)e^{t^2}. \tag{20}$$

Then by differentiation of $F_0(z)$ as

$$F_0(z) = \frac{\sqrt{\pi}}{2} W_0(t) \tag{21}$$

we obtain for the lowest three $F_m(z)$ functions

$$F_1(z) = -\frac{\sqrt{\pi}}{2}\frac{dW_0(t)}{dt}\frac{dt}{dz} \tag{22}$$

$$F_2(z) = \frac{\sqrt{\pi}}{2}\frac{d^2W_0(t)}{dt^2}\left(\frac{dt}{dz}\right)^2 + \frac{\sqrt{\pi}}{z}\frac{dW_0(t)}{dt}\frac{d^2t}{dz^2} \tag{23}$$

$$F_3(z) = -\frac{\sqrt{\pi}}{2}\frac{d^3W_0(t)}{dt^3}\left(\frac{dt}{dz}\right)^3 - \frac{\sqrt{\pi}}{2}3\frac{d^2W_0(t)}{dt^2}\frac{dt}{dz}\frac{d^2t}{dz^2} - \frac{\sqrt{\pi}}{2}\frac{dW_0(t)}{dt}\frac{d^3t}{dz^3}, \tag{24}$$

where for the derivatives of W_0 it holds

$$\frac{d^nW_0(t)}{dt^n} = -\frac{n}{t}\frac{d^{n-1}W_0(t)}{dt^{n-1}} + \frac{i}{t}\frac{d^nb(t)}{dt^n} \tag{25}$$

and

$$\frac{d^nb(t)}{dt^n} = \left[(n-1)^i \sum_{i=0}^{[(n-1)/2]} \frac{(2t)^{n-1-2i}}{i!(n-1-2i)!}\right]\frac{db(t)}{dt}. \tag{26}$$

The term in brackets is equal to the expression for the Hermite polynomial $H_{n-1}(t)$ in which the factor for sign was dropped. For $db(t)/dt$ it holds

$$\frac{db(t)}{dt} = -\frac{2i}{\sqrt{\pi}}e^{t^2} \tag{27}$$

and the derivatives of t may be expressed as

$$dt/dz = i/(2\sqrt{z}) \tag{28}$$

and for $n \geq 2$,

$$\frac{d^nt}{dz^n} = (-1)^{n+1}\frac{i(2n-3)!!}{2^n}z^{-n+1/2}. \tag{29}$$

After an extensive numerical experimentation we recommend the following procedure for obtaining $F_m(z)$ functions with $m > 0$. For z falling into the region 1 of Fig. 1 we recommend using routine FMTGEN from Gaussian 94 [13] or some other routine for real $F_m(x)$ functions and rewriting it with double complex arithmetics. For region 4 of Fig. 1, we recommend the use of Eq. (16). The upward formula, in a form somewhat different from Eq. (16),

$$F_m(z) = [(2m-1)F_{m-1}(z) - e^{-z}]/2z, \tag{30}$$

may also be used for regions 2 and 3. The referee of this paper made a careful analysis of the numerical stability of Eq. (30) and showed that outside the small $|z|$ region 1, the upward recurrence for $m \leq 10$ loses no more than one significant decimal place.

V. UPPER BOUNDS OF $F_m(z)$ FUNCTIONS

For real positive arguments it holds

$$F_0(x) \leq 1, \tag{31}$$

which is used in programs for electronic structure *ab initio* calculations for skipping calculations of small two-electron integrals in a Gaussian basis set. The upper bound for such an integral may be taken as a product of an "pre-exponential factor" and $F_0(x)$. The pre-exponential factor is easy to calculate and if it is smaller than an *a priori* chosen threshold, then calculation of that integral may be skipped. Considerable time may also be saved in electron scattering calculations in this way. Upper bounds of hybrid two-electron integrals in a mixed Gaussian and plane-wave basis set may also be expressed as a product of a simple pre-exponential factor and the upper bound of $F_0(z)$. For the complex arguments we have

$$|F_0(z)| \leq 1 \qquad \text{for } \mathrm{Re}\, z \geq 0 \tag{32}$$

and the asymptotic expression

$$|F_0(z)| \leq \left| \frac{e^{-z}}{-2z} \right| \qquad \text{for } \mathrm{Re}\, z < 0 \tag{33}$$

following from Eq. (14) for z with a large negative real part. For the purpose of pretesting integrals the condition (33) may be used for any z with $\mathrm{Re}\, z < 0$.

VI. SUMMARY

Properties of the complex incomplete gamma functions $F_m(z)$ were discussed from the viewpoint of effective calculation of hybrid two-electron integrals in a mixed Gaussian and plane-wave basis set. Different ways of calculations are recommended for different regions of the complex argument z. Asymptotes and upper bounds for $F_m(z)$ were determined.

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