Journal of Mathematical Chemistry Vol. 38, No. 4, November 2005 (© 2005)
DOI: 10.1007/s10910-005-6904-4

Use of recursion and analytical relations in evaluation of hypergeometric functions arising in multicenter integrals with noninteger n Slater type orbitals

I.I. Guseinov

Department of Physics, Faculty of Arts and Sciences, Onsekiz Mart University, Çanakkale, Turkey
E-mail: iguseinov@cheerful.com

B.A. Mamedov*,**

Department of Physics, Faculty of Arts and Sciences, Gaziosmanpaşa University, Tokat, Turkey
E-mail: bamamedov@yahoo.com

Received 15 December 2004; revised 4 January 2005

In this work we present the new recursion and analytical relations for the calculation of hypergeometric functions $F(1, b; c; z)$ occurring in multicenter integrals of noninteger n Slater type orbitals. The formulas obtained are numerically stable for $0 < z < 1$ and all integer and noninteger values of parameters b and c.

KEY WORDS: hypergeometric functions, Slater type orbitals, multicenter integrals

PACS No: 31.15.+q; 31.20.Ej

AMS subject classification: 81-V55; 81V45

1. Introduction

The hypergeometric functions play an important role in the solution of many physical problems [1–9]. It is found [10], for example, for the evaluation of multicenter integrals over noninteger n Slater type orbitals (STOs) one has to use the hypergeometric function $F(1, b; c; z)$ defined by the series [11]

$$F(1, b; c; z) = \sum_{n=0}^{\infty} \frac{(b, n)}{(c, n)} z^n, \tag{1}$$

where b and c are constants independent of $z (0 < z < 1)$ and (b, n) is the Pochhammer symbol defined by

*Corresponding author.
**The Author cordially congratulates Prof. I.I. Guseinov on his 70th birthday

$$(b, n) = \begin{cases} 1 & \text{for } n = 0 \\ b(b+1)...(b+n-1) & \text{for } n = 1, 2, ... \end{cases}. \tag{2}$$

The application that has motivated the present work is the need to evaluate multicenter integrals of noninteger n STOs occurring in the study of electronic structure of atoms, molecules, and solids, where the Hartree–Fock–Roothaan and explicitly correlated methods are employed. It was shown in previous work [10] that the required multicenter electron-repulsion integrals with noninteger n STOs could be evaluated from the matrix elements that are expressible in terms of hypergeometric functions $F(1, b; c; z)$. Thus it is still of interest to have an accurate algorithm for the evaluation of $F(1, b; c; z)$ with arbitrary values of b, c *and* z using recursion relations and analytical formulas. Such an algorithm is described in the present paper.

2. Definitions

In order to obtain the recursion and analytical relations for the hypergeometric functions $F(1, b; c; z)$ we shall use the following definitions [11]:

$$F\left(1, \mu+\nu; \nu+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{\nu(\alpha+\beta)^{\mu+\nu}}{\alpha^{\nu}\Gamma(\mu+\nu)} \int_0^{\infty} x^{\mu-1} \mathrm{e}^{-\beta x} \gamma(\nu, \alpha x) \mathrm{d}x \tag{3}$$

$$F\left(1, \mu+\nu; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{\mu(\alpha+\beta)^{\mu+\nu}}{\alpha^{\nu}\Gamma(\mu+\nu)} \int_0^{\infty} x^{\mu-1} \mathrm{e}^{-\beta x} \Gamma(\nu, \alpha x) \mathrm{d}x, \tag{4}$$

where $\alpha > 0, \beta > 0, \mu \geqslant 1, \nu = n + \varepsilon, 0 < \varepsilon < 1$ and $n = 0, 1, 2, ...$ The gamma functions in these equations are defined by

$$\gamma(\nu, \alpha x) = \textstyle\int_0^{\alpha x} t^{\nu-1} \mathrm{e}^{-t} \mathrm{d}t \tag{5}$$

$$\Gamma(\nu, \alpha x) = \textstyle\int_{\alpha x}^{\infty} t^{\nu-1} \mathrm{e}^{-t} \mathrm{d}t \tag{6}$$

$$\Gamma(\nu) = \Gamma(\nu, \alpha x) + \gamma(\nu, \alpha x) = \textstyle\int_0^{\infty} t^{\nu-1} \mathrm{e}^{-t} \mathrm{d}t. \tag{7}$$

The upward and downward recurrences, and the analytical relations for the incomplete gamma functions $\gamma(\nu, \alpha x)$ and $\Gamma(\nu, \alpha x)$ occurring in equation (3) and (4) are presented in Ref. [12].

3. Recursion relations for hypergemetric functions

The recursion relations of hypergeometric functions with respect to the indices ν can be established using in equations (3) and (4) the recurrences of

the incomplete gamma functions which are given in Ref. [12]. Then, we obtain:
Upward recurrences

$$F\left(1, \mu+\nu; \nu+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{\nu(\alpha+\beta)\Gamma(\mu+\nu-1)}{\alpha\Gamma(\mu+\nu)} \times\left[F\left(1, \mu+\nu-1; \nu; \frac{\alpha}{\alpha+\beta}\right)-1\right] \tag{8}$$

$$F\left(1, \mu+\nu; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{(\nu-1)(\alpha+\beta)\Gamma(\mu+\nu-1)}{\alpha\Gamma(\mu+\nu)} \times\left[F\left(1, \mu+\nu-1; \mu+1; \frac{\beta}{\alpha+\beta}\right)+\frac{\mu}{\nu-1}\right] \tag{9}$$

Downward recurrences

$$F\left(1, \mu+\nu; \nu+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{\alpha\Gamma(\mu+\nu+1)}{(\nu+1)(\alpha+\beta)\Gamma(\mu+\nu)} F\left(1, \mu+\nu+1; \nu+2; \frac{\alpha}{\alpha+\beta}\right)+1 \tag{10}$$

$$F\left(1, \mu+\nu; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{\alpha\Gamma(\mu+\nu+1)}{\nu(\alpha+\beta)\Gamma(\mu+\nu)} F\left(1, \mu+\nu+1; \mu+1; \frac{\beta}{\alpha+\beta}\right)-\frac{\mu}{\nu}. \tag{11}$$

The starting terms in recurrences (8)–(11) are determined by a

$$F\left(1, \mu+1+\varepsilon; 1+\varepsilon+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{(1+\varepsilon)(\alpha+\beta)^{\mu+1+\varepsilon}}{\alpha^{1+\varepsilon}\Gamma(\mu+1+\varepsilon)} \times \begin{cases} \left(\frac{1}{\beta^{\mu}}-\frac{1}{(\alpha+\beta)^{\mu}}\right)\Gamma(\mu) & \text{for } \varepsilon=0 \\ \frac{1}{\beta^{\mu}}\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(\mu+1+\varepsilon+m)}{m!(1+\varepsilon+m)}\left(\frac{\alpha}{\beta}\right)^{1+\varepsilon+m} & \text{for } 0<\varepsilon<1 \end{cases} \tag{8a}$$

$$F\left(1, \mu+1+\varepsilon; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{\mu(\alpha+\beta)^{\mu+1+\varepsilon}}{\alpha^{1+\varepsilon}\Gamma(\mu+1+\varepsilon)} \times \begin{cases} \frac{\Gamma(\mu)}{(\alpha+\beta)^{\mu}} & \text{for } \varepsilon=0 \\ \frac{1}{\beta^{\mu}}\left[\Gamma(1+\varepsilon)\Gamma(\mu)-\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(\mu+1+\varepsilon+m)}{m!(1+\varepsilon+m)}\left(\frac{\alpha}{\beta}\right)^{1+\varepsilon+m}\right] & \text{for } 0<\varepsilon<1 \end{cases} \tag{9a}$$

$$F\left(1, \mu + n_t + \varepsilon; n_t + \varepsilon + 1; \frac{\alpha}{\alpha+\beta}\right) \cong \frac{(1+\varepsilon)(\alpha+\beta)^{\mu+1+\varepsilon}}{\alpha^{1+\varepsilon}\Gamma(\mu+1+\varepsilon)} \times \begin{cases} \left(\frac{1}{\beta^\mu} - \frac{1}{(\alpha+\beta)^\mu}\right)\Gamma(\mu) & \text{for } \varepsilon = 0 \\ \frac{1}{\beta^\mu}\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(\mu+1+\varepsilon+m)}{m!(1+\varepsilon+m)}\left(\frac{\alpha}{\beta}\right)^{1+\varepsilon+m} & \text{for } 0 < \varepsilon < 1 \end{cases} \tag{10a}$$

$$F\left(1, \mu + n_t + \varepsilon; \mu + 1; \frac{\beta}{\alpha+\beta}\right) \cong \frac{\mu(\alpha+\beta)^{\mu+1+\varepsilon}}{\alpha^{1+\varepsilon}\Gamma(\mu+1+\varepsilon)} \times \begin{cases} \frac{\Gamma(\mu)}{(\alpha+\beta)^\mu} & \text{for } \varepsilon = 0 \\ \frac{1}{\beta^\mu}\left[\Gamma(1+\varepsilon)\Gamma(\mu) - \sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(\mu+1+\varepsilon+m)}{m!(1+\varepsilon+m)}\left(\frac{\alpha}{\beta}\right)^{1+\varepsilon+m}\right] & \text{for } 0 < \varepsilon < 1 \end{cases} \tag{11a}$$

See Ref. [12] for the exact definition of n_t occurring in equations (10a) and (11a).

4. Analytical relations for hypergeometric functions

In order to establish the analytical formulae for the functions $F\left(1, \mu + \nu; \nu + 1; \frac{\alpha}{\alpha+\beta}\right)$ and $F\left(1, \mu + \nu; \mu + 1; \frac{\beta}{\alpha+\beta}\right)$ we shall use in equations (3) and (4) the analytical relations of incomplete gamma functions derived in Ref. [12]. Then, it is easy to present the recursive relations (8) and (9) in the following analytical form:

$$F\left(1, \mu+\nu; \nu+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{\nu(\alpha+\beta)^{\mu+\nu}}{\alpha^k\Gamma(\mu+\nu)}\left\{\frac{(\nu)_k\Gamma(\mu+\nu-k)}{(\nu-k)(\alpha+\beta)^{\mu+\nu-k}} \times F\left(1, \mu+\nu-k; \nu-k+1; \frac{\alpha}{\alpha+\beta}\right) - \sum_{i=1}^{k}\frac{(\nu)_{k-i}\alpha^{i-1}}{(\alpha+\beta)^{\mu-1+\nu-k+i}}\Gamma(\mu-1+\nu-k+i)\right\} \tag{12}$$

$$F\left(1, \mu+\nu; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{\mu(\alpha+\beta)^{\mu+\nu}}{\alpha^k\Gamma(\mu+\nu)}\left\{\frac{(\nu)_k\Gamma(\mu+\nu-k)}{\mu(\alpha+\beta)^{\mu+\nu-k}} \times F\left(1, \mu+\nu-k; \mu+1; \frac{\beta}{\alpha+\beta}\right) + \sum_{i=1}^{k}\frac{(\nu)_{k-i}\alpha^{i-1}}{(\alpha+\beta)^{\mu-1+\nu-k+i}}\Gamma(\mu-1+\nu-k+i)\right\}, \tag{13}$$

where $0 \leqslant k \leqslant n-1$.

In special cases of equations (12) and (13) for $k = n-1$ and $\nu = n+\varepsilon$ we obtain for the hypergeometric functions the following analytical relations in terms of initial values:

$$F\left(1, \mu+n+\varepsilon; n+\varepsilon+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{(n+\varepsilon)(\alpha+\beta)^{\mu+n+\varepsilon}}{\alpha^n \Gamma(\mu+n+\varepsilon)} \left\{ \frac{(n+\varepsilon)_{n-1}\alpha\Gamma(\mu+1+\varepsilon)}{(1+\varepsilon)(\alpha+\beta)^{\mu+1+\varepsilon}} \times F\left(1, \mu+1+\varepsilon; 1+\varepsilon+1; \frac{\alpha}{\alpha+\beta}\right) - \sum_{i=1}^{n-1} \frac{(n+\varepsilon)_{n-1-i}\alpha^i}{(\alpha+\beta)^{\mu+\varepsilon+i}} \Gamma(\mu+\varepsilon+i) \right\} \tag{14}$$

$$F\left(1, \mu+n+\varepsilon; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{\mu(\alpha+\beta)^{\mu+n+\varepsilon}}{\alpha^n \Gamma(\mu+n+\varepsilon)} \left\{ \frac{(n+\varepsilon)_{n-1}\alpha\Gamma(\mu+1+\varepsilon)}{\mu(\alpha+\beta)^{\mu+1+\varepsilon}} \times F\left(1, \mu+1+\varepsilon; \mu+1; \frac{\beta}{\alpha+\beta}\right) + \sum_{i=1}^{n-1} \frac{(n+\varepsilon)_{n-1-i}\alpha^i}{(\alpha+\beta)^{\mu+\varepsilon+i}} \Gamma(\mu+\varepsilon+i) \right\}. \tag{15}$$

See Ref. [12] for the exact definition of coefficients $(n+\varepsilon)_k$.

We notice that the hypergeometric functions with integer values of the indices μ can also be evaluated from the following analytical relations:

$$F\left(1, \mu+\nu; \nu+1; \frac{\alpha}{\alpha+\beta}\right) = \frac{\nu(\mu-1)!}{\Gamma(\mu+\nu)} \sum_{k=0}^{\mu-1} \frac{\Gamma(\nu+k)}{k![\beta/(\alpha+\beta)]^{\mu-k}} \tag{16}$$

$$F\left(1, \mu+\nu; \mu+1; \frac{\beta}{\alpha+\beta}\right) = \frac{\mu!}{\Gamma(\mu+\nu)} \left\{ \frac{\Gamma(\nu)}{[\alpha/(\alpha+\beta)]^{\nu}[\beta/(\alpha+\beta)]^{\mu}} - \sum_{k=0}^{\mu-1} \frac{\Gamma(\nu+k)}{k![\beta/(\alpha+\beta)]^{\mu-k}} \right\}. \tag{17}$$

These formulae can easily be established from equations (3) and (4) by partial integration.

5. Numerical results and discussion

The use of the newly derived closed-form expressions equations (12)–(17), for hypergeometric functions $F(1, b; c; z)$ can significantly improve the accuracy

Table 1
Numbers of correct decimal figures a_k for hypergeometric functions $F(1, b; c; z)$.

					a_k	
μ	ν	α	β	k	Equation (12)	Equation (13)
5.3	6.8	6.5	2.4	5	14	14
13.5	16.8	14.6	12.4	15	16	15
0.3	3.4	1.8	2.1	2	16	17
11.5	20.3	17.1	15.2	19	20	20
23.1	25.6	21.7	19.5	24	14	15
32.3	32.5	12.1	9.5	31	13	13
43.2	53.2	40.2	29.7	52	13	13
64.3	55.3	41.4	29.7	54	13	12
70.6	35.5	58.4	42.9	34	14	14
87.2	63.5	65.8	64.2	62	16	16
100.8	9.3	106.5	86.4	8	13	14

and efficiency of the evaluation of multicenter integrals over noninteger n STOs. These approaches can be used for arbitrary values of indices b and c.

On the basis of formulas (equations (12)–(17)) obtained in this paper we constructed a program for computation of hypergeometric functions on a computer Pentium III 800 MHz (using Turbo Pascal language) in double precision with an accuracy of significant digits. One can determine the accuracy of computer results obtained from analytical relations (12) and (13) by the use of upward and downward recurrences, equations (8)–(11). The examples of computer calculation of equations (12) and (13) for the $F(1, b; c; z)$ are shown in Table 1. The numbers of correct decimal figures a_k $(|\Delta f_k| \cong 10^{-a_k})$ determined with the help of equations (8)–(11) are given in this table, where $\Delta f_k = f_k - f_{k-1}$. Here, the values f_k and f_{k-1} are obtained from equations (12) and (13).

The use of formulas established in this work for the calculation of hypergeometric functions $F(1, b; c; z)$ makes it possible to considerable simplify and speed up calculations of the multicenter integrals over noninteger n STOs.

Acknowledgment

This work was financially supported by the TÜBITAK Project No. TBAG-2396.

References

[1] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics-Non-relativistic Theory* (Pergamon, New York, 1965).

[2] H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1977).
[3] D.S.F. Crothers, J. Phys. B. 18 (1985) 2893.
[4] H.E. Moses and R.T. Prosser, J. Math. Anal. Appl. 173 (1993) 390.
[5] J.B. Seaborn, *Hypergeometric Functions and Their Applications* (Springer Verlag, New York, 1991).
[6] A.M. Mathai, R.K. Saxena, *Generalized Hypergeometric Functions with Applications in Statistics and Physical Sciences* (Springer Verlag, Heidelberg, 1973).
[7] C. Snow, *Hypergeometric and Legendre Functions with Applications to Integral Equations of Potential Theory*. 2nd ed. (U.S.Govt. Printing Office, Washington, D.C., 1952).
[8] H. Buchholz, *The Confluent Hypergeometric Function with Special Emphasis on its Applications* (Springer Verlag, 1969).
[9] H. Exton, *Multiple Hypergeometric Functions and Applications* (Ellis Horwood, 1976).
[10] I.I. Guseinov and B.A. Mamedov, Theor. Chem. Acc. 108 (2002) 21.
[11] I.S. Gradshteyn and I.M. Ryzhik, *Tables of Integrals, Sums, Series and Products*, 4th ed. (Academic Press, New York, 1980).
[12] I.I. Guseinov and B.A. Mamedov, J. Mat. Chem. 36 (2004) 341.