Computing the Hypergeometric Function

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The hypergeometric function of a real variable is computed for arbitrary real parameters. The transformation theory of the hypergeometric function is used to obtain rapidly convergent power series. The divergences that occur in the individual terms of the transformation for integer parameters are removed using a finite difference technique. © 1997 Academic Press

I. INTRODUCTION

The hypergeometric function $_2F_1$ occurs in many areas of physics. For example, the matrix elements for radiation processes in hydrogen atoms [1] and form factors for atomic collisions [2] can be expressed in terms of hypergeometric functions. The Wigner simplified rotation matrices [3] can be written in terms of Jacobi polynomials which are particular cases of the hypergeometric function. The radial momentum space wave functions for a Coulomb potential are given by Gegenbauer functions [4] which are related to hypergeometric functions. The application that has motivated the present work is the need to evaluate Bethe logarithms [5] for theoretical calculations of the QED Lamb shift. It was shown [5] for hydrogen and helium that the required Bethe logarithms could be evaluated from matrix elements that are expressible in terms of hypergeometric functions of a real variable. Therefore, it was desirable to have an efficient computer program that could evaluate the hypergeometric function for an arbitrary real variable. Such a program is now available [6] and is described in the present paper.

II. THEORY

The hypergeometric function $_2F_1$ is defined by the series

$$_{2}F_{1}(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a)_{n}(b)_{n}z^{n}}{(c)_{n}n!},$$
 (1)

C	ase I	Interval	Γransformation
	I –∞	< z < -1	$w = \frac{1}{1 - z}$
1	II -1	$\leq z < 0$	$w = \frac{z}{z - 1}$
I	II 0	$\leq z \leq .5$	w = z
I	V .5	$< z \le 1$	w = 1 - z
,	V 1	$< z \le 2$	$w = 1 - \frac{1}{z}$
7	/I 2	$< z < +\infty$	$w = \frac{1}{z}$

TABLE I
Transformation of the Hypergeometric Function

which converges for |z| < 1 as can be seen by the ratio test. For z outside the circle of convergence, it is necessary to transform z in such a way that the hypergeometric function can be expressed in terms of other hypergeometric functions of a new argument w such that |w| < 1. To do this, the real axis was divided into six intervals as shown in Table I. In each case, the new independent variable w lies in the range zero to one-half, so that the series in powers of w not only converges, but converges rapidly.

A. Transformation Equations

With the real axis divided into the six intervals shown in Table I, the transformation theory [7] for the hypergeometric function can be used as follows. For case I, the identity

$${}_{2}F_{1}(a,b;c;z) = w^{a} \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} {}_{2}F_{1}(a,c-b;a-b+1;w)$$

$$+ w^{b} \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} {}_{2}F_{1}(b,c-a;b-a+1;w)$$
(2)

is used to calculate ${}_2F_1$. If a-b is equal to an integer, one of the terms in (2) will diverge due to a gamma function of negative argument in the numerator and the other term will diverge because the third parameter of the ${}_2F_1$ is a negative integer. The sum of the two terms, however, remains finite as a-b approaches an integer. This problem is discussed in detail in the next section. For case II, the identity

$$_{2}F_{1}(a,b;c;z) = (1-w)^{a}{_{2}F_{1}(a,c-b;c;w)}$$
 (3)

is used. No transformation is needed for case III. For case IV, the identity

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} {}_{2}F_{1}(a,b;a+b-c+1;w) + w^{(c-a-b)} \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} {}_{2}F_{1}(c-a,c-b;c-a-b+1;w)$$
(4)

is used. If c - a - b is equal to an integer, both of the terms in (4) diverge for the same reason as in case I. For case V, the branch which is obtained by letting z approach the real axis from above is chosen yielding the identity

$$\lim_{\varepsilon \to 0^{+}} {}_{2}F_{1}(a,b;c;z+i\varepsilon)$$

$$= (1-w)^{a} \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} {}_{2}F_{1}(a,a-c+1;a+b-c+1;w)$$

$$+ (1-w)^{b} |w|^{(c-a-b)} e^{-i\pi(c-a-b)} \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} {}_{2}F_{1}(c-a,1-a;c-a-b+1;w).$$
(5)

Using the identity ${}_2F_1(\alpha, \beta; \gamma; w) = (1 - w)^{\gamma - \alpha - \beta} {}_2F_1(\gamma - \alpha, \gamma - \beta; \gamma; w)$ where $\alpha = c - a$, $\beta = 1 - a$, and $\gamma = c - a - b + 1$, Eq. (5) can be expressed as

$$\lim_{\varepsilon \to 0^{+}} {}_{2}F_{1}(a, b; c; z + i\varepsilon)$$

$$= (1 - w)^{a} \frac{\Gamma(c)\Gamma(c - a - b)}{\Gamma(c - a)\Gamma(c - b)} {}_{2}F_{1}(a, a - c + 1; a + b - c + 1; w)$$

$$+ (1 - w)^{a} |w|^{(c - a - b)} e^{-i\pi(c - a - b)} \frac{\Gamma(c)\Gamma(a + b - c)}{\Gamma(a)\Gamma(b)} {}_{2}F_{1}(1 - b, c - b; c - a - b + 1; w).$$
(6)

If c - a - b is equal to an integer, the two terms on the right-hand side again diverge if taken separately. Finally for case VI, with z approaching the real axis from above, the identity

$$\lim_{\varepsilon \to 0^{+}} {}_{2}F_{1}(a,b;c;z+i\varepsilon) = |w|^{a} e^{i\pi a} \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} {}_{2}F_{1}(a,a-c+1;a-b+1;w)$$

$$+ |w|^{b} e^{i\pi b} \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} {}_{2}F_{1}(b-c+1,b;b-a+1;w)$$
 (7)

is used. If a - b is equal to an integer, there is again a problem with divergent terms.

B. Exceptional Cases

In the previous section it was noted that a problem arises when either a - b is an integer (cases I and VI) or c - a - b is an integer (cases IV and V). In all of these cases, each of the two terms is infinite, but their sum remains finite. Near

these cases, i.e. for a-b close to an integer or c-a-b close to an integer, the two terms are large and of opposite sign and must be combined analytically to avoid excessive roundoff error. To carry out this combining for case I, we let $a-b=k+\varepsilon$, where k is an integer greater than or equal to zero and $|\varepsilon|$ is small. If k is negative, it can be made positive by interchanging a and b (note that ${}_2F_1(b,a;c;z)={}_2F_1(a,b;c;z)$). Equation (2) can be written in the form

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-b)} \sum_{n=0}^{k-1} \frac{(b)_{n}(c-a)_{n}\Gamma(k-n+\varepsilon)(-1)^{n}w^{b+n}}{n!}$$

$$+ \Gamma(c) \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(c-a+k+n+\varepsilon)\Gamma(-k-n-\varepsilon)(-1)^{n}w^{a+n}}{\Gamma(a)\Gamma(b)\Gamma(c-a)\Gamma(c-b)n!}$$

$$+ \Gamma(c) \sum_{n=0}^{\infty} \frac{\Gamma(a+n-\varepsilon)\Gamma(c-a+k+n)\Gamma(-n+\varepsilon)(-1)^{n+k}w^{a+n-\varepsilon}}{\Gamma(a)\Gamma(b)\Gamma(c-a)\Gamma(c-b)(n+k)!}.$$

$$(8)$$

Equation (8) can be expressed [8] in terms of finite differences (see Section IIC) which allow all of the terms to remain finite. The remaining cases are similar. For case IV, if $c - a - b = k + \varepsilon$, where $k \ge 0$ and $|\varepsilon|$ is small, (4) can be brought to the form

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(c-a)\Gamma(c-b)} \sum_{n=0}^{k-1} \frac{(a)_{n}(b)_{n}\Gamma(k+\varepsilon-n)(-1)^{n}w^{n}}{n!}$$

$$+ \Gamma(c) \sum_{n=0}^{\infty} \frac{\Gamma(c-a+n)\Gamma(c-b+n)\Gamma(-n-k-\varepsilon)(-1)^{n}w^{n+k+\varepsilon}}{\Gamma(a)\Gamma(b)\Gamma(c-a)\Gamma(c-b)n!}$$

$$+ \Gamma(c) \sum_{n=0}^{\infty} \frac{\Gamma(a+n+k)\Gamma(b+n+k)\Gamma(\varepsilon-n)(-w)^{n+k}}{\Gamma(a)\Gamma(b)\Gamma(c-a)\Gamma(c-b)(n+k)!}.$$

$$(9)$$

If $c - a - b = -k + \varepsilon$ with k > 0, a slightly different approach must be used to fix up case IV. In this case (4) can be rewritten as

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{k-1} \frac{(c-a)_{n}(c-b)_{n}\Gamma(k-\varepsilon-n)(-1)^{n}w^{n-k+\varepsilon}}{n!}$$

$$+ \Gamma(c) \sum_{n=0}^{\infty} \frac{\Gamma(a+n+\varepsilon)\Gamma(b+n+\varepsilon)\Gamma(-n-\varepsilon)(-1)^{n+k}w^{n+\varepsilon}}{\Gamma(a)\Gamma(b)\Gamma(c-a)\Gamma(c-b)(n+k)!}$$

$$+ \Gamma(c) \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)\Gamma(\varepsilon-n-k)(-w)^{n}}{\Gamma(a)\Gamma(b)\Gamma(c-a)\Gamma(c-b)n!}.$$

$$(10)$$

The notation IVa and IVb is used to refer to (9) and (10). For case V, if $c - a - b = k + \varepsilon$, where $k \ge 0$ and $|\varepsilon|$ is small, then (6) can be written as

$$\lim_{\delta \to 0^{+}} {}_{2}F_{1}(a, b; c; z + i\delta)
= (1 - w)^{a}\Gamma(c) \left\{ \sum_{n=0}^{k-1} \frac{(a)_{n}(1 + a - c)_{n}\Gamma(k - n + \varepsilon)(-w)^{n}}{\Gamma(c - a)\Gamma(c - b)n!} \right.
+ \sum_{n=0}^{\infty} \frac{(a)_{n+k}(1 + a - c)_{n+k}\Gamma(\varepsilon - n)(-w)^{n+k}}{\Gamma(c - a)\Gamma(c - b)(n + k)!}
+ \left\{ \cos[\pi(k + \varepsilon)] - i\sin[\pi(k + \varepsilon)] \right\}
\sum_{n=0}^{\infty} \frac{(1 - b)_{n}(c - b)_{n}\Gamma(-k - n - \varepsilon)(-1)^{n}w^{n+k+\varepsilon}}{\Gamma(a)\Gamma(b)n!} \right\}.$$
(11)

The real part of the infinite series can be expressed as

$$(1-w)^{a}\Gamma(c)\sum_{n=0}^{\infty}\left\{\frac{(a)_{n+k}\Gamma(\varepsilon-n)(w)^{n+k}}{\Gamma(b-n+\varepsilon)\Gamma(c-b)(n+k)!} + \cos(\pi\varepsilon)\frac{(c-b)_{n}\Gamma(-k-n-\varepsilon)(-1)^{k}w^{n+k+\varepsilon}}{\Gamma(a)\Gamma(b-n)n!}\right\}.$$

As in case IV when $c - a - b = -k + \varepsilon$, a slightly different approach must be used to fix up case V. In this case Eq. (6) can be written as

$$\lim_{\delta \to 0^{+}} {}_{2}F_{1}(a,b;c;z+i\delta)$$

$$= (1-w)^{a}\Gamma(c)\{\cos[\pi(\varepsilon-k)] - i\sin[\pi(\varepsilon-k)]\}$$

$$\left\{\sum_{n=0}^{k-1} \frac{(1-b)_{n}(c-b)_{n}\Gamma(k-n-\varepsilon)(-1)^{n}w^{n-k+\varepsilon}}{\Gamma(a)\Gamma(b)n!} + \sum_{n=0}^{\infty} \frac{(1-b)_{n+k}(c-b)_{n+k}\Gamma(-\varepsilon-n)(-1)^{n+k}w^{n+\varepsilon}}{\Gamma(a)\Gamma(b)(n+k)!}\right\}$$

$$+ (1-w)^{a}\Gamma(c)\sum_{n=0}^{\infty} \frac{(a)_{n}(a-c+1)_{n}\Gamma(\varepsilon-k-n)(-w)^{n}}{\Gamma(a-k+\varepsilon)\Gamma(b-k+\varepsilon)n!}.$$
(12)

The notation Va and Vb is used to refer to (11) and (12). For case Vb, the real part of the hypergeometric function can be expressed as

$$\operatorname{Re}_{2}F_{1}(a,b;c;z)$$

$$= (1-w)^{a}\Gamma(c)\cos[\pi(\varepsilon-k)]\sum_{n=0}^{k-1}\frac{(1-b)_{n}(c-b)_{n}\Gamma(k-n-\varepsilon)(-1)^{n}w^{n-k+\varepsilon}}{\Gamma(a)\Gamma(b)n!}$$

$$+ (1-w)^{a}\Gamma(c)\sum_{n=0}^{\infty}\left\{\frac{\Gamma(a+n)\Gamma(-k-n+\varepsilon)w^{n}}{\Gamma(a)\Gamma(a-k+\varepsilon)\Gamma(b-k-n+\varepsilon)n!}\right\}$$

$$+ \frac{\cos(\pi\varepsilon)(-1)^{k}\Gamma(a+n+\varepsilon)\Gamma(-n-\varepsilon)w^{n+\varepsilon}}{\Gamma(a)\Gamma(a-k+\varepsilon)\Gamma(b-k-n)(n+k)!}.$$
(13)

In case VI, when $a-b=k+\varepsilon$ with $k\geq 0$ and $|\varepsilon|$ small equation (7) can be written as

$$\lim_{\delta \to 0^{+}} {}_{2}F_{1}(a,b;c;z+i\delta)
= \Gamma(c)[\cos(\pi b) + i\sin(\pi b)] \sum_{n=0}^{k-1} \frac{(b-c+1)_{n}(b)_{n}\Gamma(k+\varepsilon-n)(-1)^{n}w^{n+b}}{\Gamma(a)\Gamma(c-b)n!}
+ \Gamma(c) \sum_{n=0}^{\infty} \left\{ [\cos(\pi a) + i\sin(\pi a)] \frac{(a)_{n}(a-c+1)_{n}\Gamma(-k-\varepsilon-n)(-1)^{n}w^{n+a}}{\Gamma(b)\Gamma(c-a)n!}
+ [\cos(\pi b) + i\sin(\pi b)] \frac{(b)_{n+k}(b-c+1)_{n+k}\Gamma(\varepsilon-n)(-1)^{n+k}w^{n+k+b}}{\Gamma(a)\Gamma(c-b)(n+k)!} \right\}. (14)$$

C. Finite Difference Results

The exceptional cases of Section IIB can be expressed in terms of finite differences [8]. The results are presented in this section using the definition

$$g_k(\varepsilon; n) \equiv \frac{f_k(\varepsilon; n) - f_k(0; n)}{\varepsilon},$$
 (15)

where the specific f-functions are defined in Appendix A. For case I, the finite difference result is

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-b)} \sum_{n=0}^{k-1} \frac{(b)_{n}(c-a)_{n}\Gamma(k-n+\varepsilon)(-1)^{n}w^{b+n}}{n!}$$

$$+ (-1)^{k}\Gamma(c) \sum_{n=0}^{\infty} \{(a)_{n}f_{2}^{I}(\varepsilon;n)f_{3}^{I}(\varepsilon;n)f_{4}^{I}(0;n)f_{5}^{I}(0;n)g_{6}^{I}(\varepsilon)$$

$$- f_{1}^{I}(\varepsilon;n)(c-a)_{k+n}f_{3}^{I}(0;n)f_{4}^{I}(\varepsilon;n)f_{5}^{I}(\varepsilon;n)g_{7}^{I}(\varepsilon)$$

$$- g_{1}^{I}(\varepsilon;n)f_{2}^{I}(\varepsilon;n)f_{3}^{I}(\varepsilon;n)f_{4}^{I}(0;n)f_{5}^{I}(0;n)$$

$$+ f_{1}^{I}(\varepsilon;n)g_{2}^{I}(\varepsilon;n)f_{3}^{I}(\varepsilon;n)f_{4}^{I}(0;n)f_{5}^{I}(0;n)$$

$$+ f_{1}^{I}(\varepsilon;n)f_{2}^{I}(0;n)g_{3}^{I}(\varepsilon;n)f_{4}^{I}(0;n)f_{5}^{I}(0;n)$$

$$- f_{1}^{I}(\varepsilon;n)f_{2}^{I}(0;n)f_{3}^{I}(0;n)f_{4}^{I}(\varepsilon;n)f_{5}^{I}(\varepsilon;n)$$

$$- f_{1}^{I}(\varepsilon;n)f_{2}^{I}(0;n)f_{3}^{I}(0;n)f_{4}^{I}(\varepsilon;n)g_{5}^{I}(\varepsilon;n) \}.$$

$$(16)$$

For case IVa, the finite difference result is

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(c-a)\Gamma(c-b)} \sum_{n=0}^{k-1} \frac{(a)_{n}(b)_{n}\Gamma(k-n+\varepsilon)(-1)^{n}w^{n}}{n!}$$

$$+ (-1)^{k}\Gamma(c) \sum_{n=0}^{\infty} \left\{ -(a)_{k+n} f_{2}^{IVa}(0;n) f_{3}^{IVa}(0;n) f_{4}^{IVa}(\varepsilon;n) f_{5}^{IVa}(0;n) g_{6}^{IVa}(\varepsilon) \right.$$

$$- f_{1}^{IVa}(0;n)(b)_{k+n} f_{3}^{IVa}(0;n) f_{4}^{IVa}(\varepsilon;n) f_{5}^{IVa}(0;n) g_{7}^{IVa}(\varepsilon)$$

$$-(a)_{k+n}(b)_{k+n}\varepsilon f_{3}^{IVa}(0;n)f_{4}^{IVa}(\varepsilon;n)f_{5}^{IVa}(0;n)g_{6}^{IVa}(\varepsilon)g_{7}^{IVa}(\varepsilon)$$

$$+g_{1}^{IVa}(\varepsilon;n)f_{2}^{IVa}(\varepsilon;n)f_{3}^{IVa}(\varepsilon;n)f_{4}^{IVa}(0;n)f_{5}^{IVa}(\varepsilon;n)$$

$$+f_{1}^{IVa}(0;n)g_{2}^{IVa}(\varepsilon;n)f_{3}^{IVa}(\varepsilon;n)f_{4}^{IVa}(0;n)f_{5}^{IVa}(\varepsilon;n)$$

$$+f_{1}^{IVa}(0;n)f_{2}^{IVa}(0;n)g_{3}^{IVa}(\varepsilon;n)f_{4}^{IVa}(0;n)f_{5}^{IVa}(\varepsilon;n)$$

$$-f_{1}^{IVa}(0;n)f_{2}^{IVa}(0;n)f_{3}^{IVa}(0;n)g_{4}^{IVa}(\varepsilon;n)f_{5}^{IVa}(\varepsilon;n)$$

$$+f_{1}^{IVa}(0;n)f_{2}^{IVa}(0;n)f_{3}^{IVa}(0;n)f_{4}^{IVa}(\varepsilon;n)g_{5}^{IVa}(\varepsilon;n)\}. \tag{17}$$

For case IVb, the finite difference result is

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{k-1} \frac{(c-a)_{n}(c-b)_{n}\Gamma(k-n-\varepsilon)(-1)^{n}w^{n-k+\varepsilon}}{n!}$$

$$+ (-1)^{k}\Gamma(c) \sum_{n=0}^{\infty} \left\{ -(a)_{n}f_{2}^{IVb}(0;n)f_{3}^{IVb}(0;n)f_{4}^{IVb}(\varepsilon;n)f_{5}^{IVb}(0;n)g_{6}^{IVb}(\varepsilon) \right.$$

$$- f_{1}^{IVb}(0;n)(b)_{n}f_{3}^{IVb}(0;n)f_{4}^{IVb}(\varepsilon;n)f_{5}^{IVb}(0;n)g_{7}^{IVb}(\varepsilon)$$

$$- (a)_{n}(b)_{n}\varepsilon f_{3}^{IVb}(0;n)f_{4}^{IVb}(\varepsilon;n)f_{5}^{IVb}(0;n)g_{6}^{IVb}(\varepsilon)g_{7}^{IVb}(\varepsilon)$$

$$+ g_{1}^{IVb}(\varepsilon;n)f_{2}^{IVb}(\varepsilon;n)f_{3}^{IVb}(\varepsilon;n)f_{4}^{IVb}(0;n)f_{5}^{IVb}(\varepsilon;n)$$

$$+ f_{1}^{IVb}(0;n)g_{2}^{IVb}(\varepsilon;n)f_{3}^{IVb}(\varepsilon;n)f_{4}^{IVb}(0;n)f_{5}^{IVb}(\varepsilon;n)$$

$$+ f_{1}^{IVb}(0;n)f_{2}^{IVb}(0;n)g_{3}^{IVb}(\varepsilon;n)f_{4}^{IVb}(0;n)f_{5}^{IVb}(\varepsilon;n)$$

$$- f_{1}^{IVb}(0;n)f_{2}^{IVb}(0;n)f_{3}^{IVb}(0;n)g_{4}^{IVb}(\varepsilon;n)f_{5}^{IVb}(\varepsilon;n)$$

$$+ f_{1}^{IVb}(0;n)f_{2}^{IVb}(0;n)f_{3}^{IVb}(0;n)f_{4}^{IVb}(\varepsilon;n)f_{5}^{IVb}(\varepsilon;n)$$

For case Va, the finite difference result for the real part of the hypergeometric function is

$$\operatorname{Re}_{2}F_{1}(a,b;c;z) \\
= (1-w)^{a}\Gamma(c) \sum_{n=0}^{k-1} \frac{(a)_{n}(1+a-c)_{n}\Gamma(k-n+\varepsilon)(-w)^{n}}{\Gamma(c-a)\Gamma(c-b)n!} \\
+ (1-w)^{a}\Gamma(c) \sum_{n=0}^{\infty} (-1)^{n} \left\{ -g_{1}^{Va}(\varepsilon;n)f_{2}^{Va}(\varepsilon)f_{3}^{Va}(0;n)f_{4}^{Va}(\varepsilon;n)f_{5}^{Va}(\varepsilon;n) \right. \\
+ f_{1}^{Va}(\varepsilon;n)g_{2}^{Va}(\varepsilon)f_{3}^{Va}(0;n)f_{4}^{Va}(\varepsilon;n)f_{5}^{Va}(\varepsilon;n) \\
- f_{1}^{Va}(\varepsilon;n)f_{2}^{Va}(0)g_{3}^{Va}(\varepsilon;n)f_{4}^{Va}(\varepsilon;n)f_{5}^{Va}(\varepsilon;n) \\
+ f_{1}^{Va}(\varepsilon;n)f_{2}^{Va}(0)f_{3}^{Va}(\varepsilon;n)g_{4}^{Va}(\varepsilon;n)f_{5}^{Va}(\varepsilon;n) \\
+ f_{1}^{Va}(\varepsilon;n)f_{2}^{Va}(0)f_{3}^{Va}(\varepsilon;n)g_{4}^{Va}(\varepsilon;n)f_{5}^{Va}(\varepsilon;n) \\
- \frac{(c-b)_{n}}{\Gamma(b-n)}f_{2}^{Va}(\varepsilon)f_{3}^{Va}(0;n)f_{4}^{Va}(\varepsilon;n)f_{5}^{Va}(\varepsilon;n)g_{6}^{Va}(\varepsilon) \right\}, \tag{19}$$

and the imaginary part of the hypergeometric function becomes

$$\lim_{\delta \to 0^{+}} \operatorname{Im}_{2} F_{1}(a, b; c; z + i\delta)$$

$$= -(1 - w)^{a} \Gamma(c) \frac{\sin(\pi \varepsilon)}{\varepsilon} \sum_{n=0}^{\infty} \frac{(c - b)_{n}(-1)^{n} f_{3}^{Va}(0; n) f_{4}^{Va}(\varepsilon; n) f_{5}^{Va}(\varepsilon; n)}{\Gamma(a)\Gamma(b - n)}. \quad (20)$$

For case Vb, the finite difference result for the real part of the hypergeometric function is

$$\begin{split} &\text{Re}_{2}F_{1}(a,b;c;z) \\ &= (1-w)^{a}\Gamma(c)\cos[\pi(\varepsilon-k)]\sum_{n=0}^{k-1}\frac{(1-b)_{n}(c-b)_{n}\Gamma(k-n-\varepsilon)(-1)^{n}w^{n-k+\varepsilon}}{\Gamma(a)\Gamma(b)n!} \\ &+ (1-w)^{a}\Gamma(c)\sum_{n=0}^{\infty}(-1)^{k+n}\{-(a)_{n}f_{2}^{Vb}(\varepsilon;n)f_{3}^{Vb}(0;n)f_{4}^{Vb}(\varepsilon;n)f_{5}^{Vb}(0;n)g_{7}^{Vb}(\varepsilon) \\ &+ g_{1}^{Vb}(\varepsilon;n)f_{2}^{Vb}(0;n)f_{3}^{Vb}(\varepsilon;n)f_{4}^{Vb}(0;n)f_{5}^{Vb}(\varepsilon;n)f_{6}^{Vb}(\varepsilon) \\ &- f_{1}^{Vb}(0;n)g_{2}^{Vb}(\varepsilon;n)f_{3}^{Vb}(\varepsilon;n)f_{4}^{Vb}(0;n)f_{5}^{Vb}(\varepsilon;n)f_{6}^{Vb}(\varepsilon) \\ &+ f_{1}^{Vb}(0;n)f_{2}^{Vb}(\varepsilon;n)g_{3}^{Vb}(\varepsilon;n)f_{4}^{Vb}(0;n)f_{5}^{Vb}(\varepsilon;n)f_{6}^{Vb}(\varepsilon) \\ &- f_{1}^{Vb}(0;n)f_{2}^{Vb}(\varepsilon;n)f_{3}^{Vb}(0;n)g_{4}^{Vb}(\varepsilon;n)f_{5}^{Vb}(\varepsilon;n)f_{6}^{Vb}(\varepsilon) \\ &+ f_{1}^{Vb}(0;n)f_{2}^{Vb}(\varepsilon;n)f_{3}^{Vb}(0;n)f_{4}^{Vb}(\varepsilon;n)g_{5}^{Vb}(\varepsilon;n)f_{6}^{Vb}(\varepsilon) \\ &+ f_{1}^{Vb}(0;n)f_{2}^{Vb}(\varepsilon;n)f_{3}^{Vb}(0;n)f_{4}^{Vb}(\varepsilon;n)g_{5}^{Vb}(\varepsilon;n)f_{6}^{Vb}(\varepsilon) \\ &+ f_{1}^{Vb}(0;n)f_{2}^{Vb}(\varepsilon;n)f_{3}^{Vb}(0;n)f_{4}^{Vb}(\varepsilon;n)f_{5}^{Vb}(0;n)g_{6}^{Vb}(\varepsilon) \}, \end{split}$$

with the imaginary part

$$\lim_{\delta \to 0^{+}} \operatorname{Im}_{2} F_{1}(a, b; c; z + i\delta)$$

$$= -(1 - w)^{a} \Gamma(c) \left\{ \sin[\pi(\varepsilon - k)] \sum_{n=0}^{k-1} \frac{(1 - b)_{n}(c - b)_{n} \Gamma(k - n - \varepsilon)(-1)^{n} w^{n-k+\varepsilon}}{\Gamma(a) \Gamma(b) n!} + \frac{\sin(\pi \varepsilon)}{\varepsilon} \sum_{n=0}^{\infty} \frac{(c - b)_{k+n} (1 - b)_{k+n} f_{3}^{Vb}(\varepsilon; n) f_{4}^{Vb}(0; n) f_{5}^{Vb}(\varepsilon; n)}{\Gamma(a) \Gamma(b)} \right\}. \tag{22}$$

For case VI, the finite difference result for the real part of the hypergeometric function is

$$\begin{split} \operatorname{Re}_{2}F_{1}(a,b;c;z) \\ &= \Gamma(c)\cos(\pi b)\sum_{n=0}^{k-1}\frac{(b)_{n}(b-c+1)_{n}\Gamma(k+\varepsilon-n)(-1)^{n}w^{n+b}}{\Gamma(a)\Gamma(c-b)n!} \\ &- \Gamma(c)\sin(\pi b)\frac{\sin(\pi\varepsilon)}{\varepsilon}\sum_{n=0}^{\infty}\frac{(a)_{n}(a-c+1)_{n}f_{3}^{VI}(0;n)f_{4}^{VI}(\varepsilon;n)f_{5}^{VI}(0;n)}{\Gamma(b)\Gamma(c-a)} \\ &+ \Gamma(c)\cos(\pi b)(-1)^{k}\sum_{n=0}^{\infty}\left\{(a)_{n}f_{2}^{VI}(\varepsilon;n)f_{3}^{VI}(0;n)f_{4}^{VI}(\varepsilon;n)f_{5}^{VI}(0;n)f_{6}^{VI}(\varepsilon)g_{7}^{VI}(\varepsilon)\right\} \end{split}$$

$$-g_{1}^{VI}(\varepsilon;n)f_{2}^{VI}(\varepsilon;n)f_{3}^{VI}(0;n)f_{4}^{VI}(\varepsilon;n)f_{5}^{VI}(0;n)f_{6}^{VI}(\varepsilon) +f_{1}^{VI}(\varepsilon;n)g_{2}^{VI}(\varepsilon;n)f_{3}^{VI}(0;n)f_{4}^{VI}(\varepsilon;n)f_{5}^{VI}(0;n)f_{6}^{VI}(\varepsilon) -f_{1}^{VI}(\varepsilon;n)f_{2}^{VI}(0;n)g_{3}^{VI}(\varepsilon;n)f_{4}^{VI}(\varepsilon;n)f_{5}^{VI}(0;n)f_{6}^{VI}(\varepsilon) +f_{1}^{VI}(\varepsilon;n)f_{2}^{VI}(0;n)f_{3}^{VI}(\varepsilon;n)g_{4}^{VI}(\varepsilon;n)f_{5}^{VI}(0;n)f_{6}^{VI}(\varepsilon) -f_{1}^{VI}(\varepsilon;n)f_{2}^{VI}(0;n)f_{3}^{VI}(\varepsilon;n)f_{4}^{VI}(0;n)g_{5}^{VI}(\varepsilon;n)f_{6}^{VI}(\varepsilon) +f_{1}^{VI}(\varepsilon;n)f_{2}^{VI}(0;n)f_{3}^{VI}(\varepsilon;n)f_{4}^{VI}(0;n)g_{5}^{VI}(\varepsilon;n)f_{6}^{VI}(\varepsilon) +f_{1}^{VI}(\varepsilon;n)f_{2}^{VI}(0;n)f_{3}^{VI}(\varepsilon;n)f_{4}^{VI}(0;n)f_{5}^{VI}(\varepsilon;n)g_{6}^{VI}(\varepsilon) +(23)$$

with the imaginary part

$$\lim_{\delta \to 0^{+}} \operatorname{Im}_{2} F_{1}(a, b; c; z + i\delta) \\
= \Gamma(c) \sin(\pi b) \sum_{n=0}^{k-1} \frac{(b)_{n}(b - c + 1)_{n} \Gamma(k + \varepsilon - n)(-1)^{n} w^{n+b}}{\Gamma(a) \Gamma(c - b) n!} \\
+ \Gamma(c) \cos(\pi b) \frac{\sin(\pi \varepsilon)}{\varepsilon} \sum_{n=0}^{\infty} \frac{(a)_{n}(a - c + 1)_{n} f_{3}^{VI}(0; n) f_{4}^{VI}(\varepsilon; n) f_{5}^{VI}(0; n)}{\Gamma(b) \Gamma(c - a)} \\
+ \Gamma(c) \sin(\pi b)(-1)^{k} \sum_{n=0}^{\infty} \{(a)_{n} f_{2}^{VI}(\varepsilon; n) f_{3}^{VI}(0; n) f_{4}^{VI}(\varepsilon; n) f_{5}^{VI}(0; n) f_{6}^{VI}(\varepsilon) g_{7}^{VI}(\varepsilon) \\
- g_{1}^{VI}(\varepsilon; n) f_{2}^{VI}(\varepsilon; n) f_{3}^{VI}(0; n) f_{4}^{VI}(\varepsilon; n) f_{5}^{VI}(0; n) f_{6}^{VI}(\varepsilon) \\
+ f_{1}^{VI}(\varepsilon; n) g_{2}^{VI}(\varepsilon; n) f_{3}^{VI}(0; n) f_{4}^{VI}(\varepsilon; n) f_{5}^{VI}(0; n) f_{6}^{VI}(\varepsilon) \\
- f_{1}^{VI}(\varepsilon; n) f_{2}^{VI}(0; n) g_{3}^{VI}(\varepsilon; n) f_{4}^{VI}(\varepsilon; n) f_{5}^{VI}(0; n) f_{6}^{VI}(\varepsilon) \\
+ f_{1}^{VI}(\varepsilon; n) f_{2}^{VI}(0; n) f_{3}^{VI}(\varepsilon; n) f_{4}^{VI}(0; n) g_{5}^{VI}(\varepsilon; n) f_{6}^{VI}(\varepsilon) \\
- f_{1}^{VI}(\varepsilon; n) f_{2}^{VI}(0; n) f_{3}^{VI}(\varepsilon; n) f_{4}^{VI}(0; n) g_{5}^{VI}(\varepsilon; n) f_{6}^{VI}(\varepsilon) \\
+ f_{1}^{VI}(\varepsilon; n) f_{2}^{VI}(0; n) f_{3}^{VI}(\varepsilon; n) f_{4}^{VI}(0; n) g_{5}^{VI}(\varepsilon; n) g_{6}^{VI}(\varepsilon) \\
+ f_{1}^{VI}(\varepsilon; n) f_{2}^{VI}(0; n) f_{3}^{VI}(\varepsilon; n) f_{4}^{VI}(0; n) f_{5}^{VI}(\varepsilon; n) g_{6}^{VI}(\varepsilon) \right\}. \tag{24}$$

III. FORTRAN PROGRAM

The FORTRAN program for the hypergeometric function [6] has been written in the form of a subroutine called HYP. Some of the important programming details of HYP are given in this section.

A. Programming Details

The Pochhammer symbol is computed by the recursion relation

$$(x)_n = (x+n-1)(x)_{n-1}, (25)$$

with the starting point $(x)_0 = 1$. The terms of the hypergeometric series in the region of convergence can thus be computed recursively by applying (25) to (1) to obtain

$$\frac{(a)_n(b)_n z^n}{(c)_n n!} = \frac{(a+n-1)(b+n-1)z}{(c+n-1)n} \frac{(a)_{n-1}(b)_{n-1} z^{n-1}}{(c)_{n-1}(n-1)!},$$
(26)

with the initial condition $(a)_0(b)_0z^0/(c)_00! = 1$. These terms are calculated and summed in the subroutine HYPER. The number of terms needed to get good convergence is determined from the following algorithm [8]. Let the hypergeometric function be written in terms of the finite series expansion

$$_{2}F_{1}(a,b;c;z) = \sum_{n=0}^{N} \frac{(a)_{n}(b)_{n}z^{n}}{(c)_{n}n!}$$
 (27)

plus the remainder

$$R_N = \left[\frac{(a)_{N+1}(b)_{N+1} z^{N+1}}{(c)_{N+1}(N+1)!} \right] S_N, \tag{28}$$

where

$$S_N = \sum_{n=0}^{\infty} \frac{(a+N+1)_n(b+N+1)_n(N+1)!z^n}{(c+N+1)_n(N+n+1)!}.$$
 (29)

It is not difficult to show that

$$S_N \le \sum_{n=0}^{\infty} \frac{(\alpha + N + 1)_n (N+1)! z^n}{(N+n+1)!},\tag{30}$$

where

$$\alpha = \max(\alpha_0, \alpha_1),\tag{31}$$

with

$$\alpha_0 = \frac{(a+N+1)(b+N+1)}{(c+N+1)} - N - 1 \tag{32}$$

and

$$\alpha_1 = a + b - c. \tag{33}$$

After a few more manipulations, we can see that

$$R_N \le \frac{(a)_{N+1}(b)_{N+1}z^{N+1}}{(c)_{N+1}(k+1)_{N+1}(1-z)} \sum_{n=0}^k \frac{(N+k+1)!}{(N+k+1-n)!n!},\tag{34}$$

where

$$k = \operatorname{Int}[\max(\alpha_0, \alpha_1)]. \tag{35}$$

The series (27) is truncated when the remainder R_N is less than machine epsilon. A subroutine that determines machine epsilon is included in the code [6] in order to make it portable.

The transformation formulas used to calculate the hypergeometric function when z is not between 0 and $\frac{1}{2}$ involve gamma functions. Many programs exist for calculating the gamma function, but only for positive values of the argument. Thus it was necessary to write a more general gamma function routine, which would be portable and would allow for negative arguments. To do this, the expansions

$$\Gamma(x+1) = \sum_{k=0}^{26} c_k^I T_k(2x), \qquad -\frac{1}{2} \le x \le \frac{1}{2}$$
 (36)

$$\Gamma(x+1) = \sum_{k=0}^{26} c_k^{II} T_k(2x-1), \qquad 0 \le x \le 1$$
 (37)

$$\Gamma(x+1) = \sum_{k=0}^{26} c_k^{III} T_k(2x-2), \qquad \frac{1}{2} \le x \le \frac{3}{2}$$
 (38)

are needed, where $T_k(x)$ is a Tchebychev polynomial of the first kind which obeys the recurrence relation

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x). (39)$$

Clenshaw's recurrence formula [9] is applied to (37) with the coefficients c_k^H known to 20 significant digits [10] and tabulated in the program function G(X). If the argument of the gamma function is not in the range specified by (37), the program function GAMM(X) will either step up the argument using $\Gamma(x+1) = \Gamma(x+2)/(x+1)$ or step down the argument using $\Gamma(x+1) = x\Gamma(x)$ until the argument is in range. Once the argument is in range, GAMM calls G(X) which performs the Clenshaw recurrence. An important point to notice is that whenever $1/\Gamma(x)$ is needed, $1/\Gamma(x) = x/\Gamma(x+1)$ is used until the argument is greater than zero in order to handle any possible divergences of the gamma function. Once (37) has been calculated, it can be used to determine the unknown coefficients, c_k^I and c_k^{II} , in the other two expansions (36) and (38) which are needed when forming finite differences of gamma functions.

The majority of the program coding consists of the exceptional cases presented in Section IIB. The most tedious calculations are the finite differences of the form

$$g(\varepsilon) \equiv \left[\frac{1}{\Gamma(x+1+\varepsilon)} - \frac{1}{\Gamma(x+1)} \right] / \varepsilon. \tag{40}$$

If x > 1, we can write this as

$$g(\varepsilon) = \frac{-1}{\Gamma(x+1)\Gamma(x+1+\varepsilon)} \left[\frac{\Gamma(x+1+\varepsilon) - \Gamma(x+1)}{\varepsilon} \right]. \tag{41}$$

The gamma function arguments can be stepped down using the identity

$$\left[\frac{\Gamma(x+1+\varepsilon)-\Gamma(x+1)}{\varepsilon}\right] = \left[\frac{\Gamma(x+\varepsilon)-\Gamma(x)}{\varepsilon}\right]x + \Gamma(x+\varepsilon) \tag{42}$$

until x < 1. Applying (36), (37), and (38), we get

$$\left[\frac{\Gamma(x+1+\varepsilon)-\Gamma(x+1)}{\varepsilon}\right] = \sum_{k=0}^{26} c_k^I F_k^I(x) \tag{43}$$

when x is near zero,

$$\left[\frac{\Gamma(x+1+\varepsilon)-\Gamma(x+1)}{\varepsilon}\right] = \sum_{k=0}^{26} c_k^{II} F_k^{II}(x) \tag{44}$$

when x is in the middle of the range (0, 1), and

$$\left[\frac{\Gamma(x+1+\varepsilon)-\Gamma(x+1)}{\varepsilon}\right] = \sum_{k=0}^{26} c_k^{III} F_k^{III}(x)$$
 (45)

when x is near one, where

$$F_k^I(x) \equiv \frac{T_k(2(x+\varepsilon)) - T_k(2x)}{\varepsilon},\tag{46}$$

$$F_k^{II}(x) \equiv \frac{T_k(2(x+\varepsilon)-1) - T_k(2x-1)}{\varepsilon},\tag{47}$$

$$F_k^{III}(x) \equiv \frac{T_k(2(x+\varepsilon)-2) - T_k(2x-2)}{\varepsilon}.$$
 (48)

The recursion relations

$$F_k^I(x) = 4T_{k-1}(2(x+\varepsilon)) + (4x)F_{k-1}^I(x) - F_{k-2}^I(x), \tag{49}$$

$$F_k^{II}(x) = 4T_{k-1}(2(x+\varepsilon) - 1) + (4x - 2)F_{k-1}^{II}(x) - F_{k-2}^{II}(x), \tag{50}$$

$$F_k^{III}(x) = 4T_{k-1}(2(x+\varepsilon) - 2) + (4x - 4)F_{k-1}^{III}(x) - F_{k-2}^{III}(x)$$
 (51)

can be found, where the starting points are $T_0(x) = 1$, $T_1(x) = x$, $F_0^i(x) = 0$, and $F_1^i(x) = 2$ with i = I, III. The gamma function difference quotient can now be summed.

If x < 0, the gamma function arguments in (40) can be stepped up using the identity

$$g(\varepsilon) = \left[\frac{x+1+\varepsilon}{\Gamma(x+2+\varepsilon)} - \frac{x+1}{\Gamma(x+2)} \right] / \varepsilon$$

$$= \left[\frac{1}{\Gamma(x+2+\varepsilon)} - \frac{1}{\Gamma(x+2)} \right] \frac{x+1}{\varepsilon} + \frac{1}{\Gamma(x+2+\varepsilon)}$$
(52)

	1(, -,,	• ,	- (3)-3	
Case	z	N	Error	
I	1.2	38	5×10^{-15}	
I	1.4	31	1×10^{-16}	
I	1.6	26	1×10^{-15}	
I	1.8	23	1×10^{-16}	
I	2.0	21	4×10^{-16}	
II	0.2	9	3×10^{-16}	
II	0.4	15	1×10^{-16}	
II	0.6	22	6×10^{-16}	
II	0.8	31	1×10^{-16}	
II	1.0	43	3×10^{-16}	

TABLE II

Numerical Testing of the Hypergeometric Function Code Using the Identity ${}_2F_1(0.5, 1; 1.5; -z^2) = \tan^{-1}(z)/z$

until the arguments are in the proper range. Once in range, the term in brackets will look like

$$\left[\frac{1}{\Gamma(x'+1+\varepsilon)} - \frac{1}{\Gamma(x'+1)}\right] / \varepsilon = \frac{-1}{\Gamma(x'+1)\Gamma(x'+1+\varepsilon)} \left[\frac{\Gamma(x'+1+\varepsilon) - \Gamma(x'+1)}{\varepsilon}\right]$$
(53)

and the procedure outlined above for calculating the gamma function difference quotient can again be used. Further programming details are provided in Appendix B.

B. Numerical Testing

The program HYPTEST has been included in [6] for testing the hypergeometric function subroutine HYP using the identities:

$$_{2}F_{1}(.5, 1; 1.5; -z^{2}) = \tan^{-1}(z)/z$$
 (54)

$$_{2}F_{1}(1,1;2;z) = -\log(1-z)/z$$
 (55)

$$_{2}F_{1}(-a,b;b;-z) = (1+z)^{a}.$$
 (56)

Results of the tests are presented in Tables II–IV which indicate that the program is reliable to machine double precision. Extension to quadruple precision should be straightforward. The truncation number N is also given in Tables II–IV to indicate the efficiency of the code. In many cases, the value of N is larger than it needs to be since the algorithm (see Section IIIA) is very conservative.

The transformation equations of Section IIA were used with small values of ε to test the exceptional cases of Section IIB. Table V shows the deterioration in the numerical accuracy of the transformation equations (2), (4), (6), and (7) for

TABLE III

Numerical Testing of the Hypergeometric Function Code Using the Identity ${}_2F_1(1, 1; 2; z) = -\log(1 - z)/z$

Case	z	N	Error	
III	0.1	14	2×10^{-16}	
III	0.2	20	4×10^{-16}	
III	0.3	27	1×10^{-16}	
III	0.4	35	3×10^{-16}	
IV	0.5	60	1×10^{-15}	
IV	0.6	45	6×10^{-16}	
IV	0.7	35	1×10^{-16}	
IV	0.8	30	1×10^{-16}	
IV	0.9	20	2×10^{-16}	

 $_2F_1(1, 2 + \varepsilon; 3; z)$ as ε approaches zero. The finite difference results given in Section IIC provide the desired machine precision accuracy for such cases.

IV. CONCLUSION

We have described the details of a very efficient FORTRAN program designed to compute the hypergeometric function of a real variable for arbitrary real parameters. The transformation theory of the hypergeometric function was used to obtain rapidly convergent power series. The divergences that occur in the individual terms of the transformation for integer parameters were removed using a finite difference technique. Many of the methods used in the present work should be applicable to the more difficult problem of computing the hypergeometric function of a complex variable. Preliminary code for this extension can also be found in [6].

TABLE IV

Numerical Testing of the Hypergeometric Function Code Using the Identity $_2F_1(-a, b; b; -z) = (1 + z)^a$ for a = -5 and b = 1

Case	z	N	Error	
V	-1.2	10	3×10^{-16}	
V	-1.4	10	9×10^{-16}	
V	-1.6	10	8×10^{-16}	
V	-1.8	10	9×10^{-16}	
V	-2.0	10	1×10^{-16}	
VI	-2.2	65	1×10^{-16}	
VI	-2.4	60	3×10^{-16}	
VI	-2.6	55	1×10^{-16}	
VI	-2.8	50	4×10^{-16}	
VI	-3.0	45	6×10^{-16}	

TABLE V Numerical Roundoff Error in the Transformation Formulas of Section IIA for $_2F_1(1,\,2\,+\,\epsilon;\,3;\,z)$ as ϵ Approaches Zero

ε	z = -2	z = 0.7	z = 1.5	z = 3
10-1	4×10^{-14}	7×10^{-15}	1×10^{-15}	7×10^{-15}
10^{-2}	4×10^{-13}	4×10^{-16}	1×10^{-15}	2×10^{-13}
10^{-3}	5×10^{-12}	8×10^{-13}	2×10^{-13}	2×10^{-12}
10^{-4}	4×10^{-11}	1×10^{-11}	3×10^{-12}	2×10^{-11}
10^{-5}	5×10^{-10}	2×10^{-11}	7×10^{-12}	2×10^{-10}
10^{-6}	5×10^{-9}	5×10^{-10}	2×10^{-11}	2×10^{-9}
10^{-7}	5×10^{-8}	4×10^{-9}	3×10^{-10}	2×10^{-8}
10^{-8}	6×10^{-7}	3×10^{-9}	5×10^{-9}	2×10^{-7}
10^{-9}	5×10^{-6}	6×10^{-7}	5×10^{-8}	2×10^{-6}
10^{-10}	5×10^{-5}	8×10^{-6}	2×10^{-6}	7×10^{-6}
10-11	5×10^{-4}	5×10^{-5}	1×10^{-5}	9×10^{-5}
10^{-12}	5×10^{-3}	8×10^{-4}	1×10^{-4}	1×10^{-3}
10^{-13}	5×10^{-2}	6×10^{-3}	6×10^{-4}	4×10^{-3}
10^{-14}	5×10^{-1}	3×10^{-3}	2×10^{-3}	2×10^{-2}
10^{-15}	6×10^{-0}	3×10^{-2}	2×10^{-1}	1×10^{-1}

APPENDIX A: FUNCTION DEFINITIONS

Shown below are the definitions of the f-functions that are used to obtain the finite difference results of Section IIC

$$\begin{split} f_1^I(\varepsilon;n) &\equiv \frac{(a-k-\varepsilon)_{n+k}}{\Gamma(a)}, \\ f_2^I(\varepsilon;n) &\equiv \frac{(c-a+k+\varepsilon)_n}{\Gamma(c-a)}, \\ f_3^I(\varepsilon;n) &\equiv (-1)^{k+n}\varepsilon\Gamma(-k-n-\varepsilon), \\ f_4^I(\varepsilon;n) &\equiv (-1)^n\varepsilon\Gamma(-n+\varepsilon), \\ f_5^I(\varepsilon;n) &\equiv w^{a+n-\varepsilon}, \\ f_6^I(\varepsilon) &\equiv \frac{1}{\Gamma(a-k-\varepsilon)}, \\ f_7^I(\varepsilon) &\equiv \frac{1}{\Gamma(c-a+k+\varepsilon)}, \\ f_1^{IVa}(\varepsilon;n) &\equiv \frac{(a+k+\varepsilon)_n}{\Gamma(a)}, \\ f_2^{IVa}(\varepsilon;n) &\equiv \frac{(b+k+\varepsilon)_n}{\Gamma(b)} \\ f_3^{IVa}(\varepsilon;n) &\equiv (-1)^{k+n}\varepsilon\Gamma(-k-n-\varepsilon), \end{split}$$

$$\begin{split} f_{4}^{Va}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n+\varepsilon), \\ f_{5}^{IVa}(\varepsilon;n) &\equiv w^{k+n+\varepsilon}, \\ f_{6}^{IVa}(\varepsilon) &\equiv \frac{1}{\Gamma(a+k+\varepsilon)}, \\ f_{7}^{IVa}(\varepsilon) &\equiv \frac{1}{\Gamma(b+k+\varepsilon)}, \\ f_{1}^{IVb}(\varepsilon;n) &\equiv \frac{(a-k+\varepsilon)_{n+k}}{\Gamma(a)}, \\ f_{2}^{IVb}(\varepsilon;n) &\equiv \frac{(b-k+\varepsilon)_{n+k}}{\Gamma(b)}, \\ f_{3}^{IVb}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n-\varepsilon), \\ f_{4}^{IVb}(\varepsilon;n) &\equiv (-1)^{n+k}\varepsilon\Gamma(-k-n+\varepsilon), \\ f_{5}^{IVb}(\varepsilon;n) &\equiv w^{n+\varepsilon}, \\ f_{6}^{IVb}(\varepsilon) &\equiv \frac{1}{\Gamma(a-k+\varepsilon)}, \\ f_{7}^{IVb}(\varepsilon) &\equiv \frac{1}{\Gamma(b-k+\varepsilon)}, \\ f_{2}^{Va}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n+\varepsilon), \\ f_{3}^{Va}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n+\varepsilon), \\ f_{4}^{Va}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n+\varepsilon), \\ f_{5}^{Va}(\varepsilon;n) &\equiv \frac{1}{\Gamma(a+\varepsilon)}, \\ f_{5}^{Va}(\varepsilon;n) &\equiv \frac{1}{\Gamma(a+\varepsilon)}, \\ f_{1}^{Vb}(\varepsilon;n) &\equiv \frac{1}{\Gamma(a+\varepsilon)}, \\ f_{1}^{Vb}(\varepsilon;n) &\equiv \frac{1}{\Gamma(b-k-n+\varepsilon)}, \\ f_{2}^{Vb}(\varepsilon;n) &\equiv \frac{1}{\Gamma(b-k-n+\varepsilon)}, \\ f_{3}^{Vb}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n-\varepsilon), \\ f_{4}^{Vb}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n-\varepsilon), \\ f_{5}^{Vb}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n-\varepsilon), \\ f_{5}^{Vb}(\varepsilon;n) &\equiv (-1)^{n}\varepsilon\Gamma(-n-\varepsilon), \\ f_{5}^{Vb}(\varepsilon;n) &\equiv w^{n+\varepsilon}, \\ \end{cases}$$

$$f_{6}^{Vb}(\varepsilon) \equiv \cos(\pi\varepsilon),$$

$$f_{7}^{Vb}(\varepsilon) \equiv \frac{1}{\Gamma(a-k+\varepsilon)},$$

$$f_{1}^{VI}(\varepsilon;n) \equiv \frac{(b)_{k+n}}{\Gamma(a)},$$

$$f_{2}^{VI}(\varepsilon;n) \equiv \frac{(1-c+b+\varepsilon)_{k+n}}{\Gamma(c-b-\varepsilon)},$$

$$f_{3}^{VI}(\varepsilon;n) \equiv (-1)^{n}\varepsilon\Gamma(-n+\varepsilon),$$

$$f_{4}^{VI}(\varepsilon;n) \equiv (-1)^{n+k}\varepsilon\Gamma(-n-k-\varepsilon),$$

$$f_{5}^{VI}(\varepsilon;n) \equiv w^{a+n-\varepsilon},$$

$$f_{6}^{VI}(\varepsilon) \equiv \cos(\pi\varepsilon),$$

$$f_{7}^{VI}(\varepsilon) \equiv \frac{1}{\Gamma(a-k-\varepsilon)}.$$

APPENDIX B: FUNCTION EVALUATION

In the FORTRAN code for exceptional case I, called FIX1, the functions $f_1^I(\varepsilon; n)$ and $f_2^I(\varepsilon; n)$ are calculated using the Pochhammer recursion (25) while the functions $f_3^I(\varepsilon; n)$ and $f_4^I(\varepsilon; n)$ are calculated recursively using the formulas

$$f_3'(\varepsilon; n) = \frac{f_3'(n-1)}{k+n+\varepsilon}$$
 (B1)

and

$$f_4^I(\varepsilon; n) = \frac{f_4^I(n-1)}{n-\varepsilon},\tag{B2}$$

starting at

$$f_3^I(\varepsilon; -k) = -\Gamma(1 - \varepsilon)$$
 (B3)

and

$$f_4^I(\varepsilon;0) = \Gamma(1+\varepsilon).$$
 (B4)

The g functions are calculated as

$$g_1^I(\varepsilon;n) = \frac{1}{\Gamma(a)} \left[\frac{(a-k-\varepsilon)_{n+k} - (a-k)_{n+k}}{\varepsilon} \right]$$
$$= (a-\varepsilon+n-1)g_1^I(\varepsilon;n-1) - \frac{(a-k)_{n+k-1}}{\Gamma(a)}, \tag{B5}$$

$$g_2^I(\varepsilon; n) = \frac{1}{\Gamma(c-a)} \left[\frac{(c-a+k+\varepsilon)_n - (c-a+k)_n}{\varepsilon} \right]$$
$$= (c-a+k+\varepsilon+n-1)g_2^I(\varepsilon; n-1) + \frac{(c-a+k)_{n-1}}{\Gamma(c-a)}, \tag{B6}$$

$$g_3^I(\varepsilon;n) = \frac{g_3^I(\varepsilon;n-1)}{k+n+\varepsilon} - \frac{f_3^I(0;n-1)}{(k+n)(k+n+\varepsilon)}$$
$$= \frac{g_3^I(\varepsilon;n-1)}{k+n+\varepsilon} + \frac{1}{(k+n+\varepsilon)(k+n)!},$$
(B7)

$$g_4^I(\varepsilon;n) = \frac{g_4^I(\varepsilon;n-1)}{n-\varepsilon} + \frac{f_4^I(0;n-1)}{n(n-\varepsilon)}$$
$$= \frac{g_4^I(\varepsilon;n-1)}{n-\varepsilon} + \frac{1}{(n-\varepsilon)n!},$$
(B8)

$$g_5^I(\varepsilon; n) = wg_5^I(\varepsilon; n - 1), \tag{B9}$$

with the starting points:

$$\begin{split} g_1^I(\varepsilon;-k) &= 0, \\ g_2^I(\varepsilon;0) &= 0, \\ g_3^I(\varepsilon;-k) &= -\frac{\Gamma(1-\varepsilon) - \Gamma(1)}{\varepsilon}, \\ g_4^I(\varepsilon;0) &= \frac{\Gamma(1+\varepsilon) - \Gamma(1)}{\varepsilon}, \\ g_5^I(\varepsilon;0) &= \frac{w^{a-\varepsilon} - w^a}{\varepsilon}. \end{split}$$

The starting points, $g_3^I(\varepsilon; -k)$ and $g_4^I(\varepsilon; 0)$, are calculated using (43) while the remaining g functions, $g_6^I(\varepsilon)$ and $g_7^I(\varepsilon)$, are calculated by the method outlined beginning with Eq. (40).

The FORTRAN code for exceptional case IV was divided into two subroutines called FIX4A and FIX4B corresponding to (9) and (10), respectively. In FIX4A, the functions $f_1^{IVa}(\varepsilon;n)$ and $f_2^{IVa}(\varepsilon;n)$ are calculated using (25) while $f_3^{IVa}(\varepsilon;n)$ and $f_4^{IVa}(\varepsilon;n)$ are calculated using the formulas

$$f_3^{IVa}(\varepsilon;n) = \frac{f_3^{IVa}(n-1)}{k+n+\varepsilon}$$
 (B10)

and

(B18)

$$f_4^{IVa}(\varepsilon;n) = \frac{f_4^{IVa}(n-1)}{n-\varepsilon},\tag{B11}$$

starting at

$$f_3^{IVa}(\varepsilon; -k) = -\Gamma(1 - \varepsilon)$$
 (B12)

and

$$f_4^{IVa}(\varepsilon;0) = \Gamma(1+\varepsilon). \tag{B13}$$

The g functions are calculated as

$$g_{1}^{IVa}(\varepsilon;n) = \frac{1}{\Gamma(a)} \left[\frac{(a+k+\varepsilon)_{n} - (a+k)_{n}}{\varepsilon} \right]$$

$$= (a+k+\varepsilon+n-1)g_{1}^{IVa}(\varepsilon;n-1) + \frac{(a+k)_{n-1}}{\Gamma(a)}, \qquad (B14)$$

$$g_{2}^{IVa}(\varepsilon;n) = \frac{1}{\Gamma(b)} \left[\frac{(b+k+\varepsilon)_{n} - (b+k)_{n}}{\varepsilon} \right]$$

$$= (b+k+\varepsilon+n-1)g_{2}^{IVa}(\varepsilon;n-1) + \frac{(b+k)_{n-1}}{\Gamma(b)}, \qquad (B15)$$

$$g_{3}^{IVa}(\varepsilon;n) = \frac{g_{3}^{IVa}(\varepsilon;n-1)}{k+n+\varepsilon} - \frac{f_{3}^{IVa}(0;n-1)}{(k+n)(k+n+\varepsilon)}$$

$$= \frac{g_{3}^{IVa}(\varepsilon;n-1)}{k+n+\varepsilon} + \frac{1}{(k+n+\varepsilon)(k+n)!}, \qquad (B16)$$

$$g_{4}^{IVa}(\varepsilon;n) = \frac{g_{4}^{IVa}(\varepsilon;n-1)}{n-\varepsilon} + \frac{f_{4}^{IVa}(0;n-1)}{n(n-\varepsilon)}$$

$$= \frac{g_{4}^{IVa}(\varepsilon;n-1)}{n-\varepsilon} + \frac{1}{(n-\varepsilon)n!}, \qquad (B17)$$

$$g_{5}^{IVa}(\varepsilon;n) = wg_{5}^{IVa}(\varepsilon;n-1), \qquad (B18)$$

with the starting points:

$$\begin{split} g_1^{IVa}(\varepsilon;0) &= 0, \\ g_2^{IVa}(\varepsilon;0) &= 0, \\ g_3^{IVa}(\varepsilon;-k) &= -\frac{\Gamma(1-\varepsilon) - \Gamma(1)}{\varepsilon}, \\ g_4^{IVa}(\varepsilon;0) &= \frac{\Gamma(1+\varepsilon) - \Gamma(1)}{\varepsilon}, \\ g_5^{IVa}(\varepsilon;0) &= \frac{w^{k+\varepsilon} - w^k}{\varepsilon}. \end{split}$$

The starting points, $g_3^{IVa}(\varepsilon; -k)$ and $g_7^{IVa}(\varepsilon; 0)$, are calculated using (43) while the remaining g functions, $g_6^{IVa}(\varepsilon)$ and $g_7^{IVa}(\varepsilon)$, are calculated by the method outlined, beginning with Eq. (40).

In FIX4B, the functions $f_1^{IVb}(\varepsilon; n)$ and $f_2^{IVb}(\varepsilon; n)$ are calculated using (25) while $f_3^{IVb}(\varepsilon; n)$ and $f_4^{IVb}(\varepsilon; n)$ are calculated using the formulas

$$f_3^{IVb}(\varepsilon;n) = \frac{f_3^{IVb}(n-1)}{n+\varepsilon}$$
 (B19)

and

$$f_4^{IVb}(\varepsilon;n) = \frac{f_4^{IVb}(n-1)}{k+n-\varepsilon},\tag{B20}$$

starting at

$$f_3^{IVb}(\varepsilon;0) = -\Gamma(1-\varepsilon) \tag{B21}$$

and

$$f_4^{IVb}(\varepsilon; -k) = \Gamma(1+\varepsilon).$$
 (B22)

The g functions are calculated as

$$g_1^{IVb}(\varepsilon;n) = \frac{1}{\Gamma(a)} \left[\frac{(a-k+\varepsilon)_{k+n} - (a-k)_{k+n}}{\varepsilon} \right]$$
$$= (a+\varepsilon+n-1)g_1^{IVb}(\varepsilon;n-1) + \frac{(a-k)_{k+n-1}}{\Gamma(a)}, \tag{B23}$$

$$g_2^{IVb}(\varepsilon;n) = \frac{1}{\Gamma(b)} \left[\frac{(b-k+\varepsilon)_{k+n} - (b-k)_{k+n}}{\varepsilon} \right]$$

$$= (b + \varepsilon + n - 1)g_2^{IVb}(\varepsilon; n - 1) + \frac{(b - k)_{k+n-1}}{\Gamma(b)},$$
 (B24)

$$g_{3}^{IVb}(\varepsilon;n) = \frac{g_{3}^{IVb}(\varepsilon;n-1)}{n+\varepsilon} + \frac{1}{(n+\varepsilon)n!},$$
(B25)

$$g_4^{IVb}(\varepsilon;n) = \frac{g_4^{IVb}(\varepsilon;n-1)}{k+n-\varepsilon} + \frac{1}{(k+n-\varepsilon)(k+n)!},$$
 (B26)

$$g_5^{IVb}(\varepsilon; n) = wg_5^{IVb}(\varepsilon; n - 1), \tag{B27}$$

with the starting points:

$$\begin{split} g_1^{IVb}(\varepsilon;-k) &= 0, \\ g_2^{IVb}(\varepsilon;-k) &= 0, \\ g_3^{IVb}(\varepsilon;0) &= -\frac{\Gamma(1-\varepsilon) - \Gamma(1)}{\varepsilon}, \\ g_4^{IVb}(\varepsilon;-k) &= \frac{\Gamma(1+\varepsilon) - \Gamma(1)}{\varepsilon}, \\ g_5^{IVb}(\varepsilon;0) &= \frac{w^\varepsilon - 1}{\varepsilon}. \end{split}$$

The starting points, $g_3^{IVb}(\varepsilon; 0)$ and $g_4^{IVb}(\varepsilon; -k)$, are calculated using (43) while the remaining g functions, $g_6^{IVb}(\varepsilon)$ and $g_7^{IVb}(\varepsilon)$, are calculated by the method outlined beginning with Eq. (40).

The FORTRAN code for exceptional case V was divided into two subroutines called FIX5A and FIX5B in analogy to case IV. In FIX5A, the function $f_1^{Va}(\varepsilon; n)$ is calculated using (25) while the functions $f_3^{Va}(\varepsilon; n)$ and $f_4^{Va}(\varepsilon; n)$ are found by noticing that $f_3^{Va}(\varepsilon; n) = f_4^{IVa}(\varepsilon; n)$ and $f_4^{Va}(\varepsilon; n) = f_3^{IVa}(\varepsilon; n)$. The g functions are calculated as follows:

$$g_{1}^{Va}(\varepsilon;n) = \frac{1}{\Gamma(c-b)} \left[\frac{(c-b-k-\varepsilon)_{k+n}}{\Gamma(b-n+\varepsilon)} - \frac{(c-b-k)_{k+n}}{\Gamma(b-n)} \right] \frac{1}{\varepsilon}$$

$$= \frac{1}{\Gamma(c-b)} \left\{ \left[\frac{1}{\Gamma(b-n+\varepsilon)} - \frac{1}{\Gamma(b-n)} \right] \frac{(c-b-k-\varepsilon)_{k+n}}{\varepsilon} + \left[\frac{(c-b-k-\varepsilon)_{k+n} - (c-b-k)_{k+n}}{\varepsilon} \right] \frac{1}{\Gamma(b-n)} \right\}, \quad (B28)$$

$$g_2^{Va}(\varepsilon) = \frac{\cos(\pi\varepsilon) - 1}{\varepsilon},$$
 (B29)

$$g_3^{Va}(\varepsilon;n) = g_4^{IVa}(\varepsilon;n),$$
 (B30)

$$g_4^{Va}(\varepsilon;n) = g_3^{IVa}(\varepsilon;n),$$
 (B31)

$$g_5^{Va}(\varepsilon;n) = wg_5^{IVa}(\varepsilon;n-1). \tag{B32}$$

The quantities in brackets in the definition of $g_1^{Va}(\varepsilon; n)$ above are found in analogy with the previously discussed cases. The functions needed in FIX5B and FIX6 (the program name for exceptional case VI) are found in analogy with the functions discussed above.

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REFERENCES

- 1. H. E. Moses and R. T. Prosser, J. Math. Anal. Appl. 173, 390 (1993).
- 2. D. S. F. Crothers, J. Phys. B 18, 2893 (1985).
- 3. A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princteon Univ. Press, Princeton, NJ, 1957).
- 4. H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1977), p. 39.
- 5. R. C. Forrey and R. N. Hill, Ann. Phys. (N.Y.) 226, 88 (1993).
- 6. http://cfa-www.harvard.edu/~rcf/
- 7. A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 1.
- 8. R. N. Hill, unpublished.
- 9. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes*, 2nd ed. (Cambridge Univ. Press, Cambridge, 1992), Chap. 5.
- Y. L. Luke, Mathematical Functions and Their Approximations (Academic Press, New York, 1975),
 p. 3.