Analytic Evaluation of Two-Center STO Electron Repulsion Integrals via Ellipsoidal Expansion

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Received 25 October 2001; accepted 4 February 2002

DOI 10.1002/qua.10181

ABSTRACT: Extant analytic methods for evaluating two-center electron repulsion integrals in a Slater-type orbital (STO) basis using ellipsoidal coordinates and the Neumann expansion of $1/r_{12}$ have problems of numerical stability that are analyzed in detail using computer-assisted algebraic techniques. Some of these problems can be eliminated by use of procedures known in this field 40 years ago but seemingly forgotten now. Others can be removed by use of a formulation suitable for small values of the STO screening parameter. A recent attempt at such a formulation is corrected and extended in a way permitting its practical use. The main functions encountered in the integrations over the ellipsoidal coordinate of the range $1 \ldots \infty$ are Bessel functions or generalizations thereof, as pointed out here for the first time. This fact is used to motivate the derivation of recurrence relations additional to those previously known. Novel techniques were devised for using these recurrence relations, thereby providing new ways of calculating the quantities that enter the ellipsoidal expansion. The convergence rate of this expansion and the numerical characteristics of several computational strategies are reported in enough detail to identify the ranges where various schemes can be used. This information shows that recent discussions of the "convergence characteristics of [the] ellipsoidal coordinate expansion" are in fact not that, but are instead discussions of an inability to make accurate calculations of the individual terms of the expansion. It is also seen that the parameter range suitable for use of Kotani's well-known recursive scheme is more limited than seems generally believed. The procedures discussed in this work are capable of yielding accurate two-center electron repulsion integrals by the ellipsoidal expansion method for all reasonable STO screening parameters, and have been implemented in illustrative public-domain computer programs. Int J Quantum Chem 88: 701–734, 2002

Key words: molecular integrals; Slater orbitals; ellipsoidal expansion

Introduction

Evaluation of two-electron integrals involving Slater-type orbitals (STOs) has been a subject of systematic study ever since the landmark papers of Roothaan [1], Ruedenberg [2], and Barnett and Coulson [3] were published in 1951 and the tables by Kotani et al. [4] appeared in 1955. The present author contributed to this effort with an article, published in 1960 [5], showing how all the integrals needed for diatomic molecule energy calculations could be formulated in a numerically stable fashion using ellipsoidal coordinates and the Neumann expansion of $1/r_{12}$. Shortly after the publication of the first edition of Kotani's book, an article by Corbató [6] showed that the integrals known as $B_n(x)$ could be written as finite expansions of the modified spherical Bessel functions $i_n(x)$, giving the coefficients of the expansions and showing how the $i_n(x)$ could be generated accurately and efficiently for small x by an inverse iteration procedure now known in the applied mathematics community as a "Miller algorithm" [7]. The present author's 1960 article showed that for the electron repulsion integrals the integrations with respect to η (the ellipsoidal coordinate with range $-1 \ldots 1$) could be identified as modified spherical Bessel functions, enabling application of the known methods for their evaluation. That article also showed how all the electron repulsion integrals could be computed together in a coordinated fashion in which most of the computational effort scaled as N^2 (where N is the size of the basis set), rather than as N^4.

The scheme we used in 1960 involved a manipulation of the electron repulsion integral into a symmetrical form, at the cost of an additional, but stable numerical integration. This formulation yielded all the integrals at the accuracies needed to support configuration interaction calculations on diatomic molecules involving up to hundreds of configurations, and, in the computer program we called DIATOM, produced a large number of published results in several dozen articles over a period in excess of 20 years [8]. We are now revisiting the integral evaluation because of a need to generalize for complex scaling applications, in which complex exponents will introduce oscillatory behavior and therewith instabilities in the numerical integration. Our present interests demand a stable and completely analytic method.

In examining the work since 1960 on analytic methods for evaluating diatomic STO integrals, we note that much that was common knowledge 40 years ago seems no longer to be known. Worse, there is a pervasive lack of distinction of the difference between issues of convergence of an expansion and those related to an ability to evaluate its individual terms. We further observe that it is meaningless to give serious consideration to methods unless they are carried out in ways that provide the accuracy needed for significant use, which in the context of current applications certainly requires errors in individual integrals to be smaller than 10^{-8} hartree. One example illustrating these problems (and this is only one of many by a variety of authors) is a recent article [9] whose title refers to "complementary convergence characteristics of ellipsoidal coordinate and zeta-function expansions." The authors show several integrals calculated using the Neumann expansion, claiming them to be typical of all integrals evaluated by that method. The accompanying discussion states that the expansion converges up to a certain point and then diverges. We add here the observation that the point of optimum apparent convergence is often still at an error too large to be acceptable. What is actually occurring is that when using the "standard" methods of evaluation the successive terms of the expansion are evaluated with decreasing accuracy, eventually being inaccurate even as to order of magnitude. In contrast, our experience with DIATOM, in which we routinely kept as many as 20 terms of the Neumann expansion, gives no indication of an inherent convergence problem.

It is thus clear that a route to the successful use of the Neumann expansion in a completely analytic method must involve the finding of more stable ways of computing its individual terms, and such a development should precede a comparison of ellipsoidal coordinate methods with other methods. A partially successful contribution in this direction is provided in an article by Maslen and Trefry [10], in which they develop what they called a generalized hypergeometric function expansion of the key integral arising from the integration over ξ (the ellipsoidal coordinate of range $1 \ldots \infty$). Unfortunately, their contribution is marred by errors in almost all its working formulas and by a failure to identify various quantities as known functions. There are also numerical instabilities that it leaves unidentified and unaddressed. Nevertheless, these authors provide the main insight into STO integral evaluation gained in the last three decades. Their article also contains an admirable bibliography (lacking only a few items lost in the sands of time), and

provides a good starting point for some of the analysis of the present work.

For practical integral evaluation it is desirable to use recursive methods, especially when they connect quantities all of which will be used. We shall show that the quantities arising in the integrations over ξ are related to Bessel functions, and this fact signals the existence of recurrence formulas additional to those known in the 1950s [1, 2, 4]. We derive and analyze the use of such formulas, comparing them with the historic method of Kotani et al. [4], in the course thereof finding a novel technique for the avoidance of numerical instability.

Analytic methods alternative to the ellipsoidal coordinate expansion include the "zeta-function" expansion of Barnett and Coulson [3], and special methods for Coulomb integrals [1], one of which (almost never cited) was an approach in which those integrals were obtained efficiently as finite linear combinations of overlap and nuclear attraction integrals [11]. It should be noted that, concurrently with the present study, Barnett has again focused attention on the single-center expansion method. His current work is available electronically in preprint form [12].

In the remainder of this article we present analytic formulas that can lead to accurate STO electron repulsion integral evaluations based on the Neumann expansion, and give graphs and numerical data illustrating the relevant computational issues. All the formulas have been programmed in Maple V [13] and are available on the World Wide Web [14] (thereby providing algorithms that have a chance of being error free). At this time we are not attempting a comparison with other analytic methods.

Definitions

We consider diatomic systems in which nuclei A and B are separated by a distance R and placed at positions $\mathbf{A} = (0, 0, -R/2)$, $\mathbf{B} = (0, 0, +R/2)$ of a Cartesian coordinate system. The electronic wave functions are described by STOs of the general form

$$\psi_a = (2\pi)^{-1/2} N_a r_a^{n_a-1} e^{-\zeta_a r_a} P_{l_a}^{|m_a|}(\cos\theta_a) e^{im_a\phi}, \quad (1)$$

where (r_a, θ_a, ϕ) are spherical polar coordinates about the center of ψ_a, with polar direction toward the origin along the z axis of the Cartesian system used for the nuclei, and with the same ϕ coordinate for all STOs. The associated Legendre functions P_l^m have the definitions given in the *Handbook of Mathematical Functions* [15], and N_a is the normalization constant

$$N_a = 2^{n_a}\zeta_a^{n_a+1/2}\left(\frac{(2l_a+1)(l_a-|m_a|)!}{(2n_a)!(l_a+|m_a|)!}\right)^{1/2}. \quad (2)$$

Electron repulsion integrals, identified using Mulliken notation, are of the form

$$[ab|cd] = \int \psi_a^*(\mathbf{r}_1)\psi_b(\mathbf{r}_1)\left(\frac{1}{r_{12}}\right)\psi_c^*(\mathbf{r}_2)\psi_d(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2. \quad (3)$$

To use prolate ellipsoidal coordinates (ξ, η, ϕ), where $1 \le \xi < \infty$, $-1 \le \eta \le 1$, $0 \le \phi < 2\pi$, and

$$d\mathbf{r} = \left(\frac{R}{2}\right)^3 (\xi^2 - \eta^2) d\xi d\eta d\phi, \quad (4)$$

we introduce (for STO ψ_a)

$$r_a = \frac{R}{2}(\xi + \kappa_a\eta), \quad (5)$$

$$\cos\theta_a = \frac{1 + \kappa_a\xi\eta}{\xi + \kappa_a\eta}, \quad (6)$$

where κ_a is $+1$ if ψ_a is on nucleus A and -1 if it is on nucleus B. The charge distribution $\psi_a^*(\mathbf{r}_1)\psi_b(\mathbf{r}_1)$ can then be written (including factors arising from the volume element)

$$\left(\frac{R}{2}\right)^3 \psi_a^*\psi_b(\xi_1^2 - \eta_1^2) = \frac{K_{ab}}{2\pi}\Xi_1(\xi_1, \eta_1)e^{-\alpha_1\xi_1 - \beta_1\eta_1} \times [(\xi_1^2 - 1)(1 - \eta_1^2)]^{|M_1|/2} e^{iM_1\phi}, \quad (7)$$

where $\alpha_1 = (R/2)(\zeta_a + \zeta_b)$, $\beta_1 = (R/2)(\kappa_a\zeta_a + \kappa_b\zeta_b)$, $K_{ab} = N_a N_b (R/2)^{n_a+n_b+1}$, $M_1 = m_b - m_a$, and Ξ_1 is a polynomial in its arguments:

$$\Xi_1(\xi_1, \eta_1) = \sum_{p=0}^{\Gamma_1}\sum_{q=0}^{\Gamma_1} C_1(p, q)\xi_1^p\eta_1^q. \quad (8)$$

We are following a convention adopted by Maslen and Trefry in which sets of constant coefficients are indicated by appropriately indexed script letters. The coefficients $C_1(p, q)$ depend on the locations and quantum numbers of ψ_a and ψ_b and $\Gamma_1 = n_a +$

$n_b - |M_1|$. Similar expressions, with subscripts a, b, and 1 replaced, respectively, by c, d, and 2, describe $\psi_c^*(\mathbf{r}_2)\psi_d(\mathbf{r}_2)$. A simple way of obtaining the $C_i(p, q)$ is presented in Appendix A.

The Neumann expansion for $1/r_{12}$ is

$$\frac{1}{r_{12}} = \frac{2}{R}\sum_{\mu=0}^{\infty}\sum_{\sigma=-\mu}^{\mu}(-1)^{\sigma}(2\mu+1)\left[\frac{(\mu-|\sigma|)!}{(\mu+|\sigma|)!}\right]^2 \times P_\mu^{|\sigma|}(\xi_<)Q_\mu^{|\sigma|}(\xi_>)P_\mu^{|\sigma|}(\eta_1)P_\mu^{|\sigma|}(\eta_2)e^{i\sigma(\phi_1-\phi_2)}, \quad (9)$$

where $\xi_>$ and $\xi_<$ are, respectively, the larger and smaller of ξ_1 and ξ_2 and P_μ^σ and Q_μ^σ are associated Legendre functions as defined in the Ref. [15] for their respective argument ranges (it matters whether the argument is within or outside the range $-1 \ldots 1$).

Preliminary Reduction

Insertion of the Neumann expansion into $[ab|cd]$, use of the notations of the preceding section, and integrating over ϕ_1 and ϕ_2, we reach

$$[ab|cd] = \frac{8}{R}K_{ab}K_{cd}\delta(M_1, -M_2) \times (-1)^{\sigma}\sum_{p_1,q_1}\sum_{p_2,q_2}C_1(p_1, q_1)C_2(p_2, q_2) \times \sum_{\mu=\sigma}^{\infty}(2\mu+1)i_\mu^\sigma(q_1, \beta_1)i_\mu^\sigma(q_2, \beta_2) \times W_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2), \quad (10)$$

where $\delta(i, j)$ is the Kronecker delta and $\sigma = |M_1| = |M_2|$. For the remainder of this article, it is to be understood that $\sigma \geq 0$, and many of the formulas to follow are only valid in that regime. The new quantities appearing in Eq. (10) are

$$i_\mu^\sigma(q, \beta) = \frac{(-1)^\mu}{2}\frac{(\mu-\sigma)!}{(\mu+\sigma)!} \times \int_{-1}^{1}d\eta P_\mu^\sigma(\eta)(1-\eta^2)^{\sigma/2}\eta^q e^{-\beta\eta}, \quad (11)$$

$$W_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2) = w_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2) + w_\mu^\sigma(p_2, p_1, \alpha_2, \alpha_1), \quad (12)$$

$$w_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2) = \int_1^\infty d\xi_1 Q_\mu^\sigma(\xi_1) \times (\xi_1^2-1)^{\sigma/2}\xi_1^{p_1}e^{-\alpha_1\xi_1} \times \int_1^{\xi_1}d\xi_2 P_\mu^\sigma(\xi_2) \times (\xi_2^2-1)^{\sigma/2}\xi_2^{p_2}e^{-\alpha_2\xi_2}. \quad (13)$$

The notation i_μ^σ in Eq. (11) was selected because this quantity is a direct generalization of the modified spherical Bessel function i_μ (defined on p. 469 of Ref. [15]). To avoid future confusion, we observe at this time that the quantity $P_\mu^\sigma(x)(1-x^2)^{\sigma/2}$, using the definition of P_μ^σ for the range $-1 \ldots 1$, is equal to $P_\mu^\sigma(x)(x^2-1)^{\sigma/2}$ when the definition of P_μ^σ is for the range outside $-1 \ldots 1$.

Eq. (10) is convergent for all physically relevant α_i and β_i ($\alpha_i > 0$, $|\beta_i| \leq \alpha_i$), but the rate of convergence will depend on the parameter values. Its numerical stability depends only upon the algorithms used to evaluate the i_μ^σ and W_μ^σ.

Eta Integration

As indicated in the Introduction, efficient methods for the integrals of Eq. (11) have been known since 1960 [5], and it is therefore possible to avoid the awkward discussions for small β advanced by some authors or the rejection of the ellipsoidal expansion advocated by others for that regime. In fact, the smaller the values of β_1 and β_2, the faster the Neumann expansion converges, in the limit $\beta_1 = 0$ or $\beta_2 = 0$ reducing to a finite number of terms. We write formulas here only to keep the presentation more or less self-contained.

The starting point of this section is the following integral representation for the modified spherical Bessel function $i_\mu(\beta)$:

$$i_\mu(\beta) = \frac{(-1)^\mu}{2}\int_{-1}^{1}P_\mu(\eta)e^{-\beta\eta}d\eta. \quad (14)$$

We thus see that $i_\mu^0(0, \beta) = i_\mu(\beta)$.

The Bessel functions $i_\mu(\beta)$ can be generated using the recurrence formula

$$i_{\mu-1}(\beta) - i_{\mu+1}(\beta) = \frac{2\mu+1}{\beta}\, i_\mu(\beta) \qquad (15)$$

and the values $i_0(\beta) = \sinh\beta/\beta$, $i_{-1}(\beta) = \cosh\beta/\beta$. However, the recurrence formula is unstable when used to increase the value of μ, the instability becoming significant when $\mu > |\beta|$. When upward recursion is unsatisfactory, it is then advisable to employ downward recursion, carried out by defining $r_\mu = i_{\mu+1}/i_\mu$, recasting the recurrence formula as

$$r_{\mu-1} = \frac{\beta}{2\mu + 1 + \beta r_\mu}, \qquad (16)$$

and starting with the approximate value $r_N = 0$ for a sufficiently large N. The r_μ improve in accuracy as μ decreases, at a rate that is faster for smaller $|\beta|$. After r_0 is reached, one can start from the explicit formula for i_0 and calculate $i_1 = r_0 i_0$, $i_2 = r_1 i_1$, etc. The value chosen for N must be large enough to yield all the i_μ to be actually used at sufficient accuracy.

The $i^\sigma_\mu(q, \beta)$ for positive σ and/or q may now be obtained by inserting recurrence formulas for the Legendre functions into Eq. (11). This procedure does not generate significant numerical instability. The relevant formulas are

$$i^\sigma_\mu(q+1, \beta) = -\frac{(\mu+\sigma+1) i^\sigma_{\mu+1}(q, \beta) + (\mu-\sigma) i^\sigma_{\mu-1}(q, \beta)}{2\mu+1}, \qquad (17)$$

$$i^\sigma_\mu(q, \beta) = \frac{i^{\sigma-1}_{\mu-1}(q, \beta) - i^{\sigma-1}_{\mu+1}(q, \beta)}{2\mu+1}. \qquad (18)$$

The quantity $(\mu - \sigma) i^\sigma_{\mu-1}(q, \beta)$ in Eq. (17) is replaced by zero when $\sigma = \mu$. These formulas are stable and generate no singularities even at $\beta = 0$. When β is nonzero, an alternate way of advancing the parameter σ is via the formula [5]

$$i^\sigma_\mu(0, \beta) = \beta^{-\sigma} i^0_\mu(0, \beta). \qquad (19)$$

It is also possible to write power series expansions for the i^σ_μ. The starting point is formula 10.2.5 of Ref. [15]. In our current notation, it is

$$i^0_\mu(0, \beta) = \sum_{k=0}^{\infty} \frac{\beta^{\mu+2k}}{(2\mu+2k+1)!!(2k)!!}. \qquad (20)$$

Applying Eq. (19), we see that

$$i^\sigma_\mu(0, \beta) = \sum_{k=0}^{\infty} \frac{\beta^{\mu-\sigma+2k}}{(2\mu+2k+1)!!(2k)!!}. \qquad (21)$$

Now, noting that $-\partial i^\sigma_\mu(q, \beta)/\partial\beta = i^\sigma_\mu(q+1, \beta)$, we may differentiate Eq. (21) to obtain

$$i^\sigma_\mu(q, \beta) = \sum_{k=k_0}^{\infty} \frac{(-1)^q (\mu-\sigma+2k)! \beta^{\mu-\sigma+2k-q}}{(2\mu+2k+1)!!(2k)!!(\mu-\sigma+2k-q)!}, \qquad (22)$$

where k_0 is the smallest nonnegative integer such that $2k_0 > q - \mu + \sigma - 1$, a condition arising because $\partial\beta^n/\partial\beta = 0$ when $n = 0$. This condition is only necessary if Eq. (22) is used computationally in an environment that cannot accept $n!$ for negative integer n in a denominator. Formally one may set $k_0 = 0$. These explicit formulas are not the most efficient way to obtain the i^σ_μ; the recurrence formulas are more suitable for that purpose. However, Eq. (22) will be useful in formal manipulations to be presented later in this study. It can be regarded as extending the definition of $i^\sigma_\mu(q, \beta)$ to negative q, for which the series converges while Eq. (11), the integral representation, does not.

Xi Integrations-Closed Expressions

The integrations of Eq. (13) over ξ_1 and ξ_2 can be reduced to closed form. We follow to some extent the definitions and notations of Maslen and Trefry [10], but with some adjustments to make relationships to known functions simpler and more explicit. It is convenient to use the following finite expansions, in which the coefficients $\mathcal{A}^{\mu\sigma}_s$ are nonzero only if $0 \le s \le \mu + \sigma$, with $\mu + \sigma - s$ even. The $\mathcal{B}^{\mu\sigma}_s$ are nonzero only if $0 \le s \le \mu + \sigma - 1$, with $\mu + \sigma - s$ odd. Here P^σ_μ and Q^σ_μ are defined for the range outside $-1 \ldots 1$.

$$\frac{(\mu-\sigma)!}{(\mu+\sigma)!} P^\sigma_\mu(\xi)(\xi^2-1)^{\sigma/2} = \sum_s \mathcal{A}^{\mu\sigma}_s \xi^s, \qquad (23)$$

$$\frac{(\mu-\sigma)!}{(\mu+\sigma)!} Q^\sigma_\mu(\xi)(\xi^2-1)^{\sigma/2} = \sum_s \mathcal{A}^{\mu\sigma}_s \xi^s Q_0(\xi) + \sum_s \mathcal{B}^{\mu\sigma}_s \xi^s. \qquad (24)$$

In these equations, Q_0 and the nonzero coefficients are [10]

$$Q_0(\xi) = \frac{1}{2}\log\left(\frac{\xi+1}{\xi-1}\right), \tag{25}$$

$$\mathcal{A}_s^{\mu\sigma} = (-1)^{(\mu+\sigma-s)/2}\frac{(\mu-\sigma+s-1)!!}{s!(\mu+\sigma-s)!!}, \tag{26}$$

$$\mathcal{B}_s^{\mu\sigma} = \sum_{j=0}^{(\mu+\sigma-s-1)/2}\frac{(-1)^{j+1}(2\mu-2j-1)!!}{(\mu+\sigma-s-2j)(\mu+\sigma-2j)!(2j)!!}. \tag{27}$$

We also define the auxiliary functions

$$L_\mu^\sigma(p,\alpha) = \frac{(\mu-\sigma)!}{(\mu+\sigma)!}\int_1^\infty Q_\mu^\sigma(\xi)(\xi^2-1)^{\sigma/2}\xi^p e^{-\alpha\xi}d\xi, \tag{28}$$

$$k_\mu^\sigma(p,\alpha) = \frac{(\mu-\sigma)!}{(\mu+\sigma)!}\int_1^\infty P_\mu^\sigma(\xi)(\xi^2-1)^{\sigma/2}\xi^p e^{-\alpha\xi}d\xi. \tag{29}$$

Here we have introduced k_μ^σ and given it that name because it is a (scaled) generalization of the modified spherical Bessel function $k_\mu(\alpha)$, defined on page 469 of Ref. [15].

Calculation of the $k_\mu^\sigma(p,\alpha)$ starts from the recognition that $k_\mu^0(0,\alpha) = (2/\pi)k_\mu(\alpha)$. The $k_\mu^0(0,\alpha)$ can be generated stably by upward recursion, using the well-known recurrence formula

$$k_{\mu+1}^0(0,\alpha) - k_{\mu-1}^0(0,\alpha) = \frac{2\mu+1}{\alpha}k_\mu^0(0,\alpha) \tag{30}$$

and the starting values $k_0^0(0,\alpha) = k_{-1}^0(0,\alpha) = e^{-\alpha}/\alpha$. The $k_\mu^\sigma(p,\alpha)$ for positive σ and/or p may be obtained in a satisfactory manner by inserting recurrence formulas for the Legendre functions into Eq. (29). The formulas are

$$k_\mu^\sigma(p+1,\alpha) = \frac{(\mu+\sigma+1)k_{\mu+1}^\sigma(p,\alpha) + (\mu-\sigma)k_{\mu-1}^\sigma(p,\alpha)}{2\mu+1}, \tag{31}$$

$$k_\mu^\sigma(p,\alpha) = \frac{k_{\mu+1}^{\sigma-1}(p,\alpha) - k_{\mu-1}^{\sigma-1}(p,\alpha)}{2\mu+1}. \tag{32}$$

We replace $(\mu-\sigma)k_{\mu-1}^\sigma(p,\alpha)$ in Eq. (31) by zero when $\sigma = \mu$.

The auxiliary functions $L_\mu^\sigma(p,\alpha)$ can be formally reduced to simpler functions by inserting the explicit formula for Q_μ^σ. The result is

$$L_\mu^\sigma(p,\alpha) = \sum_s \mathcal{A}_s^{\mu\sigma}L_0^0(p+s,\alpha) + \sum_s \mathcal{B}_s^{\mu\sigma}A_{p+s}(\alpha). \tag{33}$$

Here $A_n(\alpha)$ is the well-known function

$$A_n(\alpha) = \int_1^\infty x^n e^{-\alpha x}dx = \frac{n!e^{-\alpha}}{\alpha^{n+1}}\sum_{j=0}^n\frac{\alpha^j}{j!}. \tag{34}$$

The $A_n(\alpha)$ of nonzero n can be obtained by upward recursion using

$$A_{n+1}(\alpha) = \frac{n}{\alpha}A_n(\alpha) + A_0(\alpha) \tag{35}$$

and $A_0(\alpha) = e^{-\alpha}/\alpha$. Note also that the explicit formula of Eq. (34) extends the definition of $A_n(\alpha)$ to negative α, and that (as discussed further in Appendix C) the A_n are essentially incomplete gamma functions.

The remaining function, $L_0^0(p,\alpha)$, has a closed form, given (with a sign error) by Maslen and Trefry. Their formula, corrected and written in terms of the A_n, is

$$L_0^0(p,\alpha) = \frac{1}{2}\left((-1)^{p+1}E_1(2\alpha)A_p(-\alpha) + [\gamma+\log(2\alpha)]A_p(\alpha) + \frac{p!e^{-\alpha}}{\alpha^{p+1}}\sum_{t=1}^{p-1}\mathcal{L}_{pt}\frac{\alpha^t}{t!}\right). \tag{36}$$

Here E_1 is the exponential integral (as defined in Ref. [15]), γ is Euler's constant, and [10]

$$\mathcal{L}_{pt} = \sum_{j=0}^{p-1}\frac{1}{p-j}\sum_{l=l_1}^{l_2}(-1)^l 2^{t-l}\binom{t}{l} - \sum_{j=1}^{p-t}\frac{1}{j}, \tag{37}$$

where $l_1 = \max(t-p+j+1, 0)$ and $l_2 = \min(t, j)$. We also increased the lower limit of the t summa-

tion from the Maslen/Trefry value of zero because $\mathcal{L}_{p0}$ vanishes for all p. The summation limits in Eq. (37) appear to intertwine the dependence on p and t to a greater extent than is actually the case. A more convenient expression for $\mathcal{L}_{pt}$, obtained after some manipulation, is

$$\mathcal{L}_{pt}=\sum_{j=1}^{t}\left(\frac{1}{j+p-t}-\frac{1}{j}\right)\sum_{l=j}^{t}(-1)^{t-l}2^{l}\binom{t}{l}. \quad (38)$$

Using the auxiliary functions and the explicit form for P_{μ}^{σ}, one may obtain the result

$$w_{\mu}^{\sigma}(p_1, p_2, \alpha_1, \alpha_2) = \left[\frac{(\mu+\sigma)!}{(\mu-\sigma)!}\right]^2 \times\left[L_{\mu}^{\sigma}(p_1, \alpha_1)k_{\mu}^{\sigma}(p_2, \alpha_2) - \sum_{s}\mathcal{A}_{s}^{\mu\sigma} \times\sum_{j=0}^{p_2+s}\frac{(p_2+s)!}{j!\alpha_2^{p_2+s-j+1}}L_{\mu}^{\sigma}(p_1+j, \alpha_1+\alpha_2)\right]. \quad (39)$$

This formula differs in substance, as well as form, from the corresponding equation of Maslen and Trefry.

Convergence of the Neumann Expansion

The closed formulas presented in the three preceding sections are, as we shall shortly see, not optimum for numerical computation. However, in an environment with unlimited precision such as provided by Maple, they may be used to study the convergence rate of the Neumann expansion. From the convergence characteristics we may deduce the numerical behavior to be required of actual computational schemes.

In the equation arising from the Neumann expansion, Eq. (10), we approximate the infinite sum over μ by a finite sum to $\mu = \mu_{\max}$ and identify the minimum $\mu_{\max}$ that will yield a specified relative accuracy for various values of the parameters entering the summation. The criterion we actually used was that the largest term omitted from the summation be less than 1×10^{-12} times the largest term in the sum. This is a conservative criterion comparable to that used in Gaussian orbital calculations for the neglect of integrals, and will permit energy determinations to a fraction of a kJ per mole

TABLE I

Value of μ_{max} needed in the Neumann expansion to obtain relative accuracy of 1×10^{-12} in [*ab*|*cd*] for parameter values $\sigma = 0$, $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, and $p_1 = p_2 = q_1 = q_2 = 0$.

	α_2						
α_1	0.1	0.5	1.0	2.0	5.0	10.0	20.0
0.1	3	4	4	4	5	5	5
0.5		5	5	6	7	7	8
1.0			6	7	7	9	9
2.0				8	8	11	12
5.0					12	14	16
10.0						16	19
20.0							23

TABLE II

Value of μ_{max} needed in the Neumann expansion to obtain relative accuracy of 1×10^{-12} in [*ab*|*cd*] for parameter values $\sigma = 4$, $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, and $p_1 = p_2 = q_1 = q_2 = 0$.

	α_2						
α_1	0.1	0.5	1.0	2.0	5.0	10.0	20.0
0.1	7	7	8	8	9	9	10
0.5		9	9	10	11	12	12
1.0			10	11	12	13	14
2.0				12	14	15	17
5.0					16	19	21
10.0						23	25
20.0							29

TABLE III

Value of μ_{max} needed in the Neumann expansion to obtain relative accuracy of 1×10^{-12} in [*ab*|*cd*] for parameter values $\sigma = 0$, $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, and $p_1 = p_2 = q_1 = q_2 = 4$.

	α_2						
α_1	0.1	0.5	1.0	2.0	5.0	10.0	20.0
0.1	6	7	7	8	8	8	9
0.5		8	9	9	9	10	10
1.0			10	10	11	11	12
2.0				11	12	13	14
5.0					16	17	18
10.0						19	21
20.0							25

TABLE IV

Value of μ_{max} needed in the Neumann expansion to obtain relative accuracy of 1×10^{-12} in [*ab*|*cd*] for parameter values $\sigma = 4$, $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2$, and $p_1 = p_2 = q_1 = q_2 = 4$.

	α_2						
α_1	0.1	0.5	1.0	2.0	5.0	10.0	20.0
0.1	11	11	12	12	12	12	12
0.5		13	13	13	13	14	15
1.0			14	15	16	16	17
2.0				16	17	17	19
5.0					20	22	24
10.0						24	27
20.0							32

after allowing for the loss of several significant decimal digits in the further processing of the two-electron integrals. For most values of the parameters, the last term retained in the expansion is a factor of $10–10^3$ less than the term that precedes it, so a far less conservative criterion would decrease the μ_{max} values only slightly.

We studied the convergence for α_i values ($\alpha \sim \zeta R$) ranging from 0.1–20 so as to be able to handle both highly diffuse and compact orbitals at a wide range of internuclear separations, and also considered zero and nonzero values of the discrete parameters σ, p_i, and q_i. For $\alpha_i > 20$ it probably makes sense to evaluate the integrals using a technique such as a multipole expansion, as the energies involved will be less than 10^{-8} times typical single-center contributions. For α_i values smaller than 0.1, no qualitatively new behavior will be exhibited.

Our findings, generated using Maple V, are summarized in Tables I–IV. Apart from the obvious fact that larger α_i values lead to slower convergence, we note also that μ_{max} values larger than 10 will often be required and that nonzero values of σ (the "magnetic" quantum number) lead to slower convergence. In constructing the tables, we generated "worst case" scenarios by taking the values of q_1 and q_2 equal to the value chosen for p_1 and p_2 and setting $\beta_i = \alpha_i$. In an actual molecular calculation, one can normally expect some of the integrals to approach this extreme case.

We did not find a comprehensive convergence study in the literature with which to compare. One reason such data are lacking is that they cannot be easily generated for general parameter values by any fixed-precision computational algorithm that has previously been published. In fact, we needed to evaluate the closed formulas at precision levels up to 80 significant digits to obtain the data in the tables. A partial discussion of the summation convergence is given by Yasui and Saika [16], who provide graphs showing separately the two quantities that enter the sum, $i_\mu^\sigma(q, \beta)$ and $W_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2)$. However, their data are only for $\sigma = 0$, and only relatively large values of α are included.

Numerical Behavior of the Closed Formulas

With the convergence data from the preceding section in hand, we can now examine the numerical behavior of the closed formulas for the parameter ranges that must be used. In passing, we note that the behavior to be observed will extend also to recursive methods when they involve the combination of the same building blocks in a different order.

We will find that the numerical problems to be encountered are most serious for large values of the expansion parameter μ. To start, we note that even for small α values we will already for $2p$ STOs (which include terms with $p = 4$) encounter values of μ_{max} as large as 10.

The formula for $w_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2)$ given in Eq. (39) is ill-conditioned for small α_i, with the pathology becoming more extreme as the p_i increase. This is one reason for the apparent failure of the ellipsoidal expansion methods when carried out using the closed formulas. To get a sense of the source of the problem, one can use the arbitrary precision features of Maple to examine the individual quantities entering Eq. (39).

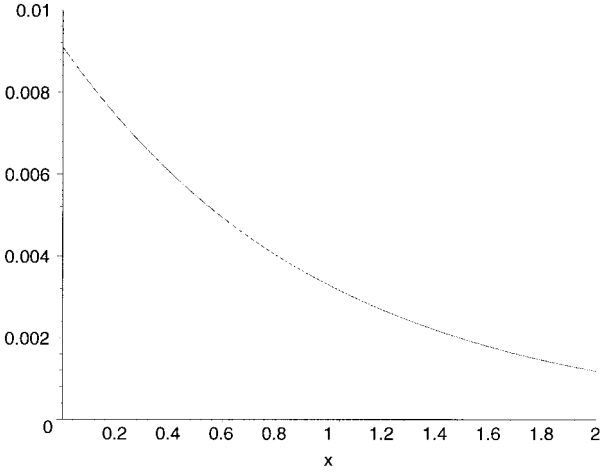

FIGURE 1. $L_{10}^0(0, \alpha)$ computed accurately.

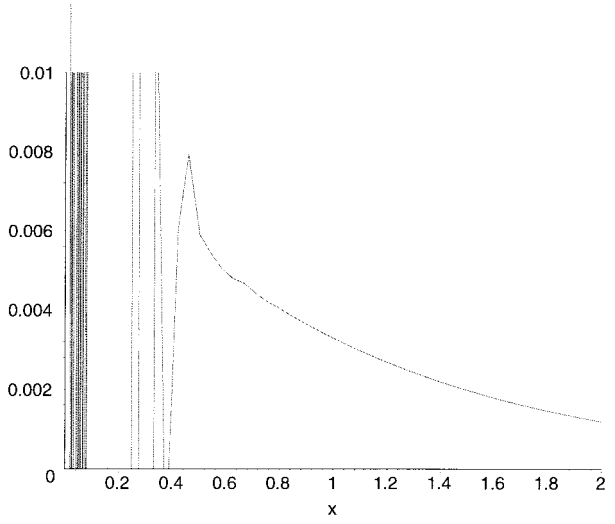

FIGURE 2. $L^0_{10}(0, \alpha)$, 64-bit floating-point computation.

We begin this process by examining $L^0_\mu(0, \alpha)$ graphically for $0 \le \alpha \le 2$ (the ill conditioning is not as serious beyond $\alpha = 2$). In Figure 1 we show $L^0_{10}(0, \alpha)$, computed to the precision needed to remove all ill-conditioning effects visible at the scale of the display. The quantity $L^0_{10}(0, 0)$ can be shown to have the exact value 1/110, so there is no pathology in the exact result, and $L^0_{10}(0, \alpha)$ is a smooth, well-behaved function for all relevant α. It required computation at 40S (40 significant decimal digits) to generate this graph. In Figure 2 we plot the same function, but computed at 16S, about the precision of 64-bit floating-point arithmetic. It is clear that no useful information remains in the computations for α smaller than about 0.6, with low precision for a range of larger α values.

The ill conditioning seen in Figure 2 does not arise from a lack of precision in evaluation of the exponential integral (as has been speculated by some authors) but from the subtraction of large numbers in Eq. (33) to yield a small result. We illustrate by tabulating separately the two summations in that equation and then their resultant. For $L^0_{10}(0, 0.1)$, we obtain at 30S the respective values

1st Sum:	+6545440445883564 97.763875452215
2nd Sum:	−6545440445883564 97.755664832610
Result:	0.008210619605.

We see that 20S has been lost due to differencing. The accurate value of $L^0_{10}(0, 0.1)$ at the precision shown is 0.008210619989, indicating that another 3S has been lost in the computation of the individual sums, leaving only 7S out of the original 30. This problem was recognized by Maslen and Trefry, and they suggested an alternate means of obtaining L^σ_μ, which we pursue in a later section of this article.

There are, however, additional ill-conditioning problems beyond those of the auxiliary functions entering Eq. (39). To observe this, we look individually at the two terms in the final square bracket of that equation. This time we illustrate for w^0_6, with $p_1 = p_2 = 0$. Taking first $w^0_6(0, 0, 0.1, 0.1)$, computed at 30S, we have

1st Term:	+2227384631.25424160888760350259
2nd Term:	−2227384631.20618767001654011371
Sum:	0.04805393887106338888.

The differencing loss in this example is 11S. A more accurate value of $w^0_6(0, 0, 0.1, 0.1)$ is 0.04805400 . . . , showing that other numerical error (from the source indicated in the preceding paragraph) has caused the loss of an additional 13S. The problem under discussion in the present paragraph is associated with the small value of α_2, as can be seen from the following two examples (computed at 30S, truncated as shown):

	$w^0_6(0, 0, 0.1, 2.)$	$w^0_6(0, 0, 2., 0.1)$
1st Term:	+1.4565207221863510545	+306864525.34360065512017449
2nd Term:	−1.4557323356323505961	−306864525.34301019961893312
Sum:	0.0007883865540004584	0.00059045550124138
Accurate value:	0.0007883865540004985	0.00059045550124133.

The first example shows only 4S of differencing error, but 13S lost in computation of the individual terms, mostly from the first term, because it contains $L^0_6(0, 0.1)$. The situation is almost reversed in the second example, which has 12S of differencing error but only 5S lost in the individual term computations.

The instability we have just examined was not discussed by Maslen and Trefry, and they presented no examples in which it would occur. Magnasco et al. [17] also advocated a method that includes this instability, but nevertheless claim to obtain integrals for small α_2 at high accuracy. This author doubts that claim, and notes that Magnasco et al. show no examples supporting it. The recursive method introduced by Kotani et al. [4] is also subject to both the instabilities discussed in this section. It is therefore apparent that we must find better ways to calculate the w_μ^σ for small α values, and if the new methods continue to use the L_μ^σ more accurate values of these functions will also be required. We address these problems in the next two sections.

Accurate Determination of the L_μ^σ for Small α

We follow the approach of Maslen and Trefry [10], in which the Legendre function $Q_\mu^\sigma(\xi)$ in the integral defining L_μ^σ is expanded in inverse powers of ξ. Using formulas 8.1.3 and 15.1.1 of Ref. [15],

$$\frac{(\mu-\sigma)!}{(\mu+\sigma)!}\,Q_\mu^\sigma(\xi)(\xi^2-1)^{\sigma/2} = \sum_{k=0}^{\infty}\frac{(-1)^\sigma(2k+\mu-\sigma)!}{(2k+2\mu+1)!!(2k)!!}\,\xi^{-(2k+\mu-\sigma+1)}. \quad (40)$$

Inserting this expansion into Eq. (28), recognizing that the integrals have a different character when the exponent of ξ is negative, and defining k_0 to be the smallest nonnegative integer such that $2k_0 > p-\mu+\sigma-1$, we thereby obtain

$$L_\mu^\sigma(p,\alpha) = \sum_{k=0}^{k_0-1}\frac{(-1)^\sigma(2k+\mu-\sigma)!}{(2k+2\mu+1)!!(2k)!!} \times A_{p-\mu+\sigma-2k-1}(\alpha) + M_\mu^\sigma(p,\alpha), \quad (41)$$

where the sum is to be omitted if $k_0 = 0$, and

$$M_\mu^\sigma(p,\alpha) = \sum_{k=k_0}^{\infty}\frac{(-1)^\sigma(2k+\mu-\sigma)!}{(2k+2\mu+1)!!(2k)!!}\,E_{\mu-\sigma-p+2k+1}(\alpha). \quad (42)$$

Here E_n is the generalized exponential integral given in formula 5.1.4 of Ref. [15].

The summation of Eq. (41), if it occurs, is finite and consists of terms all of the same sign. That of Eq. (42) is an infinite series that converges extremely slowly. However, as observed by Maslen and Trefry, it is possible to reorganize the series into a closed expression plus a rapidly convergent sum. The first step in so doing is to express each of the $E_n(\alpha)$ in terms of $E_1(\alpha)$ plus a remainder:

$$E_{n+1}(\alpha) = \frac{(-\alpha)^n E_1(\alpha)}{n!} + \frac{e^{-\alpha}}{n!}\sum_{j=1}^{n}(n-j)!(-\alpha)^{j-1}. \quad (43)$$

Then, substituting this formula into Eq. (42) and carrying out manipulations described in more detail in Appendix B, we obtain a result different and far more compact than that reported by Maslen and Trefry:

$$M_\mu^\sigma(p,\alpha) = (-1)^\mu i_\mu^\sigma(p,\alpha)E_1(\alpha) + e^{-\alpha}\sum_{t=0}^{\infty}\mathcal{M}_t^{\mu\sigma}(p)\alpha^t. \quad (44)$$

The coefficient $\mathcal{M}_t^{\mu\sigma}(p)$ is

$$\mathcal{M}_t^{\mu\sigma}(p) = \sum_{j=0}^{(\mu+\sigma)/2}\sum_{l=0}^{t}\frac{(-1)^{l+j}(2\mu-2j-1)!!}{(\mu+\sigma-2j)!!(t-l)!(2j)!!} \times T(2k_1+2\mu-2j+1, 2k_1+\mu-\sigma-p-l). \quad (45)$$

Throughout this study, sums are to be over integer values within the indicated limits and are omitted entirely if there are no such values. In Eq. (45), k_1 is the smallest nonnegative integer such that $2k_1 \geq t+p-\mu+\sigma+1$, and $T(i,j)$ stands for the summation $\Sigma_{k=0}^{\infty}\,1/(2k+i)(2k+j)$, which for the cases needed here evaluates to the closed forms

$$T(i,j) = \frac{1}{i-j}\sum_{k=0}^{(i-j-2)/2}\frac{1}{2k+j}, \quad i,j \text{ both odd},$$

$$= \frac{1}{i-j}\left[\log 2 + \sum_{k=1}^{(j-2)/2}\frac{1}{2k} - \sum_{k=0}^{(i-3)/2}\frac{1}{2k+1}\right], \quad j \text{ even}, i \text{ odd}. \quad (46)$$

Accurate Determination of w_μ^σ for Small α_2

The formulation of Eq. (39) is equivalent to partitioning w_μ^σ into two terms that we can indicate schematically as

$$w_\mu^\sigma = \int_1^\infty d\xi_1 F(\xi_1) \int_1^\infty d\xi_2 G(\xi_2) - \int_1^\infty d\xi_1 F(\xi_1) \int_{\xi_1}^\infty d\xi_2 G(\xi_2), \quad (47)$$

after which both terms of the partition can be evaluated in closed form. However, when α_2 is small the main contributions to the ξ_2 integrals are from values of ξ_2 that are larger than ξ_1 and, as we have seen, each term will be far larger than w_μ^σ itself.

The solution to this problem is obvious: If it is necessary to partition w_μ^σ at all, we must do so for small α_2 in a more suitable way, such as

$$w_\mu^\sigma = \int_1^\infty d\xi_1 F(\xi_1) \int_0^{\xi_1} d\xi_2 G(\xi_2) - \int_1^\infty d\xi_1 F(\xi_1) \int_0^1 d\xi_2 G(\xi_2). \quad (48)$$

The disadvantage to this approach is that we have not succeeded in bringing the first term of the new partitioning to a closed form, but this disadvantage is offset by the fact that a series solution for it is in positive powers of α_2 and for small α_2 converges acceptably.

In more detail, we proceed as follows. The ξ_2 integrals are of the form (with $\xi = \xi_1$ or $\xi = 1$)

$$\int_0^\xi P_\mu^\sigma(\xi_2)(\xi_2^2 - 1)^{\sigma/2} \xi_2^{p_2} e^{-\alpha_2 \xi_2} d\xi_2 = \frac{(\mu+\sigma)!}{(\mu-\sigma)!} \sum_s \mathcal{A}_s^{\mu\sigma} \xi^{p_2+s+1} a_{p_2+s}(\alpha_2 \xi), \quad (49)$$

where

$$a_n(\alpha) = \int_0^1 t^n e^{-\alpha t} dt, \quad (50)$$

so designated because

$$a_n(\alpha) + A_n(\alpha) = \int_0^\infty t^n e^{-\alpha t} dt = \frac{n!}{\alpha^{n+1}}. \quad (51)$$

As discussed in more detail in Appendix C, $a_n(\alpha)$, essentially an incomplete gamma function, has the expansion

$$a_n(\alpha) = e^{-\alpha} \sum_{j=0}^\infty \frac{n! \alpha^j}{(n+j+1)!}, \quad (52)$$

and a set of a_n can be calculated accurately for small α by a Miller algorithm.

We can now write Eq. (48) more explicitly, using Eqs. (49) and (52) in its first term, and introducing for its second term the definition

$$\bar{\imath}_\mu^\sigma(p, \alpha) = \frac{(\mu-\sigma)!}{(\mu+\sigma)!} \int_0^1 P_\mu^\sigma(\xi)(\xi^2 - 1)^{\sigma/2} \xi^p e^{-\alpha\xi} d\xi. \quad (53)$$

In Eq. (53) we use the definition of P_μ^σ valid outside the range $(-1 \ldots 1)$. The result of this processing of Eq. (48) is

$$w_\mu^\sigma(p_1, p_2, \alpha_1, \alpha_2) = \left[\frac{(\mu+\sigma)!}{(\mu-\sigma)!}\right]^2 \left[\sum_s \mathcal{A}_s^{\mu\sigma} \sum_{j=0}^\infty \times \frac{\alpha_2^j (p_2+s)!}{(p_2+s+j+1)!} L_\mu^\sigma(p_1+p_2+s+j+1, \alpha_1+\alpha_2) - L_\mu^\sigma(p_1, \alpha_1) \bar{\imath}_\mu^\sigma(p_2, \alpha_2) \right]. \quad (54)$$

Formally, $\bar{\imath}_\mu^\sigma(p, \alpha)$ can be computed by the formula of Eq. (49) with $\xi = 1$. Alternative procedures, based on the identification of $\bar{\imath}_\mu^\sigma(p, \alpha)$ as an incomplete generalized Bessel function, are discussed in Appendix C.

The formula of Eq. (54) will be most useful when α_2 is small, and particularly for larger values of μ,

where the formula of Eq. (39) becomes extremely ill-conditioned. These are also the conditions under which the L_μ^σ are best computed using Eqs. (41) and (44). The infinite sum in Eq. (54), although numerically stable, converges slowly even when α_2 is small because the L_μ^σ of argument $\alpha_1 + \alpha_2$ increases rapidly with increasing j. It is therefore useful to replace this occurrence of L_μ^σ by its explicit form and then manipulate the summations so that they can be evaluated efficiently. Because, as we shall see in a subsequent section, we need the formula only for $\sigma = p_1 = p_2 = 0$, we restrict to that case. The result, after inserting the explicit form of $\mathcal{A}_s^{\mu 0}$, is

$$w_\mu^0(0, 0, \alpha_1, \alpha_2) = \bar{k}_\mu^0(\alpha_2) \sum_{p=0}^{\infty} (-1)^{p+1} i_\mu^0(-p-1, \alpha_2) \times A_p(\alpha_1 + \alpha_2) + G_\mu(\alpha_2) + H_\mu(\alpha_2) - L_\mu^0(0, \alpha_1)\bar{i}_\mu^0(0, \alpha_2), \quad (55)$$

where

$$\bar{k}_\mu^\sigma(p, \alpha) = \int_0^\infty P_\mu^\sigma(\xi)\xi^p(\xi^2 - 1)^{\sigma/2} e^{-\alpha\xi} d\xi \quad (56)$$

and

$$G_\mu(\alpha_i) = (-1)^\mu E_1(\alpha_1 + \alpha_2) \sum_{k=0}^{\mu/2} \mathcal{G}_{\mu k} \times \sum_{j=0}^{\infty} \frac{\alpha_i^j i_\mu^0(\mu - 2k + j + 1, \alpha_1 + \alpha_2)}{(\mu - 2k + j + 1)!}, \quad (57)$$

$$H_\mu(\alpha_i) = e^{-(\alpha_1+\alpha_2)} \sum_{k=0}^{\mu/2} \mathcal{G}_{\mu k} \sum_{j=0}^{\infty} \frac{\alpha_i^j}{(\mu - 2k + j + 1)!} \times \sum_{t=0}^{\infty} \mathcal{M}_t^{\mu 0}(\mu - 2k + j + 1)(\alpha_1 + \alpha_2)^t \quad (58)$$

with

$$\mathcal{G}_{\mu k} = (\mu - 2k)!\mathcal{A}_{\mu-2k}^{\mu 0} = \frac{(-1)^k(2\mu - 2k - 1)!!}{(2k)!!}. \quad (59)$$

The derivation of Eq. (55) is presented in Appendix D and the evaluation of $\bar{k}_\mu^0$ is discussed in Appendix C. Because the first argument of $i_\mu^0(-p-1, \alpha_2)$ is negative, its evaluation requires considerations additional to those presented in the discussion of Eqs. (15)–(18). Details are in Appendix C.

The first term on the right side of Eq. (55) is the dominant part of w_μ^0. The remaining terms are the smaller contributions that arise from M_μ^0 and from the product $L_\mu^0\bar{i}_\mu^0$. We shall see that these terms are sometimes small enough that they can be neglected completely. Note that, if not negligible, $L_\mu^0\bar{i}_\mu^0$ must be evaluated by methods that are stable for small α.

TABLE V
Calculations of $L_\mu^0(0, 0.1)$.

μ	Exact	Closed	New
0	2.08622255552	2.08622255552	2.08622255552
1	0.38769568639	0.38769568639	0.38769568637
2	0.14453187663	0.14453187663	0.14453187663
3	0.07397770088	0.07397770087	0.07397770087
4	0.04475266632	0.04475266630	0.04475266632
5	0.02994928851	0.02994926000	0.02994928851
6	0.02143720306	0.02148200000	0.02143720306
7	0.01609843965	0.01650000000	0.01609843965
8	0.01253149559	−0.26000000000	0.01253149559
9	0.01003100764	*	0.01003100764
10	0.00821061999	*	0.00821061999
11	0.00684431635	*	0.00684431635
12	0.00579272708	*	0.00579272708

"Exact" is by closed formula at 60S (all digits shown are correct), "closed" is by the closed formula, and "new" is by Eqs. (41) and (44), both at 16S, with the infinite series in Eq. (44) truncated after $t = 5$. Asterisks indicate numbers too large to fit in their column.

Numerical Behavior of the Formulas for Small α

Numerical tests can now be applied both to verify the correctness of the formulas derived in the two preceding sections and assess their numerical stability and the convergence rates of the infinite series we have introduced. We start by examining the procedure for obtaining $L_\mu^\sigma(p, \alpha)$.

In Table V we compare Maple V calculations of the "new" formula for small α, Eqs. (41) and (44), with exact results and with the closed formula for $L_\mu^0(0, 0.1)$. Maple reports nonzero digits as results of additions only when the digit is significant for all addends, so the large numbers of trailing zeros in

TABLE VI

Typical values of the coefficients $\mathcal{M}_t^{\mu\sigma}(p)$ occurring in Eq. (44).

t	$\mathcal{M}_t^{00}(0)$	$\mathcal{M}_t^{00}(4)$	$\mathcal{M}_t^{10,0}(0)$	$\mathcal{M}_t^{10,4}(0)$	$\mathcal{M}_t^{10,0}(4)$	$\mathcal{M}_t^{10,4}(4)$
0	0.307	0.168	0.909 (−2)	0.352 (−7)	0.985 (−2)	0.691 (−7)
2	0.101 (−1)	0.582 (−2)	0.648 (−5)	0.777 (−9)	0.151 (−4)	0.337 (−8)
4	0.219 (−3)	0.141 (−3)	0.352 (−7)	0.849 (−10)	0.575 (−6)	0.883 (−10)
6	0.293 (−5)	0.204 (−5)	0.777 (−9)	0.169 (−11)	0.218 (−7)	0.123 (−11)
10	0.166 (−9)	0.127 (−9)	0.169 (−11)	0.100 (−15)	0.447 (−11)	0.609 (−16)

Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied.

the "closed" calculations are indications of differencing errors. For μ at and beyond 8, the closed calculations at 16S (64-bit floating point) are completely meaningless. On the other hand, we see that the small-α formula retains precision for all the μ values tabulated. The "new" entries in the table were calculated by a method giving full 16S accuracy for the spherical Bessel function and exponential integral occurring in Eq. (44), with the infinite series in that equation truncated after $t = 5$. The tabulated data, and additional calculations at higher precision and later truncation, confirm the correctness of the new formula. Test calculations were also carried out with success for nonzero values of the parameters σ and p and for larger α.

The range of practical applicability of the new formula depends upon the rate at which the infinite series in Eq. (44) converges. To this end, we list, in Table VI, representative values of the coefficients (truncated for presentation to 3S). Successive coefficients decrease on average by about a factor of 10, with an extremely weak dependence of this decrease on the parameter values, indicating that the series will be practical for use whenever α is significantly smaller than 10.

Next we study the small-α formula for w_μ^σ. In Table VII we present Maple V calculations of $w_\mu^0(0, 0, \alpha_1, \alpha_2)$, based on Eq. (54). The small-α entries, labeled "new", for α values of 0.1 and 1.0 at 16S are compared with exact results and with 16S closed-formula "closed" calculations. As expected from the behavior already noted for the closed formula for L_μ^σ, the closed results exhibit instabilities, with the pathology more extreme at small α values.

The formulation leading to the "new" entries is stable for all α values, with an accuracy limited only by the number of significant figures retained and by errors arising from truncation of the (convergent) infinite series involved. Table VII was generated using the series truncations indicated in its caption. The truncation of the L_μ^0 (in t) can be seen from Table VI to permit the t series to be correct to 11 or 12S, so that no significant portion of the errors visible in the new entries arises from this source. The bulk of the error in these entries is from the limitation to a finite number of $L_\mu^0(s + j + 1, \alpha_1 + \alpha_2)$, that is, from the truncation in j.

For small μ, it is evident that the j series converges slowly, illustrated by the fact that at $\mu = 0$, $\alpha_1 = \alpha_2 = 0.1$, the retention of 19 terms only produced 6S accuracy. The situation at small μ is worse for larger α values, in particular when α_2/α_1 is large. However, the convergence rapidly improves as μ increases. Because the contributions to $[ab|cd]$ from the η integrations [i.e., the functions $i_\mu^\sigma(q, \beta)$] decrease rapidly with increasing μ, it can be expected that reasonable expansion lengths will give w_μ^σ to sufficient accuracy when the closed formula (or other extant formulations) become unsatisfactory.

As indicated in the previous section, the small-α formulation of w_μ^0 can be rearranged as presented in Eq. (55). It is found that for small values of $\alpha_1 + \alpha_2$ the term G_μ rapidly becomes negligible as μ increases.

Recurrence Formulas for L_μ^σ

Recurrence formulas provide efficient ways to calculate a series of functions all of which are needed in a calculation. Some such formulas are known for the L_μ^σ, but additional formulas would be useful. We note that the STO integral literature does not contain a recurrence formula for $L_\mu^\sigma(p, \alpha)$ parallel to that given for the i_μ in Eq. (15); the formulas that have been reported involve changes of p or σ as well as μ. To find further formulas, we undertook an investigation of the functional properties of the $L_\mu^\sigma(p, \alpha)$. A preliminary study revealed that, for $p = 0$, these functions can be identified as Meijer's G-Functions [18]. A specific reference is formula

TABLE VII

Calculations of $w^0_\mu(0, 0, \alpha_1, \alpha_2)$.

μ	Exact	Closed	New
$\alpha_1 = 0.1, \alpha_2 = 0.1$			
0	4.369976567712 (+00)	4.369976567712 (+00)	4.369975655753 (+00)
2	3.114631145071 (−01)	3.114631151084 (−01)	3.114631137806 (−01)
4	9.941387939772 (−02)	9.116817950000 (−02)	9.941387938941 (−02)
6	4.805400299308 (−02)	4.263530556110 (+06)	4.805400299282 (−02)
8	2.819454116587 (−02)	−7.791183759105 (+14)	2.819454116585 (−02)
10	1.850695461437 (−02)	9.775085882239 (+23)	1.850695461437 (−02)
12	1.307055013596 (−02)	9.789634259042 (+32)	1.307055013596 (−02)
$\alpha_1 = 0.1, \alpha_2 = 1.0$			
0	5.100595650577 (−01)	5.100595650577 (−01)	4.504916790196 (−01)
2	2.956339442654 (−02)	2.956339442746 (−02)	2.953862925764 (−02)
4	8.531898319089 (−03)	8.531896806596 (−03)	8.531628554042 (−03)
6	3.945222336661 (−03)	4.490359688865 (−01)	3.945215008520 (−03)
8	2.259265799584 (−03)	−5.343663154686 (+05)	2.259265436565 (−03)
10	1.460596736149 (−03)	1.352030239037 (+13)	1.460596707539 (−03)
12	1.020868460904 (−03)	1.732867837568 (+20)	1.020868458609 (−03)
$\alpha_1 = 1.0, \alpha_2 = 0.1$			
0	1.415262983898 (−01)	1.415262983898 (−01)	1.415262983899 (−01)
2	1.774041533651 (−02)	1.774041533950 (−02)	1.774041533650 (−02)
4	6.326895229112 (−03)	6.327475400000 (−03)	6.326895229113 (−03)
6	3.199156628805 (−03)	1.234543000000 (−01)	3.199156628805 (−03)
8	1.923169151622 (−03)	7.236429700000 (+05)	1.923169151622 (−03)
10	1.281660279179 (−03)	−3.833773095300 (+12)	1.281660279179 (−03)
12	9.146013462021 (−04)	−1.151483334217 (+20)	9.146013462024 (−04)
$\alpha_1 = 1.0, \alpha_2 = 1.0$			
0	3.699820498504 (−02)	3.699820498504 (−02)	3.699811406358 (−02)
2	4.595396383877 (−03)	4.595396383875 (−03)	4.595396264197 (−03)
4	1.577585724033 (−03)	1.577585718679 (−03)	1.577585741028 (−03)
6	7.782802079560 (−04)	7.781465799300 (−04)	7.782802038333 (−04)
8	4.604276825712 (−04)	−4.150504798000 (−03)	4.604276837803 (−04)
10	3.034722811183 (−04)	−6.198432225820 (+02)	3.034722806248 (−04)
12	2.148285897458 (−04)	−1.563678557261 (+08)	2.148285899572 (−04)

"Exact" is by closed formula at 60S (all digits shown are correct), "closed" is by the closed formula, and "new" is by Eq. (54), both at 16S. The sum over j in Eq. (54) is truncated after $j = 18$ and the summation occurring in the evaluations therein of L^0_μ is truncated after $t = 12$. Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied.

7.141.2 of the table by Gradshteyn and Ryzhik [19]; for a general discussion of these functions, the reader is referred to the compilation by Erdélyi et al. [20]. The significance of this observation is that because the G-functions are solutions of a differential equation system it should be possible to develop families of recurrence formulas for them. Functions related, but not identical, to the usual Bessel functions have also been discussed by Agrest and Maksimov [21]. Such functions satisfy some but not all of the recurrence relationships of Bessel functions, may satisfy an inhomogeneous Bessel equation, and in some cases be identifiable as incomplete Bessel functions.

We begin by summarizing the previously known relationships. Early work [2, 4] exhibited formulas obtained by inserting the Legendre function recurrence relations into Eq. (28) for L^σ_μ. The two equations obtained in this way are

$$(\mu + 1)L^0_{\mu+1}(p, \alpha) - (2\mu + 1)L^0_\mu(p + 1, \alpha) + \mu L^0_{\mu-1}(p, \alpha) = 0, \quad (60)$$

$$L^\sigma_\mu(p, \alpha) = \frac{L^{\sigma-1}_{\mu+1}(p, \alpha) - L^{\sigma-1}_{\mu-1}(p, \alpha)}{2\mu + 1}. \quad (61)$$

Systematic use of these equations starts by making a set of $L_0^0(p, \alpha)$ for the range $p = 0 \ldots \mu_{\max} + p_{\max} + \sigma_{\max}$, where the quantities subscripted "max" indicate the largest values needed for the respective indices. To initiate the recursion process, one needs also $L_1^0(p, \alpha)$, obtainable from the formula

$$L_1^0(p, \alpha) = L_0^0(p + 1, \alpha) - A_p(\alpha). \quad (62)$$

Then Eq. (60) can be used to increase μ, followed by application of Eq. (61) to increase σ. When used as described above, Eq. (60) will always be unstable, but the instability becomes serious only for small values of α. In that case, values of $L_\mu^0(0, \alpha)$ will need to be obtained in another way, after which Eq. (60) can be used to increase p. When used in this way, the recursion is stable for all α.

The functions $L_0^0(p, \alpha)$ can be calculated by a recurrence procedure, first introduced by Ruedenberg [2], that is computationally more efficient than use of the general closed form, Eq. (36). One starts from the explicit formula for $L_0^0(0, \alpha)$:

$$L_0^0(0, \alpha) = \frac{e^{-\alpha}}{2\alpha}[\gamma + \log 2\alpha + e^{2\alpha}E_1(2\alpha)]. \quad (63)$$

Then one may introduce a set of auxiliary functions $g_n(\alpha)$ defined by the relation

$$g_n(\alpha) = (-1)^n \frac{d^n}{d\alpha^n}(\alpha L_0^0(0, \alpha)), \quad (64)$$

which satisfy the recurrence relation

$$g_n(\alpha) = g_{n-2}(\alpha) - A_{n-2}(\alpha), \quad (65)$$

and can be generated by upward recursion starting from

$$g_0(\alpha) = \alpha L_0^0(0, \alpha), \quad (66)$$

$$g_1(\alpha) = g_0(\alpha) - e^{\alpha}E_1(2\alpha). \quad (67)$$

Next, from the definition in Eq. (64) one can show that

$$L_0^0(p, \alpha) = \frac{1}{\alpha}[pL_0^0(p - 1, \alpha) + g_p(\alpha)], \quad (68)$$

which permits p to be increased. While the g_n and the L_0^0 are of opposite sign for $n > \alpha$, the g_n are far smaller and good stability is achieved for all α values.

We have succeeded in obtaining additional relationships connecting contiguous $L_\mu^\sigma(p, \alpha)$. As shown in Appendix C,

$$L_{\mu+1}^0(0, \alpha) - \frac{2\mu + 1}{\alpha} L_\mu^0(0, \alpha) - L_{\mu-1}^0(0, \alpha) = -\frac{(2\mu + 1)}{\mu(\mu + 1)} \frac{e^{-\alpha}}{\alpha}. \quad (69)$$

This recurrence formula is inhomogenous, a consequence of the fact that the L_μ^0 are, in the Agrest/Maksimov nomenclature, *semicylindrical functions.*

Eq. (69) provides a possibility not heretofore exploited in STO integral evaluation: Using it, one can generate $L_\mu^0(0, \alpha)$ for a range of μ values without having first to obtain $L_\mu^0(p, \alpha)$ of nonzero p. It is evident that this formula was not known to previous investigators.

If we set the inhomogeneous term on the right side of Eq. (69) to zero, there results an equation that we can consider as defining an associated *complementary recurrence problem.* As for differential equations, any set of functions constituting a solution to the full (inhomogeneous) Eq. (69) remains a solution if to each member of the set is added any multiple of the corresponding member of a solution set for the complementary problem. Comparing with Eq. (15), we see that the complementary problem has a solution of the form $(-1)^\mu i_\mu(\alpha) f(\alpha)$, where $f(\alpha)$ is independent of μ but otherwise arbitrary. Looking now at Eq. (44), we note that the term containing $E_1(\alpha)$ is a solution to the complementary problem, so that the remaining term (the power series in α) must (for $\sigma = 0$) satisfy the full Eq. (69).

The observations of the preceding paragraph are of particular relevance because we shall find that Eq. (69) is unstable both for upward recurrence (to increase μ) and downward recurrence. However, while upward recursion is inherently unstable, downward recursion is only unstable in that its starting values contain an uncontrolled (round-off) multiple of the solution to the complementary problem. It is therefore possible to obtain accurate results from downward recursion by (1) carrying it out, using Eq. (69) and starting values of $L_\mu^0(0, \alpha)$ for $\mu = \mu_{\max}$ and $\mu_{\max} - 1$, and then (2) adding to this result that multiple of the above identified solution to the complementary problem that yields the correct value of $L_0^0(0, \alpha)$.

We note that the complementary problem has a second solution, proportional to $k_\mu(\alpha)$, but its importance does not grow during downward recursion so its initial presence in round-off quantities is not relevant. The effectiveness of the adjustment process described here is illustrated in the section giving numerical examples.

Another new formula, useful for advancing p in $L^0_\mu(p, \alpha)$, results if we generalize Ruedenberg's procedure, Eqs. (65)–(68), to positive μ. Again the details are in Appendix C. The result is summarized as follows:

The auxiliary function $g_\mu(p, \alpha)$ satisfies the equation

$$g_\mu(p + 2, \alpha) = g_\mu(p, \alpha) + \mu[L^0_\mu(p + 1, \alpha) - L^0_{\mu-1}(p, \alpha)], \quad (70)$$

with starting values

$$g_\mu(0, \alpha) = \alpha L^0_\mu(0, \alpha), \quad (71)$$

$$g_\mu(1, \alpha) = \alpha L^0_{\mu-1}(0, \alpha) + \mu L^0_\mu(0, \alpha) - \frac{e^{-\alpha}}{\mu}. \quad (72)$$

The parameter p can be increased using

$$L^0_\mu(p, \alpha) = \frac{1}{\alpha}[pL^0_\mu(p - 1, \alpha) + g_\mu(p, \alpha)]. \quad (73)$$

The relation to Eqs. (65)–(68) becomes clear if we note that $\lim_{\mu\to 0} \mu L^0_{\mu-1}(p, \alpha) = A_p(\alpha)$.

The above equations show that a set of $L^0_\mu(p, \alpha)$, for $\mu = 1 \ldots \mu_{\max}$, $p = 0 \ldots p_{\max}$, can be constructed solely from $L^0_\mu(0, \alpha)$, $\mu = 0 \ldots \mu_{\max}$, a set of $L^0_0(p, \alpha)$, $p = 0 \ldots p_{\max}$ (made as described earlier), and starting values $g_\mu(0, \alpha)$ and $g_\mu(1, \alpha)$, $\mu = 1 \ldots \mu_{\max}$. The necessary succession of steps is:

1. Set $\mu = 1$.
2. For this μ value:
   (a) Set $p = 1$.
   (b) Use Eq. (73) to make $L^0_\mu(p, \alpha)$.
   (c) Increase p by 1. Go to step 3 if $p > p_{\max}$.
   (d) Use Eq. (70) to make $g^0_\mu(p + 1, \alpha)$.
   (e) Return to Step (b).
3. Increase μ by 1.
4. Repeat steps 2 and 3 unless $\mu > \mu_{\max}$.

It is possible to combine use of the procedure described above with the better-known formula already presented as Eq. (60) and Ruedenberg's procedure for $\mu = 0$. Starting from $L^0_\mu(p, \alpha)$ for a given p (initially zero) and $\mu = 0 \ldots \mu_{\max}$, we may employ Eq. (60) to increase p one step for $\mu = 1 \ldots \mu_{\max} - 1$. Then Ruedenberg's formula may be used to increase p for $\mu = 0$ and the new formula, based on Eqs. (73) and (70), used to increase p for $\mu = \mu_{\max}$. This approach avoids the need to generate L^0_μ values for μ values larger than $\mu_{\max}$.

Numerical Behavior of the Recurrence Formulas for L^σ_μ

If the processes involved are, or can be made, stable, the most efficient way to make the $L^\sigma_\mu(p, \alpha)$ will be to use the new recurrence formula, Eq. (69), starting from $L^0_0(0, \alpha)$ to advance μ, to then employ a procedure such as that outlined after Eq. (73) to advance p, and finally to call upon Eq. (61) to advance σ. The first step in the investigation of this approach is to examine the upward recursion in μ.

In Table VIII we present the result of upward recursion in μ for $\alpha = 0.1$ and 1.0. As might be expected from the signs of the various contributions, this process is unstable, with the instability becoming more serious at smaller α. Downward recursion is also seen to be unstable, although less severe than for the upward process. However, as noted in an earlier section, the instability under downward recursion is associated with a round-off contamination in the starting values by a solution to the corresponding complementary problem, and for small α any such contamination grows rapidly as μ is decreased.

The unwanted contributions from the complementary problem can be eliminated after identifying their magnitude from the error in $L^0_0(0, \alpha)$ as reached by downward recursion. We recall from an earlier section that the complementary problem has a solution, of arbitrary scale, whose μ member is proportional to $(-1)^\mu i_\mu(\alpha)$. Then, letting $\bar{L}$ refer to the immediate result of downward recursion, with L denoting adjusted values, we write

$$F = \frac{L^0_0(0, \alpha) - \bar{L}^0_0(0, \alpha)}{i_0(\alpha)}, \quad (74)$$

$$L^0_\mu(0, \alpha) = \bar{L}^0_\mu(0, \alpha) + (-1)^\mu i_\mu(\alpha) F, \quad (75)$$

TABLE VIII

Evaluation of $L^0_\mu(0, \alpha)$ by recurrence formulas.

μ	Exact	Up	Down	Down(adj)
$\alpha = 0.1$				
0	2.086222555524	2.086222555524	−1.722219641528	2.086222555524
1	0.387695686388	0.387695686388	0.514559208096	0.387695686388
2	0.144531876629	0.144531876629	0.141995330807	0.144531876629
3	0.073977700880	0.073977700879	0.074013931498	0.073977700880
4	0.044752666320	0.044752666306	0.044752263798	0.044752666320
5	0.029949288511	0.029949287229	0.029949292170	0.029949288511
6	0.021437203057	0.021437061999	0.021437203029	0.021437203057
7	0.016098439653	0.016080100744	0.016098439653	0.016098439653
8	0.012531495585	0.009780518169	0.012531495585	0.012531495585
9	0.010031007639	−0.457653492181	0.010031007639	0.010031007639
10	0.008210619989	*	0.008210619989	0.008210619989
$\alpha = 1.0$				
0	0.300132871667	0.300132871667	0.300132871344	0.300132871667
1	0.099460932502	0.099460932502	0.099460932603	0.099460932502
2	0.046696507415	0.046696507415	0.046696507396	0.046696507415
3	0.026377268602	0.026377268602	0.026377268605	0.026377268602
4	0.016741046944	0.016741046944	0.016741046944	0.016741046944
5	0.011500942573	0.011500942573	0.011500942573	0.011500942573
6	0.008362286816	0.008362286816	0.008362286816	0.008362286816
7	0.006343225109	0.006343225105	0.006343225109	0.006343225109
8	0.004971527416	0.004971527360	0.004971527416	0.004971527416
9	0.003998767574	0.003998766619	0.003998767574	0.003998767574
10	0.003284673748	0.003284655539	0.003284673748	0.003284673748

"Exact" is by closed formula at 60S (all digits shown are correct). The other data are by recursion at 16S using Eq. (69), "up" starting from exact values at $\mu = 0$ and 1, and "down" starting from exact values at $\mu = 10$ and 9. "Down(adj)" indicates downward recursion followed by addition of that multiple of the solution to the complementary homogeneous recurrence problem that makes $L^0_0(0, \alpha)$ correct (see text). The asterisk indicates a number too large to fit in its column.

where L^0_0 in Eq. (74) is a previously computed accurate value. The results of this adjustment are in the column of Table VIII labeled "Down(adj)"; we see that they are highly accurate.

Once a set of $L^0_\mu(p, \alpha)$ with $p = 0$ has been generated, one can increase p recursively in two ways, one of which is to use the four-step process introduced in this study and outlined after Eq. (73). This process does not use any L^0_μ with μ values larger than that of the $L^0_\mu(p, \alpha)$ to be produced; hence, we term it "vertical." If stable, this would be the more efficient of the two processes, as it does not use any function values that are needed only to generate others. The alternative is to make $L^0_\mu(p, \alpha)$ from $L^0_{\mu+1}(p-1, \alpha)$ and $L^0_{\mu-1}(p-1, \alpha)$; we label this process "oblique." The oblique process has in previous work been started with values of $L^0_0(p, \alpha)$ obtained by Ruedenberg's procedure, Eqs. (63)–(68), and with values of $L^0_\mu(0, \alpha)$ for $\mu \leq (\mu_{\max} + p_{\max})$.

Unfortunately, the vertical process does not generate the $L^0_\mu(p, \alpha)$ with sufficient stability, as can be seen from Table IX, which presents values for $p = 8$. However, it is possible to use the vertical process to avoid the necessity of computing L^0_μ with $\mu > \mu_{\max}$ by applying it only for $\mu = \mu_{\max}$, using the oblique process for $1 \leq \mu \leq (\mu_{\max} - 1)$. The data in Table IX labeled "hybrid" were obtained in this way. It is seen that the error introduced by the vertical recurrence at $\mu = \mu_{\max}$ is rapidly attenuated when the oblique algorithm is used for smaller μ values, leading to a stable and efficient way of advancing the index p.

The remaining recursive procedure is that needed to advance the index σ. In Table X we examine the result of using the previously known recurrence formula, Eq. (61), for this purpose. We note that the formula gives stable results for all α.

TABLE IX

Evaluation of $L^0_\mu(8, \alpha)$ by recurrence formulas, starting from exact values of $L^0_\mu(0, \alpha)$.

μ	Exact	Vertical	Hybrid
$\alpha = 0.1$			
0	5.04040012014316(+11)	5.04040012014313(+11)	5.04040012014313(+11)
5	2.33076289024669(+01)	2.33415326550506(+01)	2.33076289024669(+01)
6	5.80863085152762(−01)	5.44098394803513(−01)	5.80863085152762(−01)
16	3.54466697382464(−03)	−1.61809207854883(−01)	3.54466692631826(−03)
18	2.77997604166857(−03)	2.30557552456011(+00)	2.76832064382144(−03)
20	2.24174512537576(−03)	−3.36769353736485(+00)	−3.34381154353372(+00)
$\alpha = 1.0$			
0	5.08126591409885(+03)	5.08126591409886(+03)	5.08126591409886(+03)
5	4.53723389750444(−02)	4.53723389592715(−02)	4.53723389750444(−02)
6	1.77174640000642(−02)	1.77174642162433(−02)	1.77174640000642(−02)
16	1.42954404038876(−03)	1.42953476437676(−03)	1.42954404038462(−03)
18	1.12333623323820(−03)	1.12333406585736(−03)	1.12333622309907(−03)
20	9.07021794780386(−04)	9.06987581856958(−04)	9.06992679067376(−04)

"Exact" is by closed formula at 60S (all digits shown are correct), "vertical" is using Eqs. (70) and (73), and "hybrid" is using Eq. (60) with vertical recurrence for $\mu = 0$ and μ_{max} ($\mu_{max} = 20$), both at 16S. Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied.

Recurrence Formulas for W^σ_μ

Kotani's recurrence scheme for these functions [4] applies to W^σ_μ and depends only upon the properties of the Legendre functions occurring therein. We look first at his formula for increasing the index σ. This formula is based on the following identity connecting products of Legendre functions:

$$Q^{\sigma+1}_\mu(\xi_>)\,P^{\sigma+1}_\mu(\xi_<)[(\xi^2_> - 1)(\xi^2_< - 1)]^{1/2} = \frac{(\mu-\sigma)(\mu-\sigma+1)^2}{2\mu+1}\,Q^\sigma_{\mu+1}(\xi_>)\,P^\sigma_{\mu+1}(\xi_<) - (\mu-\sigma)(\mu+\sigma+1)\xi_>\xi_<Q^\sigma_\mu(\xi_>)\,P^\sigma_\mu(\xi_<) + \frac{(\mu+\sigma+1)(\mu+\sigma)^2}{2\mu+1}\,Q^\sigma_{\mu-1}(\xi_>)\,P^\sigma_{\mu-1}(\xi_<). \tag{76}$$

Substitution of Eq. (76) into Eqs. (12) and (13) yields

$$W^{\sigma+1}_\mu(p_1, p_2, \alpha_1, \alpha_2) = \frac{(\mu-\sigma)(\mu-\sigma+1)^2}{2\mu+1} \times W^\sigma_{\mu+1}(p_1, p_2, \alpha_1, \alpha_2) - (\mu-\sigma)(\mu+\sigma+1)$$

TABLE X

Evaluation of $L^3_\mu(p, \alpha)$ by recurrence formulas, starting from exact values of $L^0_\mu(p, \alpha)$.

α	μ	p	Exact	Recurrence
0.1	3	0	−1.78924176314671(−02)	−1.78924176314671(−02)
	12	0	−8.32090732491842(−08)	−8.32090732491845(−08)
1.0	3	0	−2.23557682267751(−03)	−2.23557682267751(−03)
	12	0	−3.21713098836061(−08)	−3.21713098836064(−08)
0.1	3	4	−5.71532289904843(+02)	−5.71532289904843(+02)
	12	4	−1.08200132610559(−07)	−1.08200132610559(−07)
1.0	3	4	−5.69184211748604(−02)	−5.69184211748604(−02)
	12	4	−4.07853489840676(−08)	−4.07853489840676(−08)

"Exact" is by closed formula at 60S (all digits shown are correct) and "recurrence" is using Eq. (61) at 16S. Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied.

$$\times W_\mu^\sigma(p_1+1, p_2+1, \alpha_1, \alpha_2) + \frac{(\mu+\sigma+1)(\mu+\sigma)^2}{2\mu+1} \times W_{\mu-1}^\sigma(p_1, p_2, \alpha_1, \alpha_2). \quad (77)$$

Eq. (77) is numerically satisfactory for all parameter values and leads to an efficient general method for getting W_μ^σ with $\sigma > 0$ from W_μ^0.

The remainder of Kotani's scheme connects functions $W_\mu^0(p_1, p_2, \alpha_1, \alpha_2)$ of neighboring μ, p_1, and p_2. These formulas are based on the Legendre function identities

$$Q_\mu(\xi_>) P_\mu(\xi_<) = \left(\frac{\mu-1}{\mu}\right)^2 Q_{\mu-2}(\xi_>) P_{\mu-2}(\xi_<) + \left(\frac{2\mu-1}{\mu}\right)^2 \xi_>\xi_< Q_{\mu-1}(\xi_>) P_{\mu-1}(\xi_<) - \frac{(\mu-1)(2\mu-1)}{\mu^2} [\xi_> Q_{\mu-1}(\xi_>) P_{\mu-2}(\xi_<) + \xi_< P_{\mu-1}(\xi_<) Q_{\mu-2}(\xi_>)], \quad (78)$$

$$(\mu-1)[\xi_> Q_{\mu-1}(\xi_>) P_{\mu-2}(\xi_<) + \xi_< P_{\mu-1} \times (\xi_<) Q_{\mu-2}(\xi_>)] = (2\mu-3)(\xi_>^2 + \xi_<^2) \times Q_{\mu-2}(\xi_>) P_{\mu-2}(\xi_<) - 2(2\mu-5)\xi_>\xi_< \times Q_{\mu-3}(\xi_>) P_{\mu-3}(\xi_<) + (\mu-3)[\xi_> Q_{\mu-3}(\xi_>) \times P_{\mu-4}(\xi_<) + \xi_< P_{\mu-3}(\xi_<) Q_{\mu-4}(\xi_>)], \quad (79)$$

and are framed in terms of an auxiliary function (of definition differing slightly from that of Kotani)

$$Z_\mu(p_1, p_2, \alpha_1, \alpha_2) = (2\mu-1) \times W_{\mu-1}^0(p_1+1, p_2+1, \alpha_1, \alpha_2) - (\mu-1) \int_1^\infty d\xi_1 \int_1^\infty d\xi_2 \times [\xi_> Q_{\mu-1}(\xi_>) P_{\mu-2}(\xi_<) + \xi_< P_{\mu-1}(\xi_<) \times Q_{\mu-2}(\xi_>)] \xi_1^{p_1} \xi_2^{p_2} e^{-\alpha_1\xi_1 - \alpha_2\xi_2}. \quad (80)$$

Substitution of Eq. (78) into the definition of W_μ^0 and the use of Eq. (80) yield, for $\mu > 1$, the equation

$$W_\mu^0(p_1, p_2, \alpha_1, \alpha_2) = \left(\frac{\mu-1}{\mu}\right)^2 W_{\mu-2}^0(p_1, p_2, \alpha_1, \alpha_2) + \left(\frac{2\mu-1}{\mu^2}\right) Z_\mu(p_1, p_2, \alpha_1, \alpha_2), \quad (81)$$

while insertion of Eq. (79) into the definition of Z_μ leads for $\mu > 2$ to

$$Z_\mu(p_1, p_2, \alpha_1, \alpha_2) = Z_{\mu-2}(p_1, p_2, \alpha_1, \alpha_2) - (2\mu-3) \times [W_{\mu-2}^0(p_1+2, p_2, \alpha_1, \alpha_2) + W_{\mu-2}^0(p_1, p_2 + 2, \alpha_1, \alpha_2)] + (2\mu-5) \times W_{\mu-3}^0(p_1+1, p_2+1, \alpha_1, \alpha_2) + (2\mu-1) \times W_{\mu-1}^0(p_1+1, p_2+1, \alpha_1, \alpha_2). \quad (82)$$

With suitable initial values, Eqs. (81) and (82) can be used together to obtain a set of $W_\mu^0(p_1, p_2, \alpha_1, \alpha_2)$ for a range of μ, p_1, and p_2. It can be shown that $Z_1 = 0$ for all p_1 and p_2. The other quantities needed are $Z_2(p_1, p_2, \alpha_1, \alpha_2)$ and $W_\mu^0(p_1, p_2, \alpha_1, \alpha_2)$ for $\mu = 0$ and 1. These W_μ^0 can be generated by the explicit methods already discussed; Kotani recommends obtaining them and also Z_2 via an additional auxiliary function

$$S_\mu(p_1, p_2, \alpha_1, \alpha_2) = \int_1^\infty d\xi_1 Q_\mu(\xi_1) \xi_1^{p_1} e^{-\alpha_1\xi_1} \int_1^{\xi_1} d\xi_2 \xi_2^{p_2} e^{-\alpha_2\xi_2}, \quad (83)$$

in terms of which

$$W_0^0(p_1, p_2, \alpha_1, \alpha_2) = S_0(p_1, p_2, \alpha_1, \alpha_2) + S_0(p_2, p_1, \alpha_2, \alpha_1), \quad (84)$$

$$W_1^0(p_1, p_2, \alpha_1, \alpha_2) = S_1(p_1, p_2+1, \alpha_1, \alpha_2) + S_1(p_2, p_1+1, \alpha_2, \alpha_1), \quad (85)$$

and

$$Z_2(p_1, p_2, \alpha_1, \alpha_2) = 3W_1^0(p_1+1, p_2+1, \alpha_1, \alpha_2) - S_0(p_1, p_2+2, \alpha_1, \alpha_2) - S_0(p_2, p_1+2, \alpha_2, \alpha_1) - S_1(p_1+1, p_2, \alpha_1, \alpha_2) - S_1(p_2+1, p_1, \alpha_2, \alpha_1). \quad (86)$$

The S_μ may be obtained recursively by the formula

$$\alpha_2 S_\mu(p_1, p_2, \alpha_1, \alpha_2) = p_2 S_\mu(p_1, p_2-1, \alpha_1, \alpha_2) + e^{-\alpha_2} L_\mu^0(p_1, \alpha_1) - L_\mu^0(p_1+p_2, \alpha_1+\alpha_2). \quad (87)$$

Use of this formula is self-starting, as the term with coefficient p_2 can be replaced by zero when $p_2 = 0$.

The strategy for use of these equations to obtain W for index ranges $\mu = 0 \cdots \mu_{max}$, p_1, $p_2 = 0 \cdots p_{max}$, and a given value of σ is (where $n_{max} = p_{max} + \mu_{max} + \sigma$):

1. Make W_0^0 for p_1 and p_2 over range $0 \cdots n_{max}$.
2. Make W_1^0 for p_1 and p_2 over range $0 \cdots (n_{max} - 1)$.
3. Use Eq. (86) to make Z_2 for p_1 and p_2 over range $0 \cdots (n_{max} - 2)$.
4. Use Eq. (81) to make W_2^0 for the same range.
5. For μ from 3 to $(\mu_{max} + \sigma)$,
   (a) Use Eq. (82) to make Z_μ for p_1 and p_2 over range $0 \cdots (n_{max} - \mu)$.
   (b) Use Eq. (81) to make W_μ^0 for the same range.
6. Use Eq. (77) to advance σ stepwise to the required value (reducing the range of p_1 and p_2 by one at each step).

Kotani's scheme for the W_μ^0, apart from minor variations due to Ruedenberg [2], is the only recursive procedure that has been published for these functions. Unfortunately, the scheme (in both the original and with variations) is unstable for small values of α_1 and α_2, as can be seen from numerical examples presented in the next section. We therefore needed an alternative recursive procedure. Because the instabilities are connected to the fact that W with large values of p_1 and p_2 are used to form the (inherently smaller) W with $p_1 = p_2 = 0$, we sought to develop a method that starts from functions with vanishing indices p_1 and p_2.

Our first step toward a new recursive scheme will be to introduce a quantity we designate $w_{\nu\mu}$, which can be regarded as a generalization (for $\sigma = 0$) of w_μ^σ:

$$w_{\nu\mu}(p_1, p_2, \alpha_1, \alpha_2) = \int_1^\infty d\xi_1 \int_1^{\xi_1} d\xi_2 Q_\nu(\xi_1) P_\mu(\xi_2) \xi_1^{p_1} \xi_2^{p_2} e^{-\alpha_1\xi_1 - \alpha_2\xi_2} \quad (88)$$

$$= \int_1^\infty d\xi Q_\nu(\xi) \xi^{p_1} e^{-\alpha_1\xi} k_\mu^0(p_2, \alpha_2, \xi) \quad (89)$$

$$= \int_1^\infty d\xi P_\mu(\xi) \xi^{p_2} e^{-\alpha_2\xi} L_\nu^0(p_1, \alpha_1, \xi), \quad (90)$$

where the new quantities appearing in Eqs. (89) and (90), which are incomplete analogs of the previously introduced functions $k_\mu^0(p, \alpha)$ and $L_\nu^0(p, \alpha)$, are defined as

$$k_\mu^0(p, \alpha, x) = \int_1^x P_\mu(\xi) \xi^p e^{-\alpha\xi} d\xi, \quad (91)$$

$$L_\nu^0(p, \alpha, x) = \int_x^\infty Q_\nu(\xi) \xi^p e^{-\alpha\xi} d\xi. \quad (92)$$

Eq. (90) is obtained by reversing the integration order that led to Eq. (89).

We further define

$$W_{\nu\mu}(p_1, p_2, \alpha_1, \alpha_2) = w_{\nu\mu}(p_1, p_2, \alpha_1, \alpha_2) + w_{\mu\nu}(p_2, p_1, \alpha_2, \alpha_1), \quad (93)$$

and note that

$$W_\mu^0(p_1, p_2, \alpha_1, \alpha_2) = W_{\mu\mu}(p_1, p_2, \alpha_1, \alpha_2). \quad (94)$$

We also have

$$W_{\nu\mu}(p_1, p_2, \alpha_1, \alpha_2) = W_{\mu\nu}(p_2, p_1, \alpha_2, \alpha_1). \quad (95)$$

As shown in Appendix C, the $W_{\nu\mu}$ (for $p_1 = p_2 = 0$) satisfy the following recurrence formulas:

$$W_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = \frac{\alpha_2}{2\mu + 1} (W_{\nu,\mu+1}(0, 0, \alpha_1, \alpha_2) - W_{\nu,\mu-1}(0, 0, \alpha_1, \alpha_2)) + \frac{1}{2\mu + 1} (T_{\nu,\mu+1}(\alpha_{12}) - T_{\nu,\mu-1}(\alpha_{12}) - T_{\mu+1,\nu}(\alpha_{12}) + T_{\mu-1,\nu}(\alpha_{12})), \quad (96)$$

$$W_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = \frac{\alpha_1}{2\nu + 1} (W_{\nu+1,\mu}(0, 0, \alpha_1, \alpha_2) - W_{\nu-1,\mu}(0, 0, \alpha_1, \alpha_2)) + \frac{1}{2\nu + 1} (T_{\mu,\nu+1}(\alpha_{12}) - T_{\mu,\nu-1}(\alpha_{12}) - T_{\nu+1,\mu}(\alpha_{12}) + T_{\nu-1,\mu}(\alpha_{12})), \quad (97)$$

where $\alpha_{12} = \alpha_1 + \alpha_2$ and $T_{\nu\mu}$ is an auxiliary function of definition

$$T_{\nu\mu}(\alpha) = \int_1^\infty e^{-\alpha\xi} Q_\nu(\xi) P_\mu(\xi) d\xi. \quad (98)$$

Its evaluation is also discussed in Appendix C.

The use of Eqs. (96) and (97) permits recursive generation (for $p_1 = p_2 = 0$) of a set of $W_{\nu\mu}$ from starting values of W_{00}, W_{10}, W_{01}, W_{11}, or from initial W values for any other four similarly related contiguous index pairs. The diagonal members $W_{\mu\mu}$ are, as already seen, the functions needed for the two-electron integrals. It is possible to devise recursive schemes that may be carried out either in the direction that increases the indices from (0, 0) or in the direction of decreasing index values starting at $(\mu_{\max}, \mu_{\max})$.

For upward recursion, we need starting values of W_{00}, W_{11}, W_{10}, and W_{01} for $p_1 = p_2 = 0$. The first two of these are instances of W_0^0 and W_1^0 and may be obtained by methods described earlier. From their explicit forms, the other starting values reduce to

$$W_{10}(0, 0, \alpha_1, \alpha_2) = W_0^0(1, 0, \alpha_1, \alpha_2) - \frac{e^{-(\alpha_1+\alpha_2)}}{\alpha_1(\alpha_1 + \alpha_2)}, \tag{99}$$

$$W_{01}(0, 0, \alpha_1, \alpha_2) = W_0^0(0, 1, \alpha_1, \alpha_2) - \frac{e^{-(\alpha_1+\alpha_2)}}{\alpha_2(\alpha_1 + \alpha_2)}. \tag{100}$$

For downward recursion, we require (again for $p_1 = p_2 = 0$) starting values of $W_{\mu\mu}$, $W_{\mu,\mu-1}$, $W_{\mu-1,\mu}$, and $W_{\mu-1,\mu-1}$ for $\mu = \mu_{\max}$, where $\mu_{\max}$ is the largest index value needed. These W values can be constructed from explicit formulas for the $w_{\nu\mu}$. The processes used in obtaining Eqs. (39) and (54) lead in a straightforward manner to the closed formula (suitable for large α)

$$w_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = L_\nu^0(0, \alpha_1) - \sum_s \mathcal{A}_s^{\mu 0} \times \sum_{j=0}^{s} \frac{s!}{j!\alpha_2^{s-j+1}} L_\nu^0(j, \alpha_1 + \alpha_2), \tag{101}$$

and the small-α formula

$$w_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = \sum_s \mathcal{A}_s^{\mu 0} \sum_{j=0}^{\infty} \frac{\alpha_2^j s!}{(s + j + 1)!} \times L_\nu^0(s + j + 1, \alpha_1 + \alpha_2) - L_\nu^0(0, \alpha_1)\bar{\imath}_\mu^0(0, \alpha_2). \tag{102}$$

As we shall see in the next section, both upward and downward recursion are unstable, but, as for L, the instability under downward recursion is only from an uncontrollable contamination by the solution to the homogeneous recurrence problem complementary to the inhomogeneous problem defined by Eqs. (96) and (97). Because the homogeneous parts of these equations are, apart from sign, recurrence relations for the spherical Bessel functions i_ν and i_μ, the complementary problem for $W_{\nu\mu}(0, 0, \alpha_1, \alpha_2)$ can be seen to have as a solution (that will grow on downward recursion) an arbitrary multiple of $(-1)^{\nu+\mu} i_\nu(\alpha_1) i_\mu(\alpha_2)$.

Next we need equations that can be used to increase the values of p_1 and p_2 from zero so as to make $W_{\nu\mu}(p_1, p_2, \alpha_1, \alpha_2)$. Because Q_ν and P_ν satisfy the same recurrence relation (formula 8.5.3 of Ref. [15]), insertion of that relation (for ν) into the integral forms of the $w_{\nu\mu}$ and $w_{\mu\nu}$ on the right side of Eq. (88) leads to

$$W_{\nu\mu}(p_1 + 1, p_2, \alpha_1, \alpha_2) = \frac{\nu + 1}{2\nu + 1} \times W_{\nu+1,\mu}(p_1, p_2, \alpha_1, \alpha_2) + \frac{\nu}{2\nu + 1} \times W_{\nu-1,\mu}(p_1, p_2, \alpha_1, \alpha_2). \tag{103}$$

Invoking Eq. (95), the indices and arguments in Eq. (103) can be permuted, yielding a corresponding equation that can be used to increase p_2.

Notice that Eq. (103) cannot be used without modification if $\nu = 0$ because it would then require the use of $W_{-1,\mu}$, which is singular. To obtain a formula valid for $\nu = 0$, we may insert the relation $\xi Q_0(\xi) = Q_1(\xi) + 1$ into Eq. (88), reaching after some manipulation

$$w_{0\mu}(p_1, p_2, \alpha_1, \alpha_2) = w_{1\mu}(p_1 - 1, p_2, \alpha_1, \alpha_2) + \bar{S}_\mu(p_1 - 1, p_2, \alpha_1, \alpha_2). \tag{104}$$

The function $\bar{S}$, related to that introduced for Kotani's recurrence method at Eq. (83), is

$$\bar{S}_\mu(p_1, p_2, \alpha_1, \alpha_2) = \int_1^\infty d\xi_2 P_\mu(\xi_2) \xi_2^{p_2} e^{-\alpha_2\xi_2} \times \int_{\xi_2}^\infty d\xi_1 \xi_1^{p_1} e^{-\alpha_1\xi_1}. \tag{105}$$

The $\bar{S}_\mu$ can be shown to satisfy the recurrence formula

TABLE XI

Evaluation of $W^0_\mu(0, 0, \alpha_1, \alpha_2)$ by recurrence formulas, run at 16S.

μ	Exact	Kotani	Up	Down	Down(adj)
$\alpha_1 = 0.1, \alpha_2 = 0.1$					
0	8.739953135	8.73995(+00)	8.73995(+00)	1.280151805(+25)	8.739953135
1	1.608085793	1.60809(+00)	1.60809(+00)	1.420496809(+22)	1.608085793
2	0.622926229	6.22926(−01)	6.22926(−01)	5.678742290(+18)	0.622926229
4	0.198827759	1.98828(−01)	1.99476(−01)	1.430031122(+11)	0.198827759
5	0.133813371	1.30098(−01)	5.38506(+00)	1.181678649(+07)	0.133813371
6	0.096108006	−5.20327(+00)	6.35530(+04)	6.992425292(+02)	0.096108006
7	0.072331604	1.73713(+05)	1.07419(+09)	1.034023415(−01)	0.072331604
10	0.037013909	−4.74794(+17)	2.52218(+22)	3.701390923(−02)	0.037013909
12	0.026141100	5.33699(+27)	5.88451(+31)	2.614110027(−02)	0.026141100
$\alpha_1 = 0.5, \alpha_2 = 0.1$					
0	1.916547773	1.91655(+00)	1.91655(+00)	2.776803723(+19)	1.916547773
1	0.367049738	3.67050(−01)	3.67050(−01)	1.516544091(+17)	0.367049738
2	0.141286304	1.41286(−01)	1.41286(−01)	3.010801039(+14)	0.141286304
3	0.073392802	7.33928(−02)	7.33928(−02)	3.059647499(+11)	0.073392802
4	0.044713289	4.47133(−02)	4.47242(−02)	1.883731946(+08)	0.044713289
5	0.030035927	3.00214(−02)	4.77377(−02)	7.769908661(+04)	0.030035927
6	0.021546968	4.77133(−02)	4.29720(+01)	2.297885113(+01)	0.021546968
7	0.016203671	4.03409(+01)	1.45436(+05)	2.130010139(−02)	0.016203671
10	0.008281674	−2.31852(+12)	2.73979(+16)	8.281674211(−03)	0.008281674
12	0.005846647	−4.89357(+19)	2.55970(+24)	5.846646928(−03)	0.005846647
$\alpha_1 = 1, \alpha_2 = 0.5$					
0	0.1935303369	1.93530(−01)	1.93530(−01)	1.095389712(+17)	0.1935303369
1	0.0498022201	4.98022(−02)	4.98022(−02)	5.621890929(+15)	0.0498022201
2	0.0210863237	2.10863(−02)	2.10863(−02)	1.085889703(+14)	0.0210863237
5	0.0047833533	4.78335(−03)	4.78336(−03)	2.713592361(+07)	0.0047833533
6	0.0034512124	3.45122(−03)	3.45349(−03)	7.977360317(+04)	0.0034512124
7	0.0026049521	2.60213(−03)	3.38159(−03)	1.764140967(+02)	0.0026049521
8	0.0020347736	1.41688(−03)	3.53753(−01)	3.060701290(−01)	0.0020347736
9	0.0016327382	−3.34324(−01)	2.04288(+02)	2.052526286(−03)	0.0016327382
13	0.0008123767	−2.32314(+11)	1.74073(+14)	8.123767100(−04)	0.0008123767
15	0.0006169540	−1.76890(+17)	4.28360(+20)	6.169539613(−04)	0.0006169540
$\alpha_1 = 1, \alpha_2 = 1$					
0	0.07399640997	7.39964(−02)	7.39964(−02)	6.339848479(+12)	0.07399640997
1	0.02090000776	2.09000(−02)	2.09000(−02)	6.212486627(+11)	0.02090000776
2	0.00919079277	9.19079(−03)	9.19079(−03)	2.350877131(+10)	0.00919079277
5	0.00215072856	2.15073(−03)	2.15073(−03)	4.586987797(+04)	0.00215072856
6	0.00155656041	1.55656(−03)	1.55654(−03)	2.686690959(+02)	0.00155656042
7	0.00117725821	1.17732(−03)	1.17360(−03)	1.185973194(+00)	0.00117725821
8	0.00092085537	9.20398(−04)	8.84723(−05)	4.995290663(−03)	0.00092085537
9	0.00073964501	7.01067(−04)	−2.41700(−01)	7.508752870(−04)	0.00073964501
10	0.00060694456	5.74404(−02)	−8.80607(+01)	6.069699228(−04)	0.00060694456
13	0.00036877452	1.28106(+07)	−1.30024(+10)	3.687745209(−04)	0.00036877452
15	0.00028020323	−2.77027(+12)	−8.01566(+15)	2.802032260(−04)	0.00028020323
$\alpha_1 = 2, \alpha_2 = 1$					
0	0.01602277773	1.60228(−02)	1.60228(−02)	2.080680502(+08)	0.01602277773
1	0.00483367166	4.83367(−03)	4.83367(−03)	3.499672708(+07)	0.00483367166
2	0.00218477492	2.18477(−03)	2.18477(−03)	2.458358125(+06)	0.00218477492
4	0.00076449733	7.64497(−04)	7.64497(−04)	2.189846026(+03)	0.00076449734
5	0.00052303995	5.23040(−04)	5.23040(−04)	3.498695694(+01)	0.00052303995
7	0.00028736738	2.87367(−04)	2.87326(−04)	3.807990133(−03)	0.00028736738
8	0.00022500626	2.24971(−04)	2.20270(−04)	2.490011958(−04)	0.00022500626
9	0.00018085837	1.78919(−04)	−5.16785(−04)	1.809896731(−04)	0.00018085837
10	0.00014848905	1.68632(−04)	−1.27705(−01)	1.484896371(−04)	0.00014848905
11	0.00012406506	−5.51049(−03)	−2.85419(+01)	1.240650586(−04)	0.00012406506
12	0.00010519060	7.81793(+00)	−7.62700(+03)	1.051905964(−04)	0.00010519060
13	0.00009030724	5.55287(+02)	−2.40405(+06)	9.030723619(−05)	0.00009030724
15	0.00006864211	4.40144(+08)	−3.73552(+11)	6.864211030(−05)	0.00006864211

(Continued)

TABLE XI
(Continued)

μ	Exact	Kotani	Up	Down	Down(adj)
$\alpha_1 = 2, \alpha_2 = 2$					
0	0.003596217328	3.59622(−03)	3.59622(−03)	3.272264117(+10)	0.003596217328
1	0.001192183291	1.19218(−03)	1.19218(−03)	9.447259133(+09)	0.001192183291
2	0.000564354650	5.64355(−04)	5.64355(−04)	1.231903818(+09)	0.000564354650
7	0.000078364133	7.83641(−05)	7.83641(−05)	5.013171248(+01)	0.000078364133
8	0.000061506972	6.15068(−05)	6.15071(−05)	6.772166202(−01)	0.000061506972
9	0.000049525470	4.95211(−05)	4.95326(−05)	7.405614590(−03)	0.000049525470
10	0.000040714696	4.11562(−05)	4.13759(−05)	1.063524513(−04)	0.000040714696
11	0.000034051742	1.21438(−04)	1.08401(−04)	3.454126397(−05)	0.000034051742
12	0.000028893806	8.85903(−04)	1.00236(−02)	2.889690235(−05)	0.000028893806
13	0.000024820982	−2.50015(−01)	1.58332(+00)	2.482099856(−05)	0.000024820982
16	0.000016681839	1.56036(+06)	1.50301(+07)	1.668183906(−05)	0.000016681839
18	0.000013291936	2.38977(+11)	1.27166(+12)	1.329193638(−05)	0.000013291936

"Exact" is by closed formula at 60S (all digits shown are correct). "Kotani" is Kotani's scheme; the remaining columns refer to the scheme introduced in this work: "Up" starts from $\mu = 0$ and "down" from the largest μ value shown. "Down(adj)" includes adjustment(s) based on the complementary homogeneous recurrence problem (see text). Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied.

$$\alpha_1 \bar{S}_\mu(p_1, p_2, \alpha_1, \alpha_2) = p_1 \bar{S}_\mu(p_1 - 1, p_2, \alpha_1, \alpha_2) + k^0_\mu(p_1 + p_2, \alpha_1 + \alpha_2). \quad (106)$$

This formula is parallel to but better conditioned than the corresponding formula for S_μ, Eq. (87), and is also self-starting, as the term with coefficient p_1 can be omitted when $p_1 = 0$. We also need

$$w_{\mu 0}(p_2, p_1, \alpha_2, \alpha_1) = w_{\mu 1}(p_2, p_1 - 1, \alpha_2, \alpha_1), \quad (107)$$

which follows directly from the relation $\xi P_0(\xi) = P_1(\xi)$. Combining Eqs. (104) and (107), we have

$$W_{0\mu}(p_1, p_2, \alpha_1, \alpha_2) = W_{1\mu}(p_1 - 1, p_2, \alpha_1, \alpha_2) + \bar{S}_\mu(p_1 - 1, p_2, \alpha_1, \alpha_2). \quad (108)$$

Even though our ultimate need is only for $W_{\nu\mu}(p_1, p_2, \alpha_1, \alpha_2)$ with $\nu = \mu$, the use of these recurrence relations will require generation (except when p_1 and p_2 are at their maximal values) of $W_{\nu\mu}$ with $\nu \neq \mu$.

The final stage of the new recursive process is to increase σ when necessary. This can be done with Kotani's formula, Eq. (77).

Numerical Behavior of the Recurrence Formulas for W^σ_μ

In Tables XI and XII we present data illustrative of the behavior of the recursive procedures for determining $W^0_\mu(0, 0, \alpha_1, \alpha_2)$. We chose examples with $p_1 = p_2 = 0$ because those parameter values tend to produce results subject to the largest errors. The data span a wide range of α_1, α_2 values to provide the information needed to choose among the recursive methods, and should be examined with reference to the expansion lengths that will be needed (cf. Tables I–IV). All the recursive processes were run at a precision of 16S, with any starting values that were needed obtained at full 16S accuracy.

Looking first at the W values from Kotani's scheme, we see that they become unstable for μ values that will be needed in the Neumann expansion, with the instability so extreme that for $\alpha < 1$ it is doubtful that final integrals with more than two or three significant figures can be obtained. Even at $\alpha = 10$ the instability will be significant for accurate investigations.

We turn therefore to recursion based on the formulas involving $W_{\nu\mu}$, Eqs. (96) and (97). For upward recursion (only obtaining intermediate quantities needed when $p_1 = p_2 = 0$), we proceeded as follows:

For each μ, starting with $\mu = 2$, assuming the availability of $W_{\mu-1,\mu-1}$, $W_{\mu-1,\mu-2}$, $W_{\mu-2,\mu-1}$, and $W_{\mu-2,\mu-2}$,

1. Make $W_{\mu,\mu-2}$ from $W_{\mu-2,\mu-2}$ and $W_{\mu-1,\mu-2}$.
2. Make $W_{\mu,\mu-1}$ from $W_{\mu-2,\mu-1}$ and $W_{\mu-1,\mu-1}$.
3. Make $W_{\mu-1,\mu}$ from $W_{\mu-1,\mu-1}$ and $W_{\mu-1,\mu-2}$.
4. Make $W_{\mu,\mu}$ from $W_{\mu,\mu-2}$ and $W_{\mu,\mu-1}$.

TABLE XII

Evaluation of $W^{o}_{\mu}(0, 0, \alpha_1, \alpha_2)$ by recurrence formulas, run at 16S.

μ	Exact	Kotani	Down	Down(adj)
$\alpha_1 = 5, \alpha_2 = 2$				
0	8.47144845465(−05)	8.47144845465(−05)	2.36853748291(+06)	8.47144845465(−05)
1	3.04665064084(−05)	3.04665064084(−05)	1.01823560662(+06)	3.04665064084(−05)
5	3.93929423680(−06)	3.93929423680(−06)	2.35090943327(+02)	3.93929423680(−06)
6	2.88729619242(−06)	2.88729619216(−06)	1.22018964949(+01)	2.88729619242(−06)
7	2.20230808345(−06)	2.20230808508(−06)	4.89325631427(−01)	2.20230808345(−06)
8	1.73288877107(−06)	1.73288867289(−06)	1.55897013103(−02)	1.73288877106(−06)
9	1.39786395954(−06)	1.39786897045(−06)	4.04862887590(−04)	1.39786395954(−06)
10	1.15074354340(−06)	1.15080669434(−06)	9.79554734990(−06)	1.15074354340(−06)
11	9.63428660285(−07)	9.62422878926(−07)	1.11918683478(−06)	9.63428660285(−07)
12	8.18161643957(−07)	1.02166685934(−06)	8.20553259456(−07)	8.18161643957(−07)
13	7.03291220024(−07)	−2.58044176717(−06)	7.03322876783(−07)	7.03291220024(−07)
18	3.77323093797(−07)	−2.80155329642(+04)	3.77323093797(−07)	3.77323093797(−07)
20	3.07783313682(−07)	−8.02472602537(+08)	3.07783313682(−07)	3.07783313682(−07)
$\alpha_1 = 5, \alpha_2 = 5$				
0	2.10842876143(−06)	2.10842876143(−06)	6.67524870318(−03)	2.10842876143(−06)
1	8.55733906530(−07)	8.55733906530(−07)	4.27263508089(−03)	8.55733906523(−07)
5	1.30041072522(−07)	1.30041072522(−07)	1.69529710698(−05)	1.30041072522(−07)
6	9.65066979448(−08)	9.65066979460(−08)	2.08938832630(−06)	9.65066979448(−08)
7	7.42594348696(−08)	7.42594348581(−08)	2.60167503877(−07)	7.42594348696(−08)
8	5.88040135476(−08)	5.88040134972(−08)	7.27712007040(−08)	5.88040135476(−08)
10	3.93767192938(−08)	3.93767287512(−08)	3.94210367311(−08)	3.93767192938(−08)
12	2.81372634493(−08)	2.81375582037(−08)	2.81373353536(−08)	2.81372634493(−08)
13	2.42299242168(−08)	2.42662608099(−08)	2.42299265363(−08)	2.42299242168(−08)
14	2.10782646537(−08)	2.17941330246(−08)	2.10782647190(−08)	2.10782646537(−08)
15	1.85003249207(−08)	3.85191686834(−08)	1.85003249223(−08)	1.85003249207(−08)
16	1.63655352953(−08)	1.44332546569(−06)	1.63655352954(−08)	1.63655352953(−08)
18	1.30673920615(−08)	−2.50791112630(−03)	1.30673920615(−08)	1.30673920615(−08)
20	1.06712413227(−08)	5.07367687012(+00)	1.06712413227(−08)	1.06712413227(−08)
$\alpha_1 = 10, \alpha_2 = 5$				
0	7.89634161079(−09)	7.89634161079(−09)	−8.62617909542(−03)	7.89634161079(−09)
1	3.39784882199(−09)	3.39784882199(−09)	−6.21155622758(−03)	3.39784882199(−09)
2	1.86990029556(−09)	1.86990029556(−09)	−3.27415562467(−03)	1.86990029556(−09)
3	1.16527643488(−09)	1.16527643488(−09)	−1.29287215561(−03)	1.16527643488(−09)
4	7.87317633723(−10)	7.87317633723(−10)	−3.91734393137(−04)	7.87317633723(−10)
5	5.63657375318(−10)	5.63657375318(−10)	−9.31411072730(−05)	5.63657375319(−10)
6	4.21541759504(−10)	4.21541759505(−10)	−1.77308806484(−05)	4.21541759510(−10)
8	2.59361757430(−10)	2.59361757609(−10)	−3.53077886146(−07)	2.59361757430(−10)
10	1.74640385499(−10)	1.74640377818(−10)	−3.31338774619(−09)	1.74640385499(−10)
12	1.25218122153(−10)	1.25217923776(−10)	1.06518416591(−10)	1.25218122153(−10)
14	9.40128138952(−11)	9.40483397108(−11)	9.39542658281(−11)	9.40128138952(−11)
16	7.31046871961(−11)	7.56112907411(−11)	7.31045737002(−11)	7.31046871961(−11)
17	6.51594181099(−11)	4.67648338242(−10)	6.51594138709(−11)	6.51594181099(−11)
18	5.84354634514(−11)	−1.21023719273(−09)	5.84354633085(−11)	5.84354634514(−11)
22	3.97511395681(−11)	−9.72310284317(−03)	3.97511395681(−11)	3.97511395681(−11)
24	3.35948829629(−11)	1.59838369903(+01)	3.35948829629(−11)	3.35948829629(−11)

(Continued)

TABLE XII
(Continued)

μ	Exact	Kotani	Down	Down(adj)
$\alpha_1 = 10, \alpha_2 = 10$				
0	3.04106081983(−11)	3.04106081983(−11)	9.96790106679(−10)	3.04106081983(−11)
1	1.41220853920(−11)	1.41220853920(−11)	7.96889486332(−10)	1.41220853920(−11)
2	8.18004348693(−12)	8.18004348693(−12)	5.23163676483(−10)	8.18004348693(−12)
6	2.02053511663(−12)	2.02053511663(−12)	1.56927849276(−11)	2.02053511663(−12)
8	1.26481236138(−12)	1.26481236113(−12)	2.03947055203(−12)	1.26481236138(−12)
10	8.60469052907(−13)	8.60469040668(−13)	8.84260756709(−13)	8.60469052907(−13)
12	6.21000033888(−13)	6.21000002884(−13)	6.21421492183(−13)	6.21000033888(−13)
14	4.68275821816(−13)	4.68281225234(−13)	4.68280367688(−13)	4.68275821816(−13)
16	3.65237391862(−13)	3.65099782854(−13)	3.65237423138(−13)	3.65237391862(−13)
17	3.25925288489(−13)	3.18735984836(−13)	3.25925290709(−13)	3.25925288489(−13)
18	2.92586732470(−13)	3.52937312317(−13)	2.92586732613(−13)	2.92586732470(−13)
19	2.64077991709(−13)	−1.16479619553(−13)	2.64077991718(−13)	2.64077991709(−13)
20	2.39514947181(−13)	−2.22843163621(−12)	2.39514947182(−13)	2.39514947181(−13)
22	1.99603272525(−13)	4.91366013984(−09)	1.99603272525(−13)	1.99603272525(−13)
24	1.68852732097(−13)	−1.90653796344(−06)	1.68852732097(−13)	1.68852732097(−13)

"Exact" is by closed formula at 60S (all digits shown are correct). "Kotani" is Kotani's scheme; the remaining columns refer to the scheme introduced in this work: "Down" starts from the largest μ value shown and "down(adj)" includes adjustments based on the complementary homogeneous recurrence problem (see text). Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied.

Unfortunately, as seen in the column labeled "up" in Table XI, this upward recursion procedure exhibits even greater instability than Kotani's scheme.

We then examined downward recursion based on Eqs. (96) and (97), running the four-step procedure of the preceding paragraph in reverse and starting from W values obtained from Eq. (101) or (102). The results of this process are shown, to high precision, in the table columns labeled "down." We found apparent instability at all α values.

As was the case with the inhomogeneous recurrence formula for L, the formulas in use here are only unstable for downward recurrence to the extent that they contain an uncontrollable multiple of the solution to the complementary homogeneous recurrence problem. However, in contrast to the situation for L, a round-off contamination for large μ increases so rapidly as μ decreases that (at least for small α) the result at $\mu = 0$ is in error by many orders of magnitude.

To more fully understand the implications of the use of the downward recurrence procedure for W and prepare for later use of the formulas to increase p_1 and p_2, we need to look in some detail at the sequence of operations involved. Continuing for the special case $p_1 = p_2 = 0$, we start from values of $W_{n,n}$, $W_{n,n-1}$, $W_{n-1,n}$ and $W_{n-1,n-1}$ for $n = \mu_{\max} + p_{\max} + \sigma$, where $\mu_{\max}$ and $p_{\max}$ are the maximum index values needed for the Neumann expansion. Then,

1. For each j from 2 through $2p_{\max}$:
   (a) Make $W_{n-k,n-j}$ from $W_{n-k,n-j+1}$ and $W_{n-k,n-j+2}$ for k from 0 through $j - 1$, using Eq. (96);
   (b) Make $W_{n-j,n-k}$ from $W_{n-j+1,n-k}$ and $W_{n-j+2,n-k}$ for k from 0 through j, using Eq. (97).
2. For each j from $2p_{\max} + 1$ through n:
   (a) Make $W_{n-k,n-j}$ from $W_{n-k,n-j+1}$ and $W_{n-k,n-j+2}$ for k from $j - 2p_{\max}$ through $j - 1$, using Eq. (96);
   (b) Make $W_{n-j,n-k}$ from $W_{n-j+1,n-k}$ and $W_{n-j+2,n-k}$ for k from $j - 2p_{\max}$ through j, using Eq. (97).

In general, this recursive scheme uses steps that further reduce the smaller of the two indices of W. However, some of the iterative steps combine entries on both sides of the diagonal (in index space), and this will cause the W of small indices to have an ancestry that includes substantial contributions from all four starting W values. The result is that, to high accuracy, the entire set of W contains a con-

TABLE XIII

Evaluation of $W_{\nu\mu}(0, 0, 0.1, 0.1)$, run at 16S.

ν	μ	Exact	Down	Down(adj)
A. Original calculation and adjustment				
⋆0	0	8.739953135424(+00)	1.280151804946(+25)	0.000000000000(−01)
⋆0	1	1.872679386332(+01)	−4.264330607973(+23)	1.000000000000(+08)
⋆0	2	2.021149301499(+02)	8.526225538084(+21)	−5.000000000000(+06)
⋆0	3	3.949878871895(+03)	−1.217838931482(+20)	0.000000000000(−01)
⋆0	4	1.135717675464(+05)	1.353017709414(+18)	1.120000000000(+05)
⋆0	5	4.340660907517(+06)	−1.229930094346(+16)	4.340660000000(+06)
⋆0	6	2.076037287380(+08)	9.460536353828(+13)	2.076037285700(+08)
⋆1	1	1.608085792767(+00)	1.420496808569(+22)	0.000000000000(−01)
⋆1	2	5.564561165474(+00)	−2.840182265264(+20)	2.000000000000(+05)
⋆1	3	7.515345579695(+01)	4.056759371065(+18)	−3.000000000000(+03)
⋆1	4	1.660479775271(+03)	−4.507055186028(+16)	1.730000000000(+03)
⋆1	5	5.162065025776(+04)	4.097036405554(+14)	5.162040000000(+04)
⋆1	6	2.083355609407(+06)	−3.151402777890(+12)	2.083355615000(+06)
1	7	1.037477079394(+08)	2.111228961069(+10)	1.037477079393(+08)
⋆2	2	6.229262290143(−01)	5.678742290204(+18)	−2.000000000000(+03)
⋆2	3	2.597091237938(+00)	−8.111201623712(+16)	4.000000000000(+01)
⋆2	4	3.914143109603(+01)	9.011536056049(+14)	3.790000000000(+01)
⋆2	5	9.279025757406(+02)	−8.191732685505(+12)	9.279060000000(+02)
⋆2	6	3.030778454450(+04)	6.301012750463(+10)	3.030778443000(+04)
2	7	1.269066662741(+06)	−4.187817759108(+08)	1.269066662742(+06)
2	8	6.503209870616(+07)	6.750290952165(+07)	6.503209870616(+07)
⋆3	3	3.253294243531(−01)	1.158559209387(+15)	−1.000000000000(+00)
⋆3	4	1.490503977877(+00)	−1.287158003561(+13)	1.510000000000(+00)
⋆3	5	2.394203576779(+01)	1.170061821531(+11)	2.394200000000(+01)
⋆3	6	5.937457607600(+02)	−9.000008089856(+08)	5.937457626000(+02)
3	7	2.005909831212(+04)	6.019833171881(+06)	2.005909831210(+04)
3	8	8.623517128234(+05)	8.270600167501(+05)	8.623517128233(+05)
⋆4	4	1.988277587954(−01)	1.430031122026(+11)	1.985000000000(−01)
⋆4	5	9.635603252119(−01)	−1.299937391734(+09)	9.635630000000(−01)
⋆4	6	1.613008069353(+01)	9.999021786034(+06)	1.613008067200(+01)
4	7	4.126532503980(+02)	−6.624477052026(+04)	4.126532503982(+02)
4	8	1.428518708968(+04)	1.467727744373(+04)	1.428518708968(+04)
⋆5	5	1.338133713293(−01)	1.181678648838(+07)	1.338133600000(−01)
⋆5	6	6.729673650094(−01)	−9.089302257384(+04)	6.729673651500(−01)
5	7	1.159457232246(+01)	6.175287812069(+02)	1.159457232246(+01)
5	8	3.034249498425(+02)	2.998607413110(+02)	3.034249498425(+02)
⋆6	6	9.610800598616(−02)	6.992425291432(+02)	9.610800598510(−02)
6	7	4.961750598599(−01)	−4.164618310502(+00)	4.961750598600(−01)
6	8	8.731502898355(+00)	8.758918481187(+00)	8.731502898355(+00)
7	7	7.233160415365(−02)	1.034023415335(−01)	7.233160415365(−02)
7	8	3.807716684707(−01)	3.805889050854(−01)	3.807716684707(−01)
11	11	3.087264619485(−02)	3.087264619485(−02)	3.087264619485(−02)
11	12	1.699650665672(−01)	1.699650665672(−01)	1.699650665672(−01)
12	12	2.614110027192(−02)	2.614110027192(−02)	2.614110027192(−02)

(Continued)

sistent amount of contamination by the solution to the complementary recurrence problem.

Based on the above observation, we remove the complementary solution contamination by requiring a correct value for W_{00}, recalling from the preceding section that the complementary problem has for indices ν, μ the relevant solution $(-1)^{\nu+\mu} i_\nu(\alpha_1) i_\mu(\alpha_2)$. Formulas for the adjustment are therefore

TABLE XIII
(Continued)

ν	μ	Exact	Down	Down(adj)
B. Recalculation, from $W_{7,7}$, $W_{8,7}$, $W_{7,8}$, and $W_{8,8}$				
⋆0	0	8.739953135424(+00)	−4.862723891941(+09)	8.739953000000(+00)
⋆0	1	1.872679386332(+01)	1.619828576970(+08)	1.872679380000(+01)
⋆0	2	2.021149301499(+02)	−3.238529459439(+06)	2.021149301520(+02)
0	3	3.949878871895(+03)	5.021013063593(+04)	3.949878871895(+03)
0	4	1.135717675464(+05)	1.130578166597(+05)	1.135717675464(+05)
0	5	4.340660907517(+06)	4.340665579472(+06)	4.340660907517(+06)
0	6	2.076037287380(+08)	2.076037287020(+08)	2.076037287380(+08)
⋆1	1	1.608085792767(+00)	−5.395830163728(+06)	1.608085797000(+00)
⋆1	2	5.564561165474(+00)	1.078913803702(+05)	5.564561165400(+00)
1	3	7.515345579695(+01)	−1.465827908818(+03)	7.515345579695(+01)
1	4	1.660479775271(+03)	1.677600061232(+03)	1.660479775271(+03)
1	5	5.162065025776(+04)	5.162049462968(+04)	5.162065025776(+04)
⋆2	2	6.229262290143(−01)	−2.156477173439(+03)	6.229262290150(−01)
2	3	2.597091237938(+00)	3.340791683416(+01)	2.597091237938(+00)
2	4	3.914143109603(+01)	3.879912316354(+01)	3.914143109603(+01)
2	5	9.279025757406(+02)	9.279056874133(+02)	9.279025757406(+02)
2	6	3.030778454450(+04)	3.030778452057(+04)	3.030778454450(+04)
3	3	3.253294243531(−01)	−1.147553793456(−01)	3.253294243531(−01)
3	4	1.490503977877(+00)	1.495393315192(+00)	1.490503977877(+00)
3	5	2.394203576779(+01)	2.394199132237(+01)	2.394203576779(+01)
3	6	5.937457607600(+02)	5.937457611019(+02)	5.937457607600(+02)
4	4	1.988277587954(−01)	1.987734383118(−01)	1.988277587954(−01)
4	5	9.635603252119(−01)	9.635608189999(−01)	9.635603252119(−01)
4	6	1.613008069353(+01)	1.613008068973(+01)	1.613008069353(+01)
5	5	1.338133713293(−01)	1.338133668407(−01)	1.338133713293(−01)
5	6	6.729673650094(−01)	6.729673650440(−01)	6.729673650094(−01)
6	6	9.610800598616(−02)	9.610800598589(−02)	9.610800598616(−02)
C. Second recalculation, from $W_{3,3}$, $W_{4,3}$, $W_{3,4}$, and $W_{4,4}$				
0	0	8.739953135424(+00)	8.739957476798(+00)	8.739953135424(+00)
0	1	1.872679386332(+01)	1.872679371870(+01)	1.872679386332(+01)
0	2	2.021149301499(+02)	2.021149301528(+02)	2.021149301499(+02)
1	1	1.608085792767(+00)	1.608085797584(+00)	1.608085792767(+00)
1	2	5.564561165474(+00)	5.564561165377(+00)	5.564561165474(+00)
2	2	6.229262290143(−01)	6.229262290162(−01)	6.229262290143(−01)

"Exact" is by closed formula at 60S (all digits shown are correct), "down" is by downward recursion, and "down(adj)" includes an adjustment based on the complementary homogeneous recurrence problem (see text). Numbers in parentheses are powers of 10 by which the preceding numbers must be multiplied. Starred entries are recalculated in a following section of the table.

$$F = \frac{W_{00}(0, 0, \alpha_1, \alpha_2) - \bar{W}_{00}(0, 0, \alpha_1, \alpha_2)}{i_0(\alpha_1) i_0(\alpha_2)}, \quad (109)$$

$$W_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = \bar{W}_{\nu\mu}(0, 0, \alpha_1, \alpha_2) + (-1)^{\nu+\mu} i_\nu(\alpha_1) i_\mu(\alpha_2) F, \quad (110)$$

where $\bar{W}$ is an immediate result of the recursion and W_{00} in Eq. (109) is a previously computed accurate value.

The recursive process and its adjustment are illustrated by the entries in Table XIII, section A, where we compare exact W values with the result of downward recursion before and after adjustment. Except where differencing errors in the adjustment cause a large loss in precision, we see that even values that were in error by orders of magnitude become highly accurate when adjusted. This observation confirms our claim that the recursive process is generating information of high-precision content.

The differencing errors noted in the previous paragraph arise because the complementary solu-

tion is present with a large coefficient F. It is therefore possible to improve the situation by restarting the downward recursion, using as initial values adjusted W for the smallest μ at which the adjustment was not subject to excessive differencing error. Our working criterion, applied to the diagonal $W_{\mu\mu}$, was the smallest μ for which $|\bar{W}/W|$ did not exceed 10^3. Using this criterion, the data in Table XIII, section A, indicated a need to recalculate for $\mu = 6$, which (referring to the detailed scheme) meant starting from the adjusted values of $W_{7,7}$, $W_{7,8}$, $W_{8,7}$, and $W_{8,8}$ and therefrom regenerating all W with index values ≤ 6. The recalculated numbers are shown in Table XIII, section B, together with adjustments based on the recalculated values. The validity of this technique is attested by the convergence toward exact W values.

The above-described process can be repeated as needed. In the case tabulated, the recalculated values exhibit an excessive differencing error at $\mu = 2$, and a second recalculation and subsequent adjustment are shown in Table XIII, section C. All values are now highly accurate. Similar accuracy patterns are obtained for larger α values and for $\alpha_1 \neq \alpha_2$.

Returning now to Tables XI and XII, we call attention to the column labeled "down(adj)," which includes an automatic application of the above-described iterative adjustment. The μ values at which additional adjustments occur depend both upon the α values and upon the starting point for the downward recursion. In particular, for $\alpha_1 = 2$, $\alpha_2 = 1$, a second adjustment was needed at $\mu = 5$; for α_1, α_2 pairs (0.5, 0.1) and (10, 5) it was needed at $\mu = 6$; for (1, 0.5) and (1, 1) at $\mu = 7$; for (5, 2) at $\mu = 8$; and for (0.1, 0.1) two additional adjustments were required, at $\mu = 6$ and $\mu = 2$. Only the initial adjustment was needed for (5, 5) and (10, 10). The essentially complete agreement between the "exact" and "down(adj)" columns attests to the validity and effectiveness of this approach for general values of α_1 and α_2.

Once a highly accurate set of $W_{\nu\mu}(0, 0, \alpha_1, \alpha_2)$ has been obtained, Eqs. (103) and (108) can be used to increase p_1 and p_2. Because all the W are positive and the coefficients in Eq. (103) are positive and sum to unity, these equations will always exhibit stable behavior and there is no need to examine test calculations. Eq. (77), for advancing σ, has also been found to be stable and its use will not be illustrated here.

ACKNOWLEDGMENT

This work was supported by U.S. National Science Foundation Grant DMR-9980015.

Appendix A: Evaluation of Coefficients $C_i(p, q)$

We illustrate with the array $C_1(p, q)$. Using Maple, we form $r_a^{n_a-1} r_b^{n_b-1} P_{l_a}^{|m_a|}(\cos\theta_a) P_{l_b}^{|m_b|}(\cos\theta_b)(\xi^2 - \eta^2)[(\xi^2 - 1)(1 - \eta^2)]^{-|M_1|/2}$, and substitute therein the explicit forms given in Eqs. (5) and (6) for r_a, r_b, $\cos\theta_a$, and $\cos\theta_b$. As of Maple V release 6, explicit forms can be obtained for the Legendre polynomials $P_l(x)$ using the package `orthopoly`, but associated Legendre functions must be obtained by repeated differentiation of the P_l [use `diff(f, x$n)` to obtain the nth derivative of f with respect to x]. The substitutions are conveniently carried out using the `subs` command. When this process has been completed, the result will be a polynomial in ξ and η.

The easiest way to extract the coefficients from a multivariate polynomial in Maple is by repeated differentiation, with the result evaluated at $\xi = \eta = 0$. The coefficients may then be stored in arrays and exported into a production computer program.

Appendix B: Evaluation of $M_\mu^\sigma(p, \alpha)$

After substituting for E_n using Eq. (43), we can write $M_\mu^\sigma(p, \alpha) = S_1 + S_2$, where

$$S_1 = E_1(\alpha) \sum_{k=k_0}^{\infty} \times \frac{(-1)^{p+\mu}(2k + \mu - \sigma)!\alpha^{2k-p+\mu-\sigma}}{(2k + 2\mu + 1)!!(2k)!!(2k + \mu - \sigma - p)!}, \quad (111)$$

$$S_2 = e^{-\alpha} \sum_{k=k_0}^{\infty} \sum_{t=0}^{2k+\mu-\sigma-p-1} \times \frac{(-1)^{\sigma+t}(2k + \mu - \sigma)!(2k + \mu - \sigma - p - t - 1)!\alpha^t}{(2k + 2\mu + 1)!!(2k)!!(2k + \mu - \sigma - p)!}, \quad (112)$$

where, as defined in the main text, k_0 is the smallest nonnegative integer such that $2k_0 > p - \mu + \sigma - 1$. S_1 is dealt with easily. We simply recognize that, apart from a factor $(-1)^\mu$, the summation is exactly that appearing in Eq. (22), so that

$$S_1 = E_1(\alpha)(-1)^\mu i_\mu^\sigma(p, \alpha). \quad (113)$$

S_2 may be processed along the lines suggested by Maslen and Trefry [10]. A preliminary cancellation of common factors leads to

$$S_2 = e^{-\alpha} \sum_{k=k_0}^{\infty} \sum_{t=0}^{2k+\mu-\sigma-p-1} \frac{(-1)^{\sigma+t}\alpha^t \prod_{i=0}^{\mu-1}(2k+2\mu-2i)}{\prod_{i=0}^{\mu+\sigma}(2k+\mu-\sigma+i+1)\prod_{i=0}^{t}(2k+\mu-\sigma-p-t+i)}. \quad (114)$$

We next insert partial fraction decompositions for each of the products in the denominator. The general form of the decomposition is

$$\frac{1}{a(a+1)\cdots(a+n)} = \sum_{j=0}^{n} \frac{(-1)^j}{j!(n-j)!(a+j)}, \quad (115)$$

and this operation leads to the result

$$S_2 = e^{-\alpha} \sum_{k=k_0}^{\infty} \sum_{t=0}^{2k+\mu-\sigma-p-1} \sum_{j=0}^{\mu+\sigma} \sum_{l=0}^{t} \frac{(-1)^{\sigma+t+j+l}\alpha^t}{j!(\mu+\sigma-j)!l!(t-l)!} \times \frac{\prod_{i=0}^{\mu-1}(2k+2\mu-2i)}{(2k+\mu-\sigma+j+1)(2k+\mu-\sigma-p-t+l)}. \quad (116)$$

We now wish to remove the k-dependence from the numerator of Eq. (116). We do so by taking advantage of the identity

$$\sum_{j=0}^{n} \frac{(-1)^j j^m}{j!(n-j)!} = 0, \quad 0 \le m < n, \quad (117)$$

which also implies a zero result if j^m is replaced by any polynomial in j of degree less than n. The technique is as follows: Take the first factor of the product in Eq. (116) and the factor $2k + \mu - \sigma + j + 1$ from the denominator of that equation, and note that

$$\frac{2k+2\mu-2i}{2k+\mu-\sigma+j+1} = 1 + \frac{\mu+\sigma-2i-j-1}{2k+\mu-\sigma+j+1}. \quad (118)$$

Making this substitution into the formula for S_2, the "1" will lead to a vanishing contribution when summed over j so it therefore can be omitted. The net effect is the replacement of the factor $2k + 2\mu - 2i$ by $\mu + \sigma - 2i - j - 1$ in the numerator. This process can be repeated for each remaining factor of the numerator, and we thereby reach (after moving the k summation as far to the right as possible)

$$S_2 = e^{-\alpha} \sum_{t=0}^{\infty} \alpha^t {\sum_{j=0}^{\mu+\sigma}}' \sum_{l=0}^{t} \times \frac{(-1)^{\sigma+t+j+l}}{j!(\mu+\sigma-j)!l!(t-l)!} \left(\prod_{i=0}^{\mu-1} (\mu+\sigma-2i-j-1) \right) S_4, \quad (119)$$

where

$$S_4 = \sum_{k=k_1}^{\infty} \times \frac{1}{(2k+\mu-\sigma+j+1)(2k+\mu-\sigma-p-t+l)}. \quad (120)$$

Here k_1 is the smallest nonnegative integer such that $2k_1 \ge t + p - \mu + \sigma + 1$, and we note by placing a prime on the j sum that it is to be restricted to j values of the same parity as $\mu + \sigma$. Changing the summation variable to $k - k_1$, and defining a function

$$T(i,j) = \sum_{k=0}^{\infty} \frac{1}{(2k+i)(2k+j)}, \quad (121)$$

we identify S_4 as $T(2k_1 + \mu - \sigma + j + 1, 2k_1 + \mu - \sigma - p - t + l)$.

The final steps in reducing S_2 are (1) replacement of the product notation by $(\mu + \sigma - j - 1)!!(-1)^{(\mu-\sigma+j)/2}(\mu - \sigma + j - 1)!!$, a replacement that is valid because the elements of the product are odd integers and therefore cannot include zero; (2) changing the summation variable j to $\mu + \sigma - 2j$; and (3) changing the summation variable l to $t - l$. The final result, together with the formula previously obtained for S_1, confirm Eq. (45) of the main text.

Appendix C: Details of Special Function Evaluations

INCOMPLETE GAMMA FUNCTIONS

The functions $A_n(\alpha)$ and $a_n(\alpha)$ introduced respectively in Eqs. (34) and (50) are closely related to the

incomplete gamma functions defined in section 6.5 of Ref. [15]. In particular,

$$A_n(\alpha) = \alpha^{-n-1}\Gamma(n+1, \alpha), \tag{122}$$

$$a_n(\alpha) = \alpha^{-n-1}\gamma(n+1, \alpha). \tag{123}$$

Eq. (51) is thus a statement of the obvious relation

$$\gamma(n+1, \alpha) + \Gamma(n+1, \alpha) = \Gamma(n+1). \tag{124}$$

The A_n are computed stably from A_0 by upward recurrence using Eq. (35). The a_n could in principle be obtained from the A_n by solving Eq. (51), but unless $n > \alpha$ this process produces large differencing errors. Reliable evaluation of the a_n can result from the use of Eq. (52), but a series of a_n may be more conveniently generated recursively.

A suitable recurrence formula can be obtained by first integrating the integral representation of a_n by parts, reaching the formula

$$a_n(\alpha) = \frac{n}{\alpha}\, a_{n-1}(\alpha) - \frac{e^{-\alpha}}{\alpha}. \tag{125}$$

This equation is unstable if used to increase n. Instead, we combine it, in the form written, by an instance of the same equation with n replaced by $n+1$, obtaining

$$a_{n+1}(\alpha) = \left(1 + \frac{n+1}{\alpha}\right) a_n(\alpha) - \frac{n}{\alpha}\, a_{n-1}(\alpha). \tag{126}$$

Because Eq. (126) is homogeneous, it may be used to construct a Miller algorithm similar to that used for the $i_\mu(\beta)$ at Eq. (16). Defining $r_n = a_{n+1}/a_n$, substitution into Eq. (126) yields

$$r_{n-1} = \frac{n}{n+1+\alpha(1-r_n)}, \tag{127}$$

which is used to recur downward in n from an initial approximate value $r_{N+1} = 1$. Then, starting from the explicit formula $a_0(\alpha) = (1 - e^{-\alpha})/\alpha$, we have $a_1 = r_0 a_0$, $a_2 = r_1 a_1$, etc.

INCOMPLETE BESSEL FUNCTIONS

The functions $\bar{\imath}_\mu^\sigma(p, \alpha)$ defined in Eq. (53) can be regarded as incomplete Bessel functions in that the range of integration, $0 \cdots 1$, differs from the ranges $-1 \cdots 1$ and $1 \cdots \infty$, which yield (for $\sigma = p = 0$) the respective spherical Bessel functions $i_\mu(\alpha)$ and $k_\mu(\alpha)$. Similar observations apply to the functions $\bar{k}_\mu^\sigma(p, \alpha)$ defined in Eq. (56). These functions are related to corresponding generalized Bessel functions by the identities

$$i_\mu^\sigma(p, \alpha) = (-1)^\mu \bar{\imath}_\mu^\sigma(p, \alpha) + (-1)^{\sigma+p}\bar{\imath}_\mu^\sigma(p, -\alpha), \tag{128}$$

$$\bar{k}_\mu^\sigma(p, \alpha) = \bar{\imath}_\mu^\sigma(p, \alpha) + k_\mu^\sigma(p, \alpha). \tag{129}$$

Substitution of the Legendre function recurrence relations in Eqs. (53) and (56) leads to the formulas

$$\bar{\imath}_\mu^\sigma(p+1, \alpha) = \frac{(\mu+\sigma+1)\bar{\imath}_{\mu+1}^\sigma(p, \alpha) + (\mu-\sigma)\bar{\imath}_{\mu-1}^\sigma(p, \alpha)}{2\mu+1}, \tag{130}$$

$$\bar{k}_\mu^\sigma(p+1, \alpha) = \frac{(\mu+\sigma+1)\bar{k}_{\mu+1}^\sigma(p, \alpha) + (\mu-\sigma)\bar{k}_{\mu-1}^\sigma(p, \alpha)}{2\mu+1}, \tag{131}$$

$$\bar{\imath}_\mu^\sigma(p, \alpha) = \frac{\bar{\imath}_{\mu+1}^{\sigma-1}(p, \alpha) - \bar{\imath}_{\mu-1}^{\sigma-1}(p, \alpha)}{2\mu+1}, \tag{132}$$

$$\bar{k}_\mu^\sigma(p, \alpha) = \frac{\bar{k}_{\mu+1}^{\sigma-1}(p, \alpha) - \bar{k}_{\mu-1}^{\sigma-1}(p, \alpha)}{2\mu+1}. \tag{133}$$

These formulas can be used to obtain function values for positive σ and/or p; the terms involving $\mu - \sigma$ are replaced by zero if $\mu = \sigma$. Values of $\bar{\imath}_\mu^0(0, \alpha)$ or $\bar{k}_\mu^0(0, \alpha)$ will be needed to start the process.

Another possibility is to obtain $\bar{\imath}_\mu^\sigma(0, \alpha)$ for nonzero σ by a formula analogous to Eq. (19). Making the substitution (cf. formula 8.2.5 of Ref. [15])

$$\frac{(\mu-\sigma)!}{(\mu+\sigma)!}\,(\xi^2-1)^{\sigma/2}P_\mu^\sigma(\xi) = \frac{1}{2^\mu \mu!}\,\frac{d^{\mu-\sigma}}{d\xi^{\mu-\sigma}}\,(\xi^2-1)^\mu \tag{134}$$

in Eq. (53) and integrating by parts, we find (for nonzero α)

$$\bar{\imath}_\mu^\sigma(0, \alpha) = \frac{1}{\alpha}\,(\bar{\imath}_\mu^{\sigma-1}(0, \alpha) + \mathcal{P}_{\mu\sigma}), \tag{135}$$

where

$$\mathcal{P}_{\mu\sigma} = \frac{(-1)^{(\mu+\sigma)/2}(\mu-\sigma)!}{2^\mu\left(\frac{\mu+\sigma}{2}\right)!\left(\frac{\mu-\sigma}{2}\right)!} \quad \mu-\sigma \text{ even},$$
$$= 0 \quad \text{otherwise}. \tag{136}$$

If $\alpha = 0$, the result is

$$\bar{\imath}_\mu^\sigma(0, 0) = -\mathcal{P}_{\mu,\sigma+1} \quad \mu > \sigma$$
$$= \frac{(-1)^\sigma}{(2\sigma+1)!!} \quad \mu = \sigma. \tag{137}$$

The function $\bar{k}_\mu^0(0, \alpha)$ is algebraic and can be written as the finite sum

$$\bar{k}_\mu^0(0, \alpha) = \sum_{p=0}^{\mu/2} \mathcal{G}_{\mu p}\alpha^{2p-\mu-1}, \tag{138}$$

where $\mathcal{G}_{\mu p}$ are the coefficients defined in Eq. (59). This result can be derived by insertion of Eq. (23) into Eq. (56) and integrating term by term. If α is sufficiently large, $\bar{\imath}_\mu^0(0, \alpha)$ can then be obtained from Eq. (129). For small α it is better to use the power series expansion

$$\bar{\imath}_\mu^0(p, \alpha) = \sum_{k=0}^{\infty} (-1)^k \mathcal{I}_{\mu,k+p}\alpha^k, \tag{139}$$

where

$$\mathcal{I}_{\mu k} = \frac{\pi^{1/2}2^{-k-1}}{\Gamma(\frac{1}{2}k - \frac{1}{2}\mu + 1)\Gamma(\frac{1}{2}k + \frac{1}{2}k + \frac{3}{2})}$$
$$= \frac{1}{(k-\mu)!!(k+\mu+1)!!} \quad k \geq \mu,$$
$$= \frac{(-1)^{(\mu-k-1)/2}(\mu-k-2)!!}{(\mu+k+1)!!}$$
$$k < \mu, \text{ different parity},$$
$$= 0 \quad \text{otherwise}. \tag{140}$$

The first line of Eq. (140) follows from insertion of the Maclaurin expansion of $\exp(-\alpha\xi)$ into Eq. (53) and use of formula 8.14.15 of Ref. [15] for the resulting integrals. The remaining lines are the same thing in a more computation-friendly form.

RECURRENCE FORMULAS FOR L_μ^σ

We give here derivations of the additional recurrence formulas that were developed for this work.

First, consider the integral

$$I = \int_1^\infty Q'_\mu(\xi)(\xi^2-1)e^{-\alpha\xi}d\xi. \tag{141}$$

Using formula 8.5.4 of Ref. [15] and the definition of L_μ^0, we find

$$I = \mu(L_\mu^0(1, \alpha) - L_{\mu-1}^0(0, \alpha)). \tag{142}$$

On the other hand, we may integrate Eq. (141) by parts to reach the form

$$I = \frac{1}{\alpha}\int_1^\infty [Q'_\mu(\xi)(\xi^2-1)]' e^{-\alpha\xi}d\xi$$
$$- \left[\frac{1}{\alpha}Q'_\mu(\xi)(\xi^2-1)e^{-\alpha\xi}\right]_1^\infty. \tag{143}$$

The two terms on the right side of this equation can be reduced by observing that

$$\lim_{\xi\to 1+}[Q'_\mu(\xi)(\xi^2-1)] = \lim_{\xi\to 1+}\mu[\xi Q_\mu(\xi) - Q_{\mu-1}(\xi)]$$
$$= \mu \lim_{\xi\to 1+}[(\xi P_\mu(\xi) - P_{\mu-1}(\xi))Q_0(\xi)$$
$$- \xi W_{\mu-1}(\xi) + W_{\mu-2}(\xi)]$$
$$= -1, \tag{144}$$

$$[Q'_\mu(\xi)(\xi^2-1)]' = \mu(\mu+1)Q_\mu(\xi). \tag{145}$$

The quantities $W_{\mu-1}$ and $W_{\mu-2}$ are not related to the W functions introduced earlier in this study, but are the algebraic parts of the Legendre functions Q_μ and $Q_{\mu-1}$. When the limit $\xi \to 1+$ is taken in Eq. (144), the Q_0 term vanishes and the remainder can be evaluated using the summation appearing in formula 8.6.19 of Ref. [15]. Eq. (145) follows from the Legendre differential equation.

The use of Eqs. (144) and (145) leads to

$$I = \frac{\mu(\mu+1)}{\alpha}L_\mu^0(0, \alpha) - \frac{e^{-\alpha}}{\alpha}. \tag{146}$$

From Eqs. (142) and (146), we find

$$L_\mu^0(1, \alpha) - L_{\mu-1}^0(0, \alpha) = \frac{\mu+1}{\alpha}L_\mu^0(0, \alpha) - \frac{e^{-\alpha}}{\mu\alpha}. \tag{147}$$

Finally, combining Eq. (147) with an instance of Eq. (60) for $p = 0$ in such a way as to eliminate $L^0_\mu(1, \alpha)$, we obtain the formula given as Eq. (69) of the main text.

The technique used above also permits generation of another new formula, specifically one permitting an increase of p in $L^0_\mu(p, \alpha)$ without requiring a prior evaluation of L^0_μ of larger μ values. To that end, consider now the integral

$$J = \int_1^\infty Q_\mu(\xi)\xi^p[2\xi - \alpha(\xi^2 - 1)]e^{-\alpha\xi}d\xi. \quad (148)$$

Integrating by parts, we obtain

$$J = -\int_1^\infty [Q'_\mu(\xi)\xi^p + pQ_\mu(\xi)\xi^{p-1}](\xi^2 - 1)e^{-\alpha\xi}d\xi. \quad (149)$$

We now equate the right sides of Eqs. (148) and (149), using Ref. [15] formula 8.5.4 to rewrite Q'_μ in terms of Q_μ and $Q_{\mu-1}$ and identifying each term as a L^0_μ function. The result can be brought to the form

$$g_\mu(p + 2, \alpha) = g_\mu(p, \alpha) + \mu[L^0_\mu(p + 1, \alpha) - L^0_{\mu-1}(p, \alpha)], \quad (150)$$

where

$$g_\mu(p, \alpha) = \alpha L^0_\mu(p, \alpha) - pL^0_\mu(p - 1, \alpha). \quad (151)$$

Eq. (150) is Eq. (70) of the main text; Eq. (73) is obtained by solving Eq. (151) for $L^0_\mu(p, \alpha)$.

To use these equations recursively requires starting values. Because $L^0_\mu(-1, \alpha)$ is finite for nonzero α, we can from Eq. (151) obtain the formula for $g_\mu(0, \alpha)$ given as Eq. (66). The formula for $g_\mu(1, \alpha)$ is obtained from Eq. (151) with $p = 1$ by substituting for $L_\mu(1, \alpha)$ from Eq. (147). The result of this operation is Eq. (67).

RECURRENCE FORMULAS FOR $W_{\nu\mu}$

As a preliminary to the development of new recurrence formulas, integrations by parts were performed on the right sides of Eqs. (91) and (92) for the special case $p = 0$. With the aid of the relation (also valid if P is replaced by Q)

$$\frac{d}{dx}(P_{n+1}(x) - P_{n-1}(x)) = (2n + 1)P_n(x), \quad (152)$$

we find

$$k^0_\mu(0, \alpha_2, x) = \frac{\alpha_2}{2\mu + 1}(k^0_{\mu+1}(0, \alpha_2, x) - k^0_{\mu-1}(0, \alpha_2, x)) + \frac{P_{\mu+1}(x) - P_{\mu-1}(x)}{2\mu + 1}e^{-\alpha_2 x}, \quad (153)$$

$$L^0_\nu(0, \alpha_1, x) = \frac{\alpha_1}{2\nu + 1}(L^0_{\nu+1}(0, \alpha_1, x) - L^0_{\nu-1}(0, \alpha_1, x)) - \frac{Q_{\nu+1}(x) - Q_{\nu-1}(x)}{2\nu + 1}e^{-\alpha_1 x}. \quad (154)$$

Now, substituting Eq. (153) into Eq. (89) and using Eq. (98) for $T_{\nu\mu}$, we obtain

$$w_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = \frac{\alpha_2}{2\mu + 1}(w_{\nu,\mu+1}(0, 0, \alpha_1, \alpha_2) - w_{\nu,\mu-1}(0, 0, \alpha_1, \alpha_2)) + \frac{1}{2\mu + 1}(T_{\nu,\mu+1}(\alpha_{12}) - T_{\nu,\mu-1}(\alpha_{12})), \quad (155)$$

where $\alpha_{12} = \alpha_1 + \alpha_2$. A similar process, substituting Eq. (154) into Eq. (90), yields

$$w_{\nu\mu}(0, 0, \alpha_1, \alpha_2) = \frac{\alpha_1}{2\nu + 1}(w_{\nu+1,\mu}(0, 0, \alpha_1, \alpha_2) - w_{\nu-1,\mu}(0, 0, \alpha_1, \alpha_2)) - \frac{1}{2\nu + 1}(T_{\nu+1,\mu}(\alpha_{12}) - T_{\nu-1,\mu}(\alpha_{12})). \quad (156)$$

If we now add Eq. (155), as written above, to an instance of Eq. (156) for the quantity $w_{\mu\nu}(0, 0, \alpha_2, \alpha_1)$, we reach Eq. (96) of the main text. Alternatively, if we add $w_{\mu\nu}(0, 0, \alpha_2, \alpha_1)$, evaluated according to Eq. (155), to Eq. (156) as written above, we obtain the result presented as Eq. (97).

AUXILIARY FUNCTION $T_{\nu\mu}$

This function arises in the new recursive procedure for $W_{\nu\mu}(0, 0, \alpha_1, \alpha_2)$. Starting from its definition in Eq. (98), application of the recurrence formulas for the Legendre functions leads to

$$\frac{(\nu+1)T_{\nu+1,\mu}+\nu T_{\nu-1,\mu}}{2\nu+1}=\frac{(\mu+1)T_{\nu,\mu+1}+\mu T_{\nu,\mu-1}}{2\mu+1}, \tag{157}$$

which will permit numerically stable generation of all $T_{\nu\mu}$ of nonnegative index values from starting values of $T_{\nu 0}$, $T_{\nu,-1}$, and $T_{-1,\mu}$. We have directly from their explicit forms

$$T_{\nu 0}(\alpha)=L_\nu^0(0,\alpha), \tag{158}$$

$$T_{\nu,-1}(\alpha)=0, \tag{159}$$

where L_ν^0 is the function defined in Eq. (28). The quantity $T_{-1,\mu}$ is singular, but it is only needed when multiplied by $\nu=0$, and it is possible to show that

$$\lim_{\nu\to 0}\nu T_{\nu-1,\mu}(\alpha)=k_\mu^0(0,\alpha), \tag{160}$$

where k_μ^0 is defined in Eq. (29).

GENERALIZED BESSEL FUNCTIONS

The main text uses $i_\mu^\sigma(q,\beta)$ with negative values of q. It is, at least in principle, possible to generate these functions from the series expansion, Eq. (22). However, particularly for larger β, recursive procedures will be more efficient. The recurrence formulas of Eqs. (17) and (18) can be demonstrated directly from the series expansion in a manner that is independent of the sign of q. It is also possible to develop a recurrence formula similar to that given for $L_\mu^0(p,\alpha)$ in Eq. (70). That formula, valid irrespective of the sign of q, can be written

$$\begin{aligned}qi_\mu^0(q-1,\beta)&=\mu i_{\mu-1}^0(q,\beta)-\beta i_\mu^0(q+2,\beta)\\&\quad+(\mu+q+2)i_\mu^0(q+1,\beta)+\beta i_\mu^0(q,\beta)\end{aligned} \tag{161}$$

and can also be proved directly from the series expansion for $i_\mu^0(q,\beta)$. What is relevant to note now is that Eq. (161) cannot be used to obtain values of i_μ^0 for $q=-1$ from values for nonnegative q because the coefficient of $i_\mu^0(-1,\beta)$ will be found to vanish.

A practical route for recursive generation of i_μ^0 of negative q does, however, exist. We first need $i_0^0(-1,\beta)$, the expansion for which can be recognized as that of the hyperbolic sine integral, denoted Shi, as given in formula 5.2.17 of Ref. [15]. Specifically,

$$i_0^0(-1,\beta)=-\mathrm{Shi}(\beta). \tag{162}$$

We next observe that for $q\geq 0$, $i_{-1}^0(q,\beta)$ is finite, so that $\lim_{\mu\to 0}\mu i_{\mu-1}^0(q,\beta)$ vanishes and we do not need an actual value for $i_{-1}^0(q,\beta)$ to use Eq. (17) to obtain $i_0^0(q,\beta)$ from $i_1^0(q-1,\beta)$, and thereby reach an arbitrary range of $i_\mu^\sigma(q,\beta)$ with positive q values. However, $i_{-1}^0(q,\beta)$ is singular for negative q, but, because the pole of the gamma function at argument zero has residue $+1$, it is possible to show that

$$\lim_{\mu\to 0}\mu i_{\mu-1}^0(q,\beta)=\frac{(-1)^q\beta^{-q-1}}{(-q-1)!}. \tag{163}$$

This fact gives the information needed to use Eqs. (17) and (161) recursively.

The recursive strategy we need can be formulated as follows:

1. Starting from a set of $i_\mu^0(q,\beta)$ of nonnegative q and a suitable range $\mu=0\cdots\mu_{\max}$, and from $i_0^0(-1,\beta)$, obtained from Eq. (162), use Eq. (161) and the limit in Eq. (163) to obtain $i_0^0(q,\beta)$ for the negative q values desired.
2. Use Eq. (17) to obtain $i_\mu^0(-1,\beta)$ from $i_{\mu-2}^0(-1,\beta)$ and $i_{\mu-1}^0(0,\beta)$ for a range of μ starting at $\mu=1$. When making $i_1^0(-1,\beta)$ the limit from Eq. (163) will need to be inserted into the recurrence formula.
3. Continue as in step 2 to make $i_\mu^0(q,\beta)$ for $q=-2$, then $-3,\ldots$.
4. The index σ can now be advanced using Eq. (18).

For small β this procedure will be unstable and it will then be preferable to evaluate the summation in Eq. (22) for at least some parameter values.

Appendix D: Reduction of Small-α Formula for w_μ^0

When the explicit form for L_μ^σ from Eq. (41) is inserted into the summation over s in the small-α formula for $w_\mu^0(0,0,\alpha_1,\alpha_2)$, Eq. (54), the terms arising from Eq. (44) can be directly identified as $G_\mu(\alpha_2)$ and $H_\mu(\alpha_2)$ and need not be discussed further. Letting S stand for the remainder of the s summation, namely, the part resulting from the insertion of the k summation from Eq. (41), we initially have

$$S = \sum_{s}{}' \frac{(-1)^{(\mu-s)/2}(\mu+s-1)!!}{s!(\mu-s)!!} \sum_{j=0}^{\infty} \frac{\alpha_2^j s!}{(s+j+1)!} \times \sum_{k=0}^{k_0-1} \frac{(2k+\mu)!}{(2k+2\mu+1)!!(2k)!!} A_{s+j-\mu-2k}(\alpha_1+\alpha_2), \quad (164)$$

where the prime indicates that s is restricted to nonnegative integers of the same parity as μ and the condition defining k_0 is equivalent to the requirement that the index of A be nonnegative.

We now change the summation variable s to $p = (\mu - s)/2$, leading to

$$S = \sum_{p=0}^{\mu/2} (-1)^p \sum_{j=0}^{\infty} \frac{(2\mu-2p-1)!!\alpha_2^j}{(2p)!!(\mu-2p+j+1)!} \times \sum_{k=0}^{(j-2p)/2} \frac{(2k+\mu)!}{(2k+2\mu+1)(2k)!!} A_{j-2p-2k}(\alpha_1+\alpha_2). \quad (165)$$

The k summation in Eq. (165) will vanish unless $j \geq 2p$, so we may change the summation variable j to $j' = j - 2p$, with the summation limits for j' remaining $0 \cdots \infty$. Thus, after minor rearrangement,

$$S = \left(\sum_{p=0}^{\mu/2} \frac{(-1)^p(2\mu-2p-1)!!}{(2p)!!} \alpha_2^{2p} \right) \times \sum_{j'=0}^{\infty} \frac{\alpha_2^{j'}}{(\mu+j'+1)!} \times \sum_{k=0}^{j'/2} \frac{(2k+\mu)!}{(2k+2\mu+1)!!(2k)!!} A_{j'-2k}(\alpha_1+\alpha_2). \quad (166)$$

Comparing with Eq. (138), we recognize the parenthesized summation over p in Eq. (166) as $\alpha_2^{\mu+1}\bar{k}_\mu^0(0, \alpha_2)$. We also interchange the order of the j' and k summations, reaching

$$S = \alpha_2^{\mu+1}\bar{k}_\mu^0(0, \alpha_2) \sum_{k=0}^{\infty} \sum_{j'=2k}^{\infty} \times \frac{(2k+\mu)!\alpha_2^{j'}}{(2k+2\mu+1)!!(2k)!!(\mu+j'+1)!} \times A_{j'-2k}(\alpha_1+\alpha_2). \quad (167)$$

Our final change of variables is to convert the summation index j' into $p = j' - 2k$, after which Eq. (167) can be brought to the form

$$S = \bar{k}_\mu^0(0, \alpha_2) \sum_{p=0}^{\infty} A_p(\alpha_1+\alpha_2) \times \left(\sum_{k=0}^{\infty} \frac{(\mu+2k)!\alpha_2^{\mu+2k+p+1}}{(2\mu+2k+1)!!(2k)!!(\mu+2k+p+1)!} \right). \quad (168)$$

Referring to Eq. (22), the parenthesized summation over k can be recognized as $(-1)^{p+1}i_\mu^0(-p-1, \alpha_2)$, completing the identification of S with the first term on the right side of Eq. (55).

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