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Note

On the Calculation of Wu's Integral

In a previously published study of band systems of diatomic molecules [1] integrals of the type

$$\int_0^\infty \Psi_{n',v'}(r)\, \Psi_{n'',v''}(r)\, dr \tag{1}$$

were encountered which involved the associated Laguerre polynomials $L_v^\beta(z)$ with argument $z = e^{-ar}$. These were expressed in terms of integrals of the form[1]

$$J_{p,\gamma}(\xi) = \int_0^\infty e^{-(1/2)(z+\xi z^\gamma)} z^p\, dz \tag{2}$$

for the purpose of numerical evaluation.

Since the integral (2) cannot, in general, be expressed in terms of known functions except in the special cases where $\gamma = 0, 1, 2, 3$ and (in the last instance, integer "p") recourse to numerical integration is necessary for its evaluation in general. ($\gamma = 0, 1$ are trivial; $\gamma = 2$ leads to parabolic cylinder functions [2, Chap. 19]; while the case $\gamma = 3$ involves Airy functions, but with considerable complications (cf. Chap. 10, loc. cit.)

The present paper derives some analytical properties of the integral (2) in the form of recurrence relations and an asymptotic approximation. In addition, a method is presented whereby a priori and a posteriori error estimates can be obtained, when the integral is approximated by quadrature.

1. Recurrence Relations

For convenience, a simpler form of the integral (2) will be adopted, namely,

$$\begin{aligned} I_{p,\gamma}(x) &= \int_0^\infty e^{-(t+xt^\gamma)} t^p\, dt \\ &= 2^{-1-p} J_{p,\gamma}(\xi), \qquad x = 2^{\gamma-1}\xi, \end{aligned} \tag{3}$$

[1] The actual integral involved has a finite upper limit but, in most problems, it is sufficiently large to allow (2) to constitute an adequate approximation.

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($\mathrm{Re}(p) > -1$, $\mathrm{Re}(x) > 0$, $\mathrm{Re}(\gamma) \geqslant 0$.) An obvious integration by parts gives

$$\gamma x I_{p+\gamma,\gamma}(x) = (p+1)\, I_{p,\gamma}(x) - I_{p+1,\gamma}(x), \tag{4a}$$

$$p \neq -1, \qquad \gamma x I_{\gamma-1,\gamma}(x) = 1 - I_{0,\gamma}(x). \tag{4b}$$

If "γ" is assumed to be a positive integer, then, ordinarily, knowledge of $I_{p,\gamma}(x)$ for "γ" contiguous values of p would be needed to give all remaining values of $I_{p,\gamma}(x)$. However, because of the relation (4b), this number can be reduced to $\gamma - 1$ if p is also a positive integer, although, in practice, it is preferable to compute the $I_{p,\gamma}(x)$ by applying (4a) in the backward direction starting with the full number of initial values, and then to use (4b) as a check relation. The reason for this is twofold: First, the relation (4a), when applied in the direction of decreasing "p," involves only addition and multiplication of positive quantities, and is therefore numerically stable. Second, as will be shown later (Art. 3), the evaluation of the integral (2) by quadrature requires fewer tabular values of the integrand to obtain a prescribed accuracy when "p" is large.

2. Asymptotic Approximation

An asymptotic approximation to $I_{p,\gamma}(x)$ can be found by writing the integral in the form

$$\int_0^\infty e^{-\phi(t)}\, dt \tag{5}$$

where

$$\phi(t) = |t + xt^\gamma - p \ln t| \tag{6}$$

and applying the "saddle point" method. This method is based on the assumption that the primary contribution to the integral comes from values of "t" in the vicinity of one or more stationary points of $\phi(t)$; i.e., at a point or points where

$$\phi'(t) = 0. \tag{7}$$

In the present example,

$$\phi'(t) = 1 + \gamma x t^{\gamma-1} - p/t \tag{8}$$

so that the saddle point (or points) occurs when

$$\gamma x t^\gamma + t - p = 0. \tag{9}$$

It is evident that the above equation has one and only one positive root, t_0, and hence only one stationary point need be considered.

Developing $\phi(t)$ in a Taylor series about t_0, we get

$$\phi(t) = a_0 + a_2(t-t_0)^2 + a_3(t-t_0)^3 + \cdots + \tag{10}$$

where

$$\begin{aligned} a_0 &= t_0 + xt_0^{\gamma} - p\ln(t_0), \\ 2!a_2 &= \gamma(\gamma-1)\,xt_0^{\gamma-2} + p/t_0^2 \end{aligned} \tag{11}$$

and in general

$$k!a_k = \gamma(\gamma-1)\cdots(\gamma-k+1)\,xt^{\gamma-k} + (-)^k(k-1)!\,p/t_0^k.$$

(Note that, if γ is a positive integer, the last relation reduces to

$$k!a_k = (-)^k(k-1)!\,p/t_0^k \tag{12}$$

for $k > \gamma$.)

For convenience set

$$u^2 = [\phi(t) - a_0]/a_2, \qquad u \geqslant 0,\ \tau = |t - t_0|. \tag{13}$$

Then, from (11),

$$u^2 = \tau^2[1 + b_1\tau + b_2\tau^2 + \cdots +] \tag{14}$$

where

$$b_k = \pm a_{k+2}/a_2 \tag{15}$$

and where the "+" sign holds for $t > t_0$ and the "−" for $t < t_0$. The integral (5) now becomes

$$\int_0^{\infty} e^{-\phi(t)}\,dt = e^{-a_0}\int_0^{\infty} e^{-a_2u^2}\left(\frac{dt}{du}\right)du. \tag{16}$$

Further, the series (14) can be inverted by writing it in the form

$$u = \tau[1 + b_1\tau + b_2\tau^2 + \cdots +]^{1/2}$$

and applying LaGrange's theorem [2, Art. 3.6.6]. This gives

$$\tau = u[1 + c_1u + c_2u^2 + \cdots +] \tag{17}$$

where

$$\begin{aligned} (k+1)\,c_k = \{&\text{coefficient of } \tau^k \text{ in the expansion of} \\ &[1 + b_1\tau + b_2\tau^2 + \cdots +]^{-(1/2)(k+1)}\}. \end{aligned} \tag{18}$$

In particular:

$$
\begin{aligned}
c_1 &= -\frac{1}{2} b_1, \\
c_2 &= \frac{5}{8} b_1^2 - \frac{1}{2} b_2, \\
c_3 &= -b_1^3 + \frac{3}{2} b_1 b_2 - \frac{1}{2} b_3, \\
c_4 &= \frac{231}{128} b_1^4 - \frac{63}{16} b_1^2 b_2 + \frac{7}{4} b_1 b_3 + \frac{7}{8} b_2^2 - \frac{1}{2} b_4.
\end{aligned} \tag{19}
$$

In changing the integration variable from t to u, distinction must be made between the regions on either side of the saddle point, t_0. From (17)

$$dt = du[1 + 2c_1 u + 3c_2 u^2 + \cdots +], \tag{20}$$

but, because of the ambiguous sign in (15), we find that when the integrals originating from the two sides of t_0 are combined, the terms in (20) with odd coefficients cancel, while the even ones combine, and hence

$$\int_0^\infty e^{-\phi(t)}\, dt \sim 2e^{-a_0} \int_0^\infty e^{-a_2 u^2} [1 + 3c_2 u^2 + 5c_4 u^4 + \cdots +]\, du. \tag{21}$$

(It should be remarked that the above result is only asymptotically true, subject to the condition that a_2 be sufficiently large to allow those contributions which originate outside the radius of convergence of the inverted series (17) to be neglected. This assumption is consistent with asymptotic analyses in general.)

The integrals involved in (21) are well known. Specifically [2, Art. 7.4.4]:

$$2\int_0^\infty e^{-a_2 u^2}\, du = \sqrt{\frac{\pi}{a_2}}, \tag{22}$$

$$2\int_0^\infty e^{-a_2 u^2} u^{2k}\, du = \sqrt{\frac{\pi}{a_2}}\, \frac{1 \cdot 3 \cdots (2k-1)}{2^k a_2^k}, \qquad k > 0 \tag{23}$$

and hence[2]

$$\int_0^\infty e^{-(t + xt^\gamma)} t^p\, dt \sim \sqrt{\frac{\pi}{a_2}}\, e^{-a_0} \left[1 + \frac{3c_2}{2a_2} + \frac{15c_4}{4a_2^2} + \cdots + \right]. \tag{24}$$

Since (24) is effectively an expansion in inverse powers of "a_2," it will be more accurate when this parameter, which, according to (11), is of the order of magnitude of "p," is large. As an illustration of the above formula, the following approximations

[2] The leading term of this expression is comparable to that obtained in [1, Eq. (16)].

to the integral for $p = 50$, $x = 8$, $y = 3$ are obtained using 1, 2, and three terms of the series (24):

$$t_0 = 1.266308; \qquad a_0 = 5.70559; \qquad a_2 = 45.9819; \qquad a_3 = -.207874$$
$$a_4 = 4.86130; \qquad c_2 = -.05285; \qquad c_4 = -.01168;$$

which give, with

$$\text{one term: } I \cong 8.69712 \times 10^{-4};$$
$$\text{two terms: } I \cong 8.68212 \times 10^{-4};$$
$$\text{three terms: } I \cong 8.68194 \times 10^{-4};$$

the last value being in close agreement with that obtained in the next section by quadrature.

3. Evaluation by Quadrature

With the aid of the Euler–McLauren formula [2, Art. 25.4.7], it is possible to evaluate the integral (3) by the trapezoidal rule, with an a priori error estimate, which may be converted to a sharper, a posteriori one by performing the integration with successive intervals of "h" and "$2h$." We introduce the notation $I_t(h)$ to denote, for a given integrand $f(x)$ and integration limits a and b, the sum

$$h[\tfrac{1}{2}f(a) + f(a+h) + f(a+2h) + \cdots + \tfrac{1}{2}f(b)]. \tag{25}$$

The Euler–McLauren formula can be written

$$\int_a^b f(t)\,dt = I_t(h) - \sum_{k=0}^{n} h^{2k} \frac{B_{2k}}{2k!} [f^{(2k-1)}(b) - f^{(2k-1)}(a)] + R_{2n}(h) \tag{26}$$

where the B_{2k} are the Bernoulli numbers, the first few of which are

$$\begin{aligned} B_2 &= 1/6, \\ B_4 &= -1/30, \\ B_6 &= 1/42, \end{aligned} \tag{27}$$

with additional values given in [2, Table 23.2].

An estimate of the remainder $R_{2n}(h)$ is given by the following

$$R_{2n}(h) \sim \frac{B_{2n} h^{2n}}{(2n!)} C_{2n} \tag{28}$$

(loc. cit., Art. 23.1.30), where C_{2n} is bounded if $f^{(2n)}(t)$ exists and is finite for $a \leqslant t \leqslant b$. It follows that, although

$$R_{2n}(h) \to \infty, \qquad h \text{ fixed}, \; n \to \infty \tag{29}$$

it still holds that

$$R_{2n}(h) \to 0, \qquad n \text{ fixed}, \; h \to 0. \tag{30}$$

In this sense, (26) is an asymptotic series, and can thus be written

$$\int_a^b f(t)\,dt \sim I_t(h) - \sum_{k=1}^{\infty} \frac{h^{2k} B_{2k}}{(2k!)} \left|f^{(2k-1)}(b) - f^{(2k-1)}(a)\right|. \tag{31}$$

In the case of the present integral, it can be seen from the Taylor series expansion of $f(t)$ that, if "P" denotes the integral part of "p," the first non-zero term in the Euler–McLauren series will be $O(h^{P+2})$ if "P" is even, and $O(h^{P+1})$ if "P" is odd. That is,

$$\begin{aligned} \int_a^b f(t)\,dt &\sim I_t(h) + ah^{P+2}, \qquad P \text{ even} \\ &\sim I_t(h) + ah^{P+1}, \qquad P \text{ odd} \end{aligned} \tag{32}$$

where "a" does not depend on "h," so that a larger interval of integration can be used to obtain a desired accuracy as "p" increases, and because of the property (30), such a value of "h" can always be found. The difficulty, of course, is that in some cases the magnitude of "a" may be fairly large, and a precise estimate difficult to obtain analytically. However, a reasonably good estimate of this quantity can be found numerically by performing the trapezoidal integration with successive intervals of "h" and "$2h$." This gives, e.g., for "P" even, the following estimate for the absolute error:

$$E_a(h) \cong ah^{P+2} \left[\frac{I_t(h) - I_t(2h)}{2^{P+2} - 1}\right]. \tag{33}$$

In some problems, such as the present one, where the integral itself is fairly small, the absolute error is less meaningful than the relative error, which is given by

$$E_r(h) = \frac{1 - (I_t(2h)/I_t(h))}{2^{P+2} - 1} \tag{34}$$

since the latter is an indication of the number of correct significant figures, rather than the number of correct decimal places.

As an example, the integral (3) with $x = 8$, $y = 3$ and $p = 10$ is approximated by

$$3.11955105 \times 10^{-4}$$

with $h = 0.1$ and by

$$3.11945302 \times 10^{-4}$$

with $h = 0.2$. Hence, from (34) the relative error for $h = 0.1$ is estimated as

$$7.7 \times 10^{-9},$$

indicating that the value of $I_t(0.1)$ is correct to within approximately 2 units in the ninth significant figure.

The results for $p = 50$ are even more surprising: With $h = 0.1$ and 0.2, the respective approximations are

$$I_t(0.1) = 8.6819219 \times 10^{-4},$$
$$I_t(0.2) = 8.64354263 \times 10^{-4},$$

so that the relative error for $I_t(0.1)$ in this case is of the order of 1×10^{-18}.

The facility with which this integral can be evaluated accurately by quadrature when p is large provides the following very simple scheme for its calculation:

"Evaluate the integral by quadrature for three fairly large and contiguous values of p, and then use the recurrence formula (4a) in the backward direction to obtain the values of the integral for all lesser values of $p \geqslant 0$, with a check on the accuracy provided by the relation (4b), in the cases where "p" is an integer."

The method is illustrated in the following tables for $x = 8$, $y = 3$. The values of $I_{12,3}(8)$, $I_{11,3}(8)$ and $I_{10,3}(8)$ are first determined by quadrature, using an integration interval of 0.1:

$$I_{12,3}(8) \cong 1.717303 \times 10^{-4},$$
$$I_{11,3}(8) \cong 2.276686 \times 10^{-4},$$
$$I_{10,3}(8) \cong 3.119549 \times 10^{-4}.$$

The error estimate (34) indicates that all of the figures in the above are correct. With the above as starting values, the recurrance relation (4a) is then applied in the backward direction to obtain $I_{p,3}(8)$ for $p = 9, 8, \ldots, 0$. The check relation gives

$$I_{0,3}(8) + 24 I_{2,3}(8) = 0.99999976.$$

The results are given in Tables I and II. An additional set of values for $p = 13, 14, 15$, obtained by applying (4a) in the forward direction, is also included. For comparison, in both tables approximate values are determined from the asymptotic series (24), with 1, 2 and 3 terms, for $p = 15(-1)8$. As would be anticipated, the asymptotic approximation improves with increasing p.

TABLE I

$I_{p,\gamma}(x) \times 10^4$ for $x = 8$, $\gamma = 3$, $p = 12(-1)0$

p	By quadrature and Eq. (4a)	Asymptotic series (Eq. (24)) 1 term	2 terms	3 terms
12	1.717303	1.73097	1.71786	1.71725
11	2.276686	2.29662	2.27755	2.27660
10	3.119551	3.14989	3.12095	3.11935
9	4.433482	4.48198	4.43592	4.43311
8	6.563772	6.64569	6.56821	6.56297
7	10.179118			
6	16.654670			
5	29.030866			
4	54.66594			
3	113.59451			
2	270.1118			
1	791.0472			
0	3517.315			

Note. Check relation: $I_0 + 24I_2 = 0.99999976$.

TABLE II

$I_{p,\gamma}(x) \times 10$ for $x = 8$, $\gamma = 3$, $p = 13, 14, 15$

p	By recurrence relation (4a)	Asymptotic series (Eq. (24)) 1 term	2 terms	3 terms
13	1.334931	1.34466	1.33530	1.33489
14	1.066789	1.07396	1.06705	1.06677
15	0.874584	0.88004	0.87477	0.87456

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