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Comparison of Some Methods for Evaluating Infinite Range Oscillatory Integrals

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A number of related methods for the evaluation of oscillatory integrals over infinite ranges which arise in physical applications are compared critically. Various modifications are suggested and recommendations made for more efficient implementation. In particular, coefficients for Gaussian trigonometric quadrature formulas are listed and an alternative Chebyshev-polynomial-based oscillatory integrator is suggested. The use of these algorithms coupled with summation accelerators in the partition–extrapolation procedure is illustrated in a number of practical examples and comparisons are made with earlier work.

1. PHYSICAL BACKGROUND AND INTRODUCTION

Integrals of the form

$$\int_0^\infty f(x)\, w(x)\, dx, \tag{1}$$

where $w(x)$ is an oscillatory function, appear in many physical applications, one of the most important cases being the evaluation of Fourier transforms in which

$$w(x) = \begin{matrix}\cos \\ \sin\end{matrix} \omega x. \tag{2}$$

Generalizations to other oscillatory weight functions such as

$$w(x) = J_0(\omega x) \tag{3}$$

also appear in many branches of applied mathematics.

An example of the latter case arises in fluid mechanics in the study of particle interaction in a slow viscous flow, as described by Evans [1]. The force on one particle due to the presence of a second particle in a given underlying flow was considered. Asymptotic expansions of the fluid velocity vector and pressure were

made with the usual inner and outer regions. Each of the terms of the expansions satisfies a linear partial differential equation and the asymptotic matching is achieved by using generalized functions. As pointed out by Evans and Ockendon [2], the problem is then solvable by taking Fourier transforms. The inversion of these transforms gave rise to the integral

$$\int_0^\infty xc^{-1}y^{-1}\exp(-y\sin\alpha) \times [2(c^2+x^2)J_0(x\cos\alpha) - 2x\sec\alpha J_1(x\cos\alpha)]\,dx, \tag{4}$$

where

$$y = (x^2 + R^2/4)^{1/2}$$

and

$$c = Ry + R^2/2.$$

The angle α relates the particle position to the flow direction and R is the Reynolds number. At $\alpha = 0$ the integral exists only in the mean but, in this case, an asymptotic estimate is available for small R which provides a check on the numerical values obtained.

The second application arose in the field of molecular physics in the evaluation of certain two-center molecular integrals involving one-electron Green's functions. These integrals arise from the variational functional

$$\eta = (\phi V, GV\phi)/(\phi, V\phi) \tag{5}$$

which has been proposed by Hall and co-workers [3, 4] as an alternative to the usual minimum energy variational principle for atoms and molecules. The Green's operator G is defined by

$$G = (\mu^2 E - T)^{-1}, \tag{6}$$

E, V, and T denoting the energy of the system, the potential energy operator, and the electronic kinetic energy operator, respectively. The arbitrary trial function $\phi(\mathbf{r})$ is adopted and μ is a scaling factor.

For applications to two-center molecular systems, a particular class of potential energy weighted trial functions involving Slater-type orbitals has been suggested by Blakemore, Evans, and Hyslop [5].

The most complicated two-center integrals arising from the numerator of functional (5) are denoted, as in [5], by g_{ab}. For the suggested Slater-type trial functions, analytical reduction is achieved by utilizing the Fourier representation

$$g(\mathbf{r}_1, \mathbf{r}_2) = -(4\pi^3)^{-1}\int (s^2 + k^2)^{-1}\exp[-i\mathbf{s}\cdot(\mathbf{r}_1 - \mathbf{r}_2)]\,d\mathbf{s} \tag{7}$$

for the one-electron Green's function

$$g(\mathbf{r}_1, \mathbf{r}_2) = -(2\pi \mid \mathbf{r}_1 - \mathbf{r}_2 \mid)^{-1} \exp(-k \mid \mathbf{r}_1 - \mathbf{r}_2 \mid), \tag{8}$$

which corresponds to the operator G with $\mu^2 E = -\frac{1}{2}k^2$. It is seen that the required integrals may be analytically reduced to the form

$$g_{ab} = \sum_l A_l \int_0^\infty s^2 j_l(Rs)\, F_a(s)\, F_b(s)(s^2 + k^2)^{-1}\, ds. \tag{9}$$

In this equation, the summation extends over the usual combinations of the azimuthal quantum numbers and j_l is the spherical Bessel function as defined by Abramowitz and Stegun [6]. The functions $F_a(s)$ and $F_b(s)$ are related to the Fourier transform of the orbitals centered on nuclei A and B, respectively, and general expressions for these functions and the constants A_l are quoted in [5]. These functions, although somewhat complicated in general form, are, in fact, rational functions of s so that the basic integrals required in Eq. (9) may be expressed generally as

$$\int_0^\infty F(s) j_l(Rs)\, ds, \tag{10}$$

in which $F(s)$ is a rational function and R denotes the internuclear separation. The simplest case treated in practice corresponded to $l = 0$ and the choice

$$F(s) = Rs^2(s^2 + 1)^{-3} \tag{11}$$

which actually leads to the integral I_9 of Table I.

For nonzero values of l, the spherical Bessel function is written in the form

$$j_l(z) = u_l(z) \sin z + v_l(z) \cos z \tag{12}$$

and the two components of the integral are evaluated separately; expressions for the rational functions $u_l(z)$ and $v_l(z)$ are quoted in [6].

The numerical evaluation of such integrals is difficult, particularly for large values of ω, and is further complicated by the infinite range. This precludes the conventional procedure of approximating $f(x)$ by a polynomial, as adopted, for example, by Filon [7], Clendenin [8], and Flinn [9] in the evaluation of finite Fourier transforms.

The procedure of integration between the successive zeros of $w(x)$, thus converting the integral to an infinite summation, has been considered by several authors [10–13]. The use of a modified version of Euler's transformation to accelerate the convergence of the resulting series of finite integrals has been investigated by Longman [14].

More recently, Alaylioglu, Evans, and Hyslop [15] have suggested the use of the more general transformations of Shanks [16] to accelerate convergence in the partition-extrapolation method, coupled with a low order Gauss–Legendre quadrature prescription for the evaluation of the half-cycle integrals. A similar technique was adopted by Squire [17], who used the Aitken extrapolation formula together with a corrected Simpson's rule. In a later paper Squire [18] compares the Aitken extrapolation approach, linked with a Gaussian quadrature rule, with the use of the ϵ-algorithm for the acceleration as suggested by Chisholm, Gentz, and Rowlands [19]. Squire also suggests that the transformations of Levin [20] would be worth investigation as alternatives to those of Shanks.

The extrapolation procedure has also been investigated by Gray and Atchison [21, 22], who introduce the G-transformation, which is a continuous analog of the Aitken transformation, and their results appear to confirm the equivalence. In a later paper, Gray, Atchison, and McWilliams [23] generalize the G-transform to give a continuous analog of Shanks' transformations with the expected improvement in convergence.

In contrast to these "integration, then summation" methods, Piessens and Haegemans [24], in a variation of the method of Hurwitz and Zweifel [10], perform the summation of the function over the half-cycles first, using Euler's transformation for acceleration purposes, and *then* perform the integration using the trapezoidal rule. This technique of summation followed by integration has also been adopted in a recent paper by Boris and Oran [25], who use the properties of the Fourier series of the summation.

In a completely different approach, Pantis [26] has proposed an extension of Filon's procedure to the infinite range. The range is split into $[0, \alpha]$ and $[\alpha, \infty]$: Filon's method is applied to the finite interval $[0, \alpha]$ and the contribution from $[\alpha, \infty]$ is estimated by utilizing an asymptotic expansion for sufficiently large α.

It is clear, therefore, that many variations of the basic procedures have been suggested, both with respect to the accelerator and the quadrature rule. It is of interest then to compare the efficiencies of these variations for the purpose of producing procedures which may be adopted in physical applications.

In the present paper, the main sources of motivation are the examples outlined above and it is worth emphasizing the particular characteristics of these problems. In many cases, the function $f(x)$ may be extremely complicated in form, and large numbers of such functions may have to be integrated for each value of the frequency ω. This is particularly true in the quantum mechanical applications where the utilization of large basis sets for the variational trial function ϕ will give rise, on optimization of functional (5), to large matrices with elements containing terms like g_{ab} of Eq. (9). Consequently, the accurate computation of these integrals with a minimum of function evaluations is of paramount importance and, indeed, is the main aim of the present work. The complexity of the functions considered

in these applications also means that estimation of the errors involved in the quadrature routines is extremely difficult. The difficulty is accentuated in cases where $f(x)$ is only available numerically as, for instance, when variational functional (5) is incorporated in a Hartree–Fock self-consistent field model and the integrands are produced numerically by iteration. Consequently, the "experimental" alternative of carrying out convergence tests with quadrature prescriptions of increasing order has been adopted for selected values of the parameters. This process, of course, involves extra function evaluations but has been used consistently for all the quadrature methods considered and thus gives a basis for comparison. In this connection, the value of quadrature routines which are adaptive is emphasized, since the earlier function evaluations may be reutilized.

The implementation of the basis procedures is therefore considered in the light of these remarks and various modifications are suggested to increase efficiency by reducing the number of function evaluations. Comparisons are carried out between the various techniques for representative examples, particular emphasis being placed on the physical applications described. Other examples illustrating specific points have also been included.

2. Formulation of the Integrals

In the case where the weight function $w(x)$ is $\sin \omega x$, integration is carried out between the zeros of $w(x)$ and a linear transformation enables the integral

$$S(\omega) = \int_0^\infty f(x) \sin \omega x \, dx \tag{13}$$

to be written in the form

$$S(\omega) = \sum_{n=0}^{\infty} u_n(\omega), \tag{14}$$

where

$$u_n(\omega) = (-1)^n \omega^{-1} \int_0^\pi f[(t + n\pi)\omega^{-1}] \sin t \, dt. \tag{15}$$

This subdivision prescription is to be contrasted with the formula of Pantis [26] where $S(\omega)$ is expressed as

$$S(\omega) = \int_0^\alpha f(x) \sin \omega x \, dx + \omega^{-1} f(\alpha) \cos \omega\alpha - \omega^{-2} f'(\alpha) \sin \omega\alpha$$
$$- \omega^{-3} f''(\alpha) \cos \omega\alpha + \cdots, \tag{16}$$

the asymptotic series being valid for large α provided $f(\alpha)$ and its derivatives fall off sufficiently rapidly. Note, in this connection, that the choice of α according to the relation

$$\omega\alpha = m\pi, \tag{17}$$

where m is an integer, would seem to produce the more convenient asymptotic series

$$(-1)^m \{\omega^{-1}f(\alpha) - \omega^{-3}f''(\alpha) + \cdots\}, \tag{18}$$

the odd derivative terms being missing. However, if the object is to evaluate the integral for many values of ω, such a restriction on α would require a new set of function evaluations for each ω and an α independent of ω would be preferable in such cases, as suggested by Pantis.

The basic oscillatory integral over a finite range which is required in (15) and (16) may be expressed in general form as

$$\int_a^b F(t) \sin \omega t \, dt \tag{19}$$

and various methods are now described for its numerical evaluation.

The most familiar method is due to Filon [7], in which the nonoscillatory part, $F(t)$, of the integrand is fitted to a parabola over the range $[a, b]$ and analytical evaluation then effected. This procedure was, in fact adopted by Pantis. Serious inaccuracies occur over the range $[0, \alpha]$ in the integral of Eq. (16) when α is large and Pantis found it necessary to subdivide the range uniformly and apply the Filon formula repeatedly, in the usual way. In most practical cases, however, the values of α required were so large that a prohibitively large number of function evaluations was necessary for a specified accuracy. Some improvement is possible by adopting a nonuniform subdivision procedure which takes the properties of $F(t)$ into account. For instance, in one of his examples, Pantis concentrates the number of points in the regions where $F(t)$ is varying most rapidly and has its largest magnitude. This procedure depends, of course, on knowledge of the properties of $F(t)$ and it is clear therefore that, if further economies are to be realized in general, more powerful integrators should be adopted.

The higher order polynomial approximations, as suggested, for example, by Flinn [9], could be introduced and give rise to the family of quadrature formulas for the oscillatory integrals of the Newton–Cotes type, based on equally spaced ordinates. The automatic generation of these quadrature rules has been considered recently by Alaylioglu, Evans, and Hyslop [27]. The higher order formulas tend to be unstable numerically, like the normal Newton–Cotes formulas for nonoscillatory integrals, and their use is not recommended in practice. It appears preferable to use the lower orders [say, 2 (which is Filon's prescription), 4, and 5]

repeatedly by subdivision of the interval of integration, although extra cancellation errors may be introduced by this means.

For this reason, an alternative scheme was investigated which is based on a suggestion by Bakhvalov and Vasil'eva [28] involving the expansion of $F(t)$ over the normalized range of integration $[-1, 1]$ in a series of Chebyshev polynomials $T_n(t)$. Bakhvalov and Vasil'eva originally adopted a quadrature procedure depending on expansion in Legendre polynomials $P_n(t)$, the resulting formulas involving a finite series of spherical Bessel functions. Their suggestion for the use of Chebyshev polynomials was subsequently adopted by Piessens and Poleunis [29], who proposed a formula involving an infinite series of Bessel functions. An alternative formulation of this Chebyshev-based algorithm has been developed by Alaylioglu, Evans, and Hyslop [30], a brief outline of which appears in Appendix A. The method is analogous to the treatment of the Newton–Cotes formulas adopted by these authors [27] and represents an extension of the well-known Clenshaw and Curtis method [31] to the case of oscillatory integrands. Some advantages of this alternative approach are: (i) The implementation is simple, (ii) the summation of an infinite series of Bessel functions is avoided, and (iii) the algorithm is adaptive. The stability of the method and limitations on its use are discussed at length in [30], where detailed comparisons with other methods have been made. Similar methods involving the use of Chebyshev polynomials which give rise to prescriptions involving finite series of Bessel functions have been developed by Patterson [32] and by Littlewood and Zakian [33]. It was found that a very significant saving in the number of function evaluations was realized, together with an increase in stability over the Newton–Cotes prescriptions, particularly the Filon procedure.

It will be noted that, in all of the methods described above, the fitting of $F(t)$ is independent of ω. Consequently, these methods will be particularly efficient if a given integral is required for a number of values of ω, since the same function evaluations may be utilized in each case.

In contrast, the integral required in the subdivision algorithm (15) is confined to the range $[0, \pi]$ but the ordinates required are clearly dependent on ω. The techniques mentioned above (particularly the Chebyshev based procedure) may also be utilized for these integrals but additional methods which may be more suited to the subdivision procedure are also developed.

In the previous work by Alaylioglu *et al.* [15] a low order Gauss–Legendre quadrature prescription [34] was used, coupled with uniform subdivision of the range. Since the integration was over one half-cycle only, it was not considered necessary to take the periodic nature of the weight function into account and consequently the quadrature prescription was applied to the entire integrand. Obviously, Gaussian quadrature formulas taking the oscillatory weight functions explicitly into account would be more efficient and these procedures have been

investigated by a number of authors including Miklosko [35], Piessens [36, 37], and Gautschi [38]. In most cases the formulas proposed are restricted to low order or the weight functions are not directly applicable to the subdivision algorithm of Eq. (15). For instance, Piessens [36] tabulates Gaussian coefficients for orders $N = 2$, 4, and 6 for the weight function $\sin x$ on the symmetrical interval $[-\pi, \pi]$ with a more extensive tabulation up to order $N = 18$ appearing on microfiche in [37]. The tabulations presented by Gautschi are for the weight functions $(1 + \cos \pi x)$ and $(1 + \sin \pi x)$ on $[-1, 1]$ and clearly require Gauss–Legendre coefficients in addition. Also, coefficients for the weight function $\cos x$ on the interval $[-\pi/2, \pi/2]$ are presented by Piessens [36]. These are reducible immediately to the forms required for $\sin x$ on $[0, \pi]$ in Eq. (15) by simply adding $\pi/2$ to the abscissas. The tables in [36] are restricted to orders $N = 1$ to 4, although extensive tabulations are presented in [39]. Extensive multiple precision computations of Gaussian quadrature coefficients for various weight functions have also been carried out recently by Alaylioglu, Evans, and Hyslop, the details of which will be reported elsewhere. This investigation included coefficients specifically for the integrals appearing in (15) according to the N-point relation

$$\int_0^{\pi} F(t) \sin t \, dt \simeq \sum_{i=1}^{N} \omega_i f(t_i), \tag{20}$$

formulas of this type having also been considered by Price [40]. A short extract from these calculations is presented in Appendix B for convenient reference, attention being confined to the lower order results which were utilized in the practical calculations described here.

It will be noticed that the formulation developed here applies to the sine transform of Eq. (13). However, the basic quadrature rule, Eq. (20), may also be applied directly to the cosine transform

$$C(\omega) = \int_0^{\infty} f(x) \cos \omega x \, dx, \tag{21}$$

since it is easily seen that $C(\omega)$ may be expressed as

$$C(\omega) = \omega^{-1} \int_0^{\pi/2} f(t/\omega) \cos t \, dt + \sum_{n=0}^{\infty} u_n(\omega), \tag{22}$$

where

$$u_n(\omega) = (-1)^{n+1} \omega^{-1} \int_0^{\pi} f[(t + n\pi + \tfrac{1}{2}\pi) \omega^{-1}] \sin t \, dt, \tag{23}$$

which is analogous to Eqs. (14) and (15). It will be necessary, of course, to evaluate the integral over $[0, \pi/2]$ separately here, and a wide choice of accurate methods

is available, ranging from Gauss–Legendre quadrature to the Chebyshev method mentioned above, or even to a special Gaussian-trigonometric procedure for the weight function cos t on the interval $[0, \pi/2]$, some coefficients being presented in Appendix B.

For the main integrals u_n, the Gauss-trigonometric prescription, Eq. (20), has proved most efficient in practice over a wide range of functions and has produced significant reductions in the number of function evaluations. However, it should be mentioned that the Chebyshev algorithm was only marginally less efficient in most cases tested and has the advantage of being adaptive in nature.

Concentrating on the sine transform, Eq. (13), it is apparent that the subdivision algorithm, Eq. (15), in conjunction with the Gaussian formula, Eq. (20), produces the quadrature rule

$$S(\omega) = \omega^{-1} \sum_{n=0}^{\infty} (-1)^n \sum_{i=1}^{N} w_i f[(t_i + n\pi)\, \omega^{-1}]. \tag{24}$$

The order N of the quadrature rule may well depend on the value of n and in most cases in practice, where the functions are falling off smoothly enough, it is possible to reduce $N(n)$ as n increases. The infinite summation over n is then evaluated once the quadrature has been completed by utilizing the acceleration–extrapolation procedures described in the next section.

For comparison purposes, the alternative procedure of summing first over the cycles, as adopted by Piessens and Haegemans [24] and by Boris and Oran [25] would produce the result

$$S(\omega) = \int_0^{\pi} \sigma(t, \omega) \sin t \, dt, \tag{25}$$

where

$$\sigma(t, \omega) = \sum_{n=0}^{\infty} (-1)^n \omega^{-1} f[(t + n\pi)\, \omega^{-1}], \tag{26}$$

and give rise to the alternative form of the quadrature rule

$$S(\omega) \simeq \omega^{-1} \sum_{i=1}^{N} w_i \sum_{n=0}^{\infty} (-1)^n f[(t_i + n\pi)\, \omega^{-1}]. \tag{27}$$

The acceleration algorithm is used here on the infinite summation *before* the integration.

Note also that in cases where $f(t)$ is an *odd* function (an *even* function for cosine transforms) it is possible to obtain a symmetrized $\sigma(t, \omega)$ which produces a periodic integrand in Eq. (25). This is the procedure suggested by Piessens and Haegemans

[24]. The trapezoidal rule is particularly efficient for such integrals and is often superior even to the Gauss-trigonometric procedure.

However, the method is limited to even or odd functions and, in the present work, the more general $\sigma(t, \omega)$ of Eq. (26) is adopted. This function does not have the periodic properties which enable the trapezoidal rule to be used effectively and it is preferable to use the integrators described in the Appendixes.

It is important in practice that an efficient "accelerator" should be built into the summations in (24) or (27), particularly in the cases of slow convergence. In fact, an accelerator may, in certain instances, produce convergent sequences even when the original sequence diverges, as in the case of integrals which converge only in the mean [15]. Procedures such as that suggested by Boris and Oran [25] which do not use an acceleration technique would fail when applied to such problems.

3. Implementation of the Acceleration Techniques

The basic mechanism here is the application of the Shanks operators e_k to accelerate the convergence of the sequences $\{A_n\}$ $(n = 0, 1, 2,...)$ of partial sums given by

$$A_n = \sum_{j=0}^{n} u_j \,. \tag{28}$$

The sequence $\{B_{k,n}\}$ $(n = k, k + 1,...)$ is produced according to

$$\{B_{k,n}\} = e_k\{A_n\}, \tag{29}$$

the terms of the sequence being defined as the ratio of two determinants of order $(k + 1)$ which may be expressed in the form

$$B_{k,n} = \begin{vmatrix} A_{n-k} & \cdots & A_n \\ u_{n-k+1} & \cdots & u_{n+1} \\ \vdots & & \vdots \\ u_n & \cdots & u_{n+k} \end{vmatrix} \div \begin{vmatrix} 1 & \cdots & 1 \\ u_{n-k+1} & \cdots & u_{n+1} \\ \vdots & & \vdots \\ u_n & \cdots & u_{n+k} \end{vmatrix}. \tag{30}$$

The case $k = 1$ is readily seen to be equivalent to the well-known Aitken Δ^2 extrapolation formula.

The direct evaluation of these determinants may lead to numerical instability due to cancellation particularly for the higher order transformations and it was found to be preferable to use the equivalent ϵ-algorithm or the implementation suggested by Longman [41] and used by Levin [20] in his comparisons. The

ϵ-algorithm was also used by Chisholm, Genz, and Rowlands [19] for a somewhat different integration problem and is defined by

$$\begin{aligned} \epsilon_n^{(-1)} &= 0; \qquad \epsilon_n^{(0)} = A_n , \\ \epsilon_n^{(p)} &= \epsilon_{n+1}^{(p-2)} + [\epsilon_{n+1}^{(p-1)} - \epsilon_n^{(p-1)}]^{-1}. \end{aligned} \tag{31}$$

It can be shown [42] that the equivalence

$$\epsilon_0^{(2k)} = e_k\{A_0 , A_1 ,..., A_{2k}\} = B_{k,k} \tag{32}$$

is then true. This algorithm is well known to be stable.

Also employed were the t-transformation and u-transformation of Levin. These were implemented via the v-transformation, which exhibits desirable properties of both the previous forms. The v-transformation is defined by

$$V_{kn} = \sum_{j=0}^{k} c(j, k, n)\, A_{n+j} \Big/ \sum_{j=0}^{k} c(j, k, n), \tag{33}$$

where

$$c(j, k, n) = (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k}\right)^{k-1} (a_{n+j}^{-1} - a_{n+j+1}^{-1}) \tag{34}$$

and

$$a_n = A_n - A_{n-1} . \tag{35}$$

Following Levin, the diagonal transformation V_{k1} was used.

4. Numerical Comparison and Discussion

To summarize, the methods considered here are as follows.

(i) Asymptotic expansion coupled with a finite interval oscillatory integrator as in Eq. (16). This is Pantis' approach.

(ii) Subdivision into half-cycles over each of which an integration is performed followed by evaluation of the resulting summation, usually with an accelerator incorporated. This is the "integration, then summation" algorithm of Eq. (14) and this category includes the work of Longman [14], Alaylioglu, Evans and Hyslop [15] and Squire [17].

(iii) Here the summation over the cycles is performed first (with or without an accelerator) and is followed by integration. This is the "summation, then integration" algorithm of Eq. (25) and includes the work of Hurwitz and Zweifel [10], Piessens and Haegemans [24], and Boris and Oran [25].

In each case, the original methods are modified by making use of the Gaussian trigonometric integrator of Eq. (20), coupled with the ϵ-algorithm. For non-trigonometric weight functions, the Clenshaw–Curtis method was used for integrations over the half-cycles.

A number of test integrals are considered for comparison purposes. These are usually taken from the original work on the methods described, although some further examples have been added to elucidate specific points. The integrals are listed in Table I together with the exact values obtained from [43].

TABLE I

Test Integrals

$$I_1 = \int_0^\infty x(1+x^2)^{-1} \sin x \, dx = 0.5778636749...$$

$$I_2 = \int_\pi^\infty x^{-2} \sin x \, dx = -0.07366791204...$$

$$I_3 = \int_0^\infty x^{-1} \sin x \exp(-x/2) \, dx = 1.107148718...$$

$$I_4 = \int_0^\infty \operatorname{sech} 2x \cos 4x \, dx = 0.06775373785...$$

$$I_5 = \int_0^\infty x^{-0.1} \sin x \, dx = 1.055472109...$$

$$I_6 = \int_0^\infty x^2 \sin 100x^2 \, dx = \tfrac{1}{2}\int_0^\infty x^{1/2} \sin 100x \, dx = 3.133285343... \times 10^{-4}$$

$$I_7 = \int_0^\infty \cos(1/x^2) \sin x^2 \, dx = 0.1969225576...$$

$$I_8 = \int_0^\infty x(1+x^2)^{-1} J_0(x) \, dx = 0.4210244382...$$

$$I_9 = \int_0^\infty x(x^2+1)^{-3} \sin x \, dx = 8.931901241... \times 10^{-2} \quad (\omega = 0.5)$$

$$= 1.173080162... \times 10^{-1} \quad (\omega = 3.0)$$

$$= 9.805680900... \times 10^{-4} \quad (\omega = 10.0)$$

The number of function evaluations required to evaluate the test integrals to nine significant figures using each of the three methods is exhibited in Table II.

In each case, an attempt was made to improve the integration procedure by reducing the total number of function evaluations required. Thus, Pantis in his

original work used Filon's rule with 702 function evaluations on the subdivided range $[0, \alpha]$ to give I_1 correct to seven figures, whereas the Gaussian trigonometric integrator, Eq. (20), again with subdivision of the range, reduced this number to 140, although 420 evaluations were necessary to obtain nine significant figures. Similar reductions were achieved in the other examples. In most cases, the maximum number of Gauss-trigonometric points required to produce the quoted accuracy was six or seven points per half-cycle. This number was rather larger for the earlier half-cycles in certain examples where the functions were varying rapidly or nonmonotonically for small x although, compensatingly, it was usually found that for the later half-cycles the order of the Gauss-trigonometric formula could be reduced, due to the ultimate smooth decay of the integrand. For methods (i)–(iii) the order N of the Gauss-trigonometric quadrature rule was

final number of function evaluations required being quoted in Table II. Of course, extra function evaluations are required in performing these convergence tests but, since this technique has been adopted for all three methods, the quoted results form a basis for comparison.

TABLE II

Comparison of Methods (i), (ii), and (iii)[a]

Integral	Number of function evaluations		
	(i)	(ii)	(iii)
I_1	420	53	143
I_2	123	51	77
I_3	35	39	100
I_4	18	23	21
I_5	fails	74	>250
I_6 (first form)	—	112	—
I_6 (second form)	fails	60	fails
I_7	—	$94 + 74$	—
I_8	—	80	—
I_9 ($\omega = 0.5$)	100	70	165
I_9 ($\omega = 3.0$)	119	68	72
I_9 ($\omega = 10.0$)	130	64	70

[a] Method (i): Pantis—Eq. (16); method (ii): Integration, then summation—Eq. (14); method (iii): Summation, then integration—Eq. (25). Accelerator used for (ii) and (iii): ϵ-algorithm—Eq. (31); integrator used for (i), (ii), and (iii): Gauss-trigonometric—Eq. (20) [Clenshaw–Curtis for I_6 (first form), I_7, I_8]. Accuracy required: nine significant figures.

It was also found that the Chebyshev-based algorithm of Appendix A was only slightly more expensive than the Gauss-trigonometric approach, requiring usually only about one extra function evaluation per half-cycle. Chebyshev procedures of this type have several useful properties which suggest that they merit consideration as practical alternatives. Thus, unlike the Gaussian-based result, the formula is adaptive in nature so that, if N is chosen to be 2^k with $k = 1, 2, 3,...$, the earlier function evaluations may be reutilized for larger k. Again, it is possible to investigate the convergence of the Chebyshev fit to the function $f(x)$ by considering successive values of the coefficients a_i of Eq. (A3), as described in the original paper by Clenshaw and Curtis [31]. Indeed, as pointed out by Piessens and Poleunis [29], in their discussion of the errors arising in quadrature formulas of this type, the integral of the Chebyshev expansion converges more rapidly than the expansion itself. In addition, since the Chebyshev fitting of $f(x)$ is independent of ω the method is therefore ideally suited to cases where it is required to evaluate a given integral for a large number of values of ω. In such instances, the Chebyshev integration method could be incorporated into the Pantis procedure to great effect.

For weights other than $\sin \omega x$ and $\cos \omega x$, the Gauss-trigonometric integrator is not applicable and the integrations over the half-cycles were performed using the Clenshaw–Curtis method [31], which is the limiting version of the Chebyshev-based algorithm of Appendix A. Of course, a Gaussian method such as Gauss–Legendre quadrature could be used here and would produce some slight reduction in the number of points quoted for integrals I_6, I_7, and I_8. However, the properties of the Chebyshev procedure listed in the preceding paragraph, particularly adaptivity and the facility for continuous monitoring of the coefficients, are still applicable and suggest that the Clenshaw–Curtis method is a feasible practical procedure. Note also that for I_7 it was necessary, because of the $1/x^2$ singularity to consider the ranges $[0, 1]$ and $[1, \infty]$ separately and to use the transformation $t = 1/x$ on the first range.

The value of α required in the method of Pantis is determined by truncating the asymptotic series in Eq. (16) to obtain the desired accuracy. Clearly, it is desirable to exclude any derivatives other than the first in practical applications and even the first derivative $f'(x)$ may be extremely difficult to compute in certain instances. The values of α used for integrals I_1–I_4 were 300, 100, 30 and 10 respectively. Obviously, the Pantis method will be efficient if the terms of the asymptotic series fall off quickly enough for the choice of α to be reasonably small. The integration over $[0, \alpha]$ may then be accomplished with a relatively small number of points. Thus, I_3 and I_4, where there is a predominantly exponential decay in $f(x)$, require small α values and these integrals, especially I_4, are evaluated extremely efficiently using Pantis' method. However, in other integrals where the falloff in $f(x)$ is slow, the required α value may be excessively large and may even result in failure of the

method, as in I_5. The same applies to the second form of I_6 which is an example of an integral converging only in the mean. Integrals such as the first form of I_6 and also I_7 and I_8 are not amenable to the Pantis approach unless special asymptotic expansions are generated appropriate to the weight functions occurring. The integral I_9 is the simplest example arising in the molecular integral applications referred to earlier and ω in this case represents the scaled internuclear separation for the H_2^+ ion. The function $f(x)$ falls off reasonably rapidly here and the α values are small enough (68, 50, 89, respectively) for fairly efficient evaluation to be possible using Pantis.

Method (ii), which is the modified version of the work of Alaylioglu *et al.* [15] and which involves integration over the half-cycles followed by summation, is clearly applicable to a wider class of problems than the other methods considered. With the modifications suggested, it proves highly competitive in terms of function evaluations, even when conditions are such as to favor the alternative techniques. For the most part, it makes little difference whether e_k or e_1^k is used as an accelerator and it was found that $k = 5$ was the largest order required and hence 11 half-cycle integrals was the maximum number needed for any of the integrals. In certain cases, the acceleration produced was extremely rapid and lower order transformations were adequate. For instance, for I_3 only 6 half-cycles were required and e_2 or e_1^2 was sufficient. Again, for I_4 where there is rapid exponential decay, only 3 half-cycles are needed and the simple Aitken transformation e_1 is adequate here. This question is discussed in more detail with reference to a particular example in the next section.

In order to decide a priori which transformation is required, it is necessary to have a detailed knowledge of the transient behavior [16] of the terms u_n of the sequences. This information is not, in general, available and in practice the convergence is best investigated empirically by setting up a Shanks table. This table would use $e_1, e_2, e_3, \ldots$, and/or $e_1, e_1^2, e_1^3, \ldots$, until convergence was exhibited to a specified tolerance, the half-cycle integrals being evaluated only as required.

The calculations based on method (iii) were introduced to see if there was any merit in performing the summations first. The results indicate that this approach is usually less economical than method (ii) and, of course, since it relies on the periodicity of the trigonometric functions it is not always applicable and cannot be used, for example, on I_7 and I_8 or the first form of I_6.

The method of Boris and Oran [25], which does not use an accelerator and employs essentially the trapezoidal rule for integration, appeared to converge extremely slowly for most of the integrals tested. The method requires the rapid decay of the Fourier transform of $f(x)$ and it was only in cases like I_4 where rapid exponential decay was exhibited that the method converged, although, even here, 100 function evaluations were required for nine figure accuracy. The method, of course, does not apply to integrals like I_7 or I_8. It appears to be most useful in

those applications for which it was specifically designed, where there is rapid exponential decay, as exemplified by their test integral

$$\int_0^\infty \exp(-40 \cosh x) \cos(39x)\, dx = 7.553050... \times 10^{-28}. \tag{36}$$

5. Two Special Examples

In examples I_1–I_9 there is no very significant variation in the number of function evaluations used when the angular frequency ω is changed, except possibly for very large and small values of ω. In the partition–extrapolation methods, an increase in ω usually results in more cycles being required but there is a compensating reduction in the number of quadrature points because of the smoother behavior of the function $f[(t + n)\,\omega^{-1}]$. On the other hand the efficiency of Pantis' asymptotic formula, Eq. (16), increases with ω.

TABLE III

Evaluation of $I_{10}(\omega)$ to Nine Decimal Places

ω	Exact value	Number of function evaluations		
		(i)	(ii)	(iii)
0.5	2.4466748187	197	60	110
1	1.9054722647	129	53	88
2	1.1557273498	120	50	77
4	0.4251683316	92	40	77
8	0.0575402766	69	45	66
16	0.0010538869	50	43	66
32	0.0000003535	40	34	66

The effect is demonstrated in Table III, which illustrates the relative efficiency of the various methods for varying angular frequency ω and introduces an additional practical difficulty which also arises in the Boris and Oran integral, Eq. (36). The example chosen is that of Piessens and Haegemans [24] and Squire [17] namely,

$$I_{10}(\omega) = \int_0^\infty (x^2 + \tfrac{1}{4})^{-1} \cos \omega x\, dx = \pi \exp(-\omega/2) \tag{37}$$

for values of ω ranging from 0.5 to 32.

The number of function evaluations using methods (i), (ii), and (iii) for an accuracy of nine decimal places is also displayed.

Once again method (ii) (integration, then summation) proves the most economical, and a further demonstration of its efficiency is provided by comparing it with the earlier results of Piessens and Haegemans [24] and Squire [17]. To provide a meaningful comparison, the present method was implemented to produce equivalent accuracy (about eight decimal places) with the earlier calculations. The accuracy of the earlier work varied slightly for the different values of ω and also from Refs. [24] to [17]. Hence, the more stringent requirement of the two earlier works was applied in each case. The results are shown in Table IV and demonstrate a considerable increase in efficiency for the present method over the earlier results.

TABLE IV

Comparisons with Earlier Methods for $I_{10}(\omega)$

	Number of function evaluations		
ω	PH[a]	S[b]	(ii)[c]
0.5	780	186	45
1	419	170	49
2	223	170	47
4	113	221	37
8	120	269	38
16	46	285	43
32	53	—	34

[a] Piessens and Haegemans [24].
[b] Squire [17].
[c] Present method: Eq. (14).

[redacted] with increasing ω. Thus, from Table III, the exact value of I_{10} when $\omega = 32$ is

$$I_{10}(32) = 3.535... \times 10^{-7}, \tag{38}$$

whereas the magnitude of the first term in the sequence (28) is given by

$$u_0 \simeq -0.24. \tag{39}$$

Hence, extremely severe cancellation will arise at the summation stage of the process, resulting in a loss of approximately six significant figures. This instability is inherent and is the reason why eight decimal places rather than eight significant digits are quoted in this particular example. The situation is worse for larger values of ω. For example,

$$I_{10}(100) = 6.059... \times 10^{-22} \tag{40}$$

and about 20 figures will be lost through cancellation and multiple precision arithmetic would be necessary to obtain an accurate result. This defect applies also to the other methods mentioned in this paper and was also discussed by Boris and Oran in connection with their example (36). In practice, of course, an acceleration algorithm will simply provide the result zero to machine accuracy for integrals such as (40) and whether this is sufficient depends on the nature of the problem in question. Special quadrature rules can always be invented for specific integrals which incorporate the required behavior, such as the $\exp(-\omega/2)$ factor, but they have no practical use outside the special case considered.

An additional test integral defined by

$$I_{11} = \int_0^\infty x^{-1/2} \sin \omega x \exp(-x - x^{-1})\, dx = -4.885538257... \times 10^{-3} \quad (\omega = 10)$$
$$= -9.769643582... \times 10^{-6} \quad (\omega = 50)$$
$$= 8.994771670... \times 10^{-8} \quad (\omega = 100)$$

was considered to provide a more critical test of the extrapolation procedure. In most of the previous examples, the function $f(x)$ decayed sufficiently rapidly for the terms u_j in the sequence $\{A_n\}$ of Eq. (28) to exhibit monotonic decrease at an early stage (I_6 being a notable exception). Consequently, the ϵ-algorithm proved to be extremely efficient in accelerating convergence. The alternative v-transformation proposed by Levin was even more efficient in these examples and generally induced convergence in one or two fewer half-cycles than the ϵ-algorithm. For instance, when applying method (ii) to I_2, the number of function evaluations was reduced from 51 to 47 and on I_6 from 112 to 104.

However, I_{11} provides a more stringent test of the accelerator used in that the half-cycle contributions increase initially before a monotonic decrease is attained. Thus, for $\omega = 10$ the half-cycle contributions have a maximum modulus in the third half-cycle and 14 terms are required to give nine figure accuracy using the ϵ-algorithm with a total of 71 function evaluations. The v-transformation achieves the same accuracy in 12 half-cycles and 63 function evaluations. At $\omega = 50$, the maximum modulus occurs in the thirteenth term and yet 16 half-cycles are sufficient to yield the maximum achievable accuracy of eight figures (with 11 figures working, see the note on I_{10}) with the ϵ-algorithm using 67 function evaluations. Only one half-cycle is gained by the v-transformation here and 64 function evaluations are necessary. Finally, at $\omega = 100$ the maximum occurs *outside* the sequence used in the accelerator but, even here, 17 terms give the expected six figure accuracy with the ϵ-algorithm, taking 71 function evaluations. The v-transformation needs 18 terms and 74 function evaluations.

It appears that marginal advantage may be gained by using a transformation suited to a given sequence and that the v-transformation of Levin seems to have

a slight edge over the ϵ-algorithm in most of the examples considered. However, both transformations are highly effective in practice and are equally easy to implement.

6. Conclusions and Physical Applications

It appears that the "integration, then summation" algorithm, Eq. (14), gives the best results over a wide range of examples. With the powerful Gauss-trigonometric integrator or the alternative Chebyshev procedure described in the Appendixes, the method is very efficient in terms of function evaluations. The Chebyshev-based integrator is usually only slightly more expensive than the Gauss-trigonometric procedure in terms of function evaluations. However, it has the advantage of being adaptive in nature and, in addition, the facility is able to monitor the Chebyshev coefficients a_i as in the Clenshaw–Curtis method. These features may be important in practice since they may be balanced against the need to conduct empirical convergence tests to determine the order of the Gauss-trigonometric rule necessary for a given half-cycle integration. The well-known and easily implemented ϵ-algorithm proves to be extremely efficient as an accelerator, although it should be mentioned that the v-transformation suggested by Levin is marginally more efficient in most of the examples considered and is also easy to implement.

There are certainly examples where the asymptotic series approach of Pantis is quicker, but this method lacks speed in many other examples and it is not so widely applicable. It appears also that it is preferable to integrate first before summation rather than to reverse the procedure, both on grounds of efficiency in most of the examples considered and also because of wider applicability. The suggested method is easily generalized to nontrigonometric oscillatory integrands, whereas "summation, then integration" does not apply here and the method of Pantis would require a modified asymptotic expansion as well as a modified integrator. For these nontrigonometric weight functions, the Clenshaw–Curtis quadrature prescription [31], which is the limiting form of the procedure outlined in Appendix A, has been utilized for the half-cycle integrals although alternative methods such as Gauss–Legendre quadrature could also be adopted here.

In the light of these conclusions, the two problems in mathematical physics which involved infinite range oscillatory integrals were considered further. For the problem in fluid mechanics with an integrand which has the Bessel functions J_0 and J_1 for its oscillatory parts, only the technique of "integration, then summation" is appropriate. This method proved extremely efficient and gave results in complete agreement with the asymptotic estimates where these were available ($\alpha = 0$, $R \to 0$). Moreover the difficulty at $\alpha = 0$ was absorbed by the method

which deals directly with mean convergence, as mentioned in Section 2. Extensive convergence tests then indicated that accurate values of the integral could be obtained economically for all values of the Reynolds number and over the complete range of the angle α and the corresponding forces were then computed as detailed in [1].

Again for the problem in quantum mechanics, the "integration, then summation" algorithm was utilized and extensive convergence tests carried out together with comparisons with selected analytical test cases. It was found that values of the infinite integrals accurate to eight significant figures are obtainable over the complete range of internuclear separation R with a total of about 50 integration points required for each value of R. These results were then used to compute approximate energy levels for the hydrogen molecular ion H_2^+, the results being presented in [5].

APPENDIX A: CHEBYSHEV BASED QUADRATURE FORMULAS FOR TRIGONOMETRIC INTEGRALS

On normalizing the interval of integration to $[-1, 1]$ by means of a linear transformation, the basic Nth order quadrature rules may be expressed as

$$\int_{-1}^{1} f(x) \cos \omega x \, dx \simeq \sum_{i=0}^{N''} a_i \sum_{r=0}^{i} D_{i,r} C_r \,, \tag{A1}$$

$$\int_{-1}^{1} f(x) \cos \omega x \, dx \simeq \sum_{i=0}^{N''} a_i \sum_{r=0}^{i} D_{i,r} S_r \,. \tag{A2}$$

The Clenshaw–Curtis coefficients a_i arise on expanding $f(x)$ terms of the Chebyshev polynomials $T_i(x)$ and are given by

$$a_i = (2/N) \sum_{j=0}^{N''} f(x_j) \cos(\pi j i / N), \tag{A3}$$

with

$$x_j = \cos(\pi j / N), \tag{A4}$$

the double primes denoting that the first and last terms in the summations are to be multiplied by $\frac{1}{2}$. $D_{i,r}$ represents the coefficients of x^r in $T_i(x)$ and is easily computed from the recurrence relation

$$D_{i,r} = 2D_{i-1,r-1} - D_{i-2,r} \,, \qquad i \geqslant 2, \quad r \leqslant i, \tag{A5}$$

the starting values being $D_{0,0} = 1$, $D_{1,0} = 0$, and $D_{1,1} = 1$.

The monomial integrals

$$C_r = \int_{-1}^{1} x^r \cos \omega x \, dx \tag{A6}$$

and

$$S_r = \int_{-1}^{1} x^r \sin \omega x \, dx \tag{A7}$$

are given by the finite series

$$C_r = \sum_{l=r}^{r} l! \binom{r}{l} \frac{x^{r-l}}{\omega^{l+1}} \sin(\omega x + \tfrac{1}{2} l\pi) \Big|_{-1}^{1} \tag{A8}$$

and

$$S_r = -\sum_{l=0}^{r} l! \binom{r}{l} \frac{x^{r-l}}{\omega^{l+1}} \cos(\omega x + \tfrac{1}{2} l\pi) \Big|_{-1}^{1} \tag{A9}$$

when ω is large ($\omega > 4$ in practice). For smaller values of ω ($\omega < 4$), these series may become unstable for large values of N and should be replaced by the rapidly converging infinite series

$$C_r = 2 \sum_{l=0}^{\infty} (-1)^l (\omega^{2l}/(2l)!)(2l + r + 1)^{-1} \tag{A10}$$

and

$$S_r = 2 \sum_{l=0}^{\infty} (-1)^l (\omega^{2l+1}/(2l + 1)!)(2l + r + 2)^{-1} \tag{A11}$$

for even and odd r, respectively. Truncation at

$$l = [2\omega] + 10 \tag{A12}$$

was found to yield double-precision accuracy (about 22 figures) for the monomials for $\omega < 4$.

The derivation and structure of these formulas are discussed in detail in [30], where the stability of the procedure with increasing N is also considered. The recommendation is that, if values of N much beyond $N = 20$ are to be used, double-precision arithmetic (22 figures) is necessary to evaluate the summations in (A1) and (A2); otherwise, single-precision (11 figures) arithmetic is adequate for most of the N values likely to be used in practice.

Note that, if ω is taken to be zero in (A10), then the quadrature rule (A1) degenerates into

$$\int_{-1}^{1} f(x) \, dx \simeq -2 \sum_{i=0}^{N''} a_i/(i^2 - 1), \tag{A13}$$

which is the Clenshaw–Curtis formula [31] and which has been used in the present work for half-cycle integration for weight functions other than $\sin \omega x$ or $\cos \omega x$.

APPENDIX B: GAUSSIAN FORMULAS FOR TRIGONOMETRIC INTEGRALS

Gaussian quadrature coefficients are presented for the weight function $\cos t$

$$\int_{-\pi/2}^{\pi/2} F(t)\cos t\,dt \simeq \sum_{i=1}^{N} w_i F(t_i) \qquad \text{(see Table B1)}, \tag{B1}$$

$$\int_{0}^{\pi/2} F(t)\cos t\,dt \simeq \sum_{i=1}^{N} \bar{w}_i F(\bar{t}_i) \qquad \text{(see Table B2)}. \tag{B2}$$

TABLE B1

Gaussian Coefficients for $\cos t$ on $[-\pi/2, \pi/2]$

Order	Abscissas[a]	Weights
2	6.8366739009 (−1)	1.0000000000 (0)
3	0.0000000000 (0)	1.0883191839 (0)
	1.0126012400 (0)	4.5584040804 (0)
4	4.3928746686 (−1)	7.7592938187 (−1)
	1.1906765639 (0)	2.2407061813 (−1)
5	0.0000000000 (0)	7.5221097881 (−1)
	7.2598673794 (−1)	5.0378251239 (−1)
	1.2964402800 (0)	1.2011199821 (−1)
6	3.2385211421 (−1)	6.0581370012 (−1)
	9.1979066552 (−1)	3.2479855138 (−1)
	1.3639113021 (0)	6.9387748500 (−2)
7	0.0000000000 (0)	5.7554040031 (−1)
	5.6350196618 (−1)	4.5607388993 (−1)
	1.0555399634 (0)	2.1353015976 (−1)
	1.4094168673 (0)	4.2625750151 (−2)
8	2.5649650742 (−1)	4.9199579660 (−1)
	7.4346864788 (−1)	3.3626447785 (−1)
	1.1537256455 (0)	1.4420409203 (−1)
	1.4414905402 (0)	2.7535633514 (−2)
9	0.0000000000 (0)	4.6630641290 (−1)
	4.5980985871 (−1)	4.0043355770 (−1)
	8.8098166893 (−1)	2.4776782327 (−1)
	1.2267607474 (0)	1.0010472234 (−1)
	1.4649150799 (0)	1.8540690233 (−2)
10	2.1234288707 (−1)	4.1271237189 (−1)
	6.2214145705 (−1)	3.1897307574 (−1)
	9.8788528562 (−1)	1.8407934564 (−1)
	1.2824218393 (0)	7.1311631869 (−2)
	1.4825294562 (0)	1.2923574871 (−2)

[a] Only positive abscissas shown.

TABLE B2

Gaussian Coefficients for cos t on $[0, \pi/2]$

Order	Abscissas	Weights
2	2.6587388056 (−1)	6.0362553281 (−1)
	1.0351526093 (0)	3.9637446719 (−1)
4	9.5669389197 (−2)	2.3783071420 (−1)
	4.5240902327 (−1)	4.0265695524 (−1)
	9.3185057672 (−1)	2.8681737949 (−1)
	1.3564439600 (0)	7.2694951083 (−2)
6	4.8337202961 (−2)	1.2233130510 (−1)
	2.4157438682 (−1)	2.4897643030 (−1)
	5.4241569594 (−1)	2.8666212347 (−1)
	8.8888235763 (−1)	2.1871922991 (−1)
	1.2145625204 (0)	1.0250866521 (−1)
	1.4579176907 (0)	2.0802246015 (−2)
8	2.9023729769 (−2)	7.3908998095 (−2)
	1.4828524405 (−1)	1.6002993702 (−1)
	3.4531111152 (−1)	2.1444434342 (−1)
	5.9447696798 (−1)	2.1979581269 (−1)
	8.6538380686 (−1)	1.7581164478 (−1)
	1.1263076093 (0)	1.0560448025 (−1)
	1.3470150460 (0)	4.2485497299 (−2)
	1.5015603622 (0)	7.9192864406 (−3)
10	1.9324468537 (−2)	4.9349210907 (−2)
	9.9799217690 (−2)	1.0982195774 (−1)
	2.3672223071 (−1)	1.5692441652 (−1)
	4.1797757474 (−1)	1.8142185381 (−1)
	6.2827073435 (−1)	1.7735663121 (−1)
	8.5057478126 (−1)	1.4671616225 (−1)
	1.0673430163 (0)	1.0046661487 (−1)
	1.2616021055 (0)	5.4074272678 (−2)
	1.4180367416 (0)	2.0246477726 (−2)
	1.5241034398 (0)	3.6224022909 (−3)

The symmetric interval $[-\pi/2, \pi/2]$ is chosen for convenience in tabulation. If the coefficients for the weight function sin t on $[0, \pi]$ are required, as in Eq. (20) of the text, then $\pi/2$ is simply added to the abscissas t_i, the weights w_i remaining the same. Here, attention is confined to the lower order results which have been most used in the practical calculations described in the present paper.

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