

**Note**

**Numerical Evaluation of Oscillatory Integrals Such as  
the Modified Bessel Function  $K_{i\zeta}(x)$**

I. INTRODUCTION

We present an "orthogonalized" Fourier method of numerically evaluating oscillatory integrals of the form

$$I(\zeta) = \int_0^\infty f(t) \begin{Bmatrix} \cos \zeta t \\ \sin \zeta t \end{Bmatrix} dt, \tag{1}$$

where  $\zeta$  is a constant. This method is particularly efficient when  $f(t)$  is a function whose Fourier transform,  $\tilde{f}(\omega)$ , decays rapidly for large  $\omega$ . Maximal efficiency is achieved as  $\zeta$  becomes large and many cycles of the sine or cosine contribute significantly. When  $\zeta$  is large enough, we need to evaluate  $f(t)$  only twice per cycle. We explicitly present an analysis of the cosine form of Eq. (1) and take advantage of the fact that for a wide class of functions  $f(t)$ , the even part of the sum

$$F(\zeta, t) \equiv \sum_{j=0} f\left(t + \frac{2\pi j}{\zeta}\right), \quad 0 \leq t \leq \frac{2\pi}{\zeta} \tag{2}$$

rapidly approaches  $A_0 + A_1 \cos \zeta t$  for large enough  $\zeta$ . Thus, a finite discrete Fourier analysis of the sum extracts  $A_1$  numerically, and the remaining quadrature is performed analytically. Difference-of-large-number errors are avoided by "orthogonalizing" the function  $f(t)$  over the successive cycles of  $\cos \zeta t$  or  $\sin \zeta t$ . The analysis and method described below extend easily to the sine function integral.

Difficulties occur in the numerical evaluation of Eq. (1) by standard quadrature methods (e.g., Simpson's rule) in the important limit when  $\zeta$  is large. In this case, approximation of the integrand by simple polynomials could only be done accurately over a prohibitively small interval of  $t$ . Further problems arise from strong cancellation of the positive and negative contributions to the integral. Methods which approximate  $f(t)$  by a low-order polynomial, such as those suggested by Filon [1], Clendenin [2], and Flinn [3], deal with the problem of the small integration interval but do not really apply here because of the infinite

integration range. Hurwitz and Zweifel [4], Hurwitz, Pfeifer, and Zweifel [5], Saenger [6], and deBalbine and Franklin [7], deal with the cancellation problem by converting the infinite integral into a summation and integrating over successive half-cycles of the sine or cosine term before summing. Attempts to accelerate the convergence of these methods have been made by Longman [8], using an Euler transformation, and Alaylioglu, Evans, and Hyslop [9], using the Shanks [10] transformation.

This study of oscillatory integrals was motivated by a need to evaluate the modified Bessel functions of imaginary order,  $K_\nu(x)$  where  $\nu = i\zeta$  and

$$K_{i\zeta}(x) = \int_0^\infty e^{-x \cosh t} \cos \zeta t \, dt, \quad (3)$$

and its derivative with respect to  $x$ ,

$$K'_{i\zeta}(x) = - \int_0^\infty \cosh t \cos \zeta t e^{-x \cosh t} \, dt \quad (3')$$

over a wide range of the parameters  $x$  and  $\zeta$ . These Bessel functions occur in calculations of quantum mechanical cross sections and reaction rates for electron impact excitation of ions and neutrals (cf. calculations of Oran and Davis [11] and references therein). The modified Bessel function is also a solution to the one-dimensional Schrodinger equation with potential energy  $V(r) = V_\infty - Ae^{-r/a}$ , where  $A$ ,  $V_\infty$ , and  $a$  are parameters and  $r$  is the distance from the center of force. This potential can represent the repulsive forces of a diatomic-molecule, as shown by Luke [12].

Hunter [13] has discussed the problems of evaluating the integrals representing this kind of Bessel function. The quadrature techniques he recommends, however, are impractical for the range of values of  $x$  and  $\zeta$  required by both the cross section and the diatomic-molecule calculations just mentioned in which many cycles of the cosine may contribute. Tables of values of  $K_{i\zeta}(x)$ , (generated by Morgan [14] and Luke and Weissman [15]) were computed laboriously by numerical integration of the associated ordinary differential equations, and accuracy was obtained to four or five decimal digits. We needed to evaluate the Bessel function *and* its derivative accurately for arbitrary values of  $x$  and  $\zeta$ . Thus a method of direct calculation was indicated as opposed to generating and interpolating in a very extensive table [16].

Section II of this paper develops the method. Section III presents two examples of its use and provides brief comparisons with two other methods in current use.

## II. METHOD

The cosine form of the desired integral, Eq. (1), can be rewritten as,

$$I(\zeta) = \int_0^{2\pi/\zeta} \cos \zeta t \, dt \, F(\zeta, t), \quad (4)$$

in which the function  $f(t)$  has been replaced by Eq. (2), a sum of all corresponding points in the successive cycles of  $\cos \zeta t$ . The sum  $F(\zeta, t)$  converges provided  $|f(t)|$  decreases rapidly enough as  $t \rightarrow \infty$ .  $F(\zeta, t)$  becomes large as  $\zeta$  increases because an increasing number of terms from the sum in Eq. (2) contribute. The integral  $I(\zeta)$  gets smaller as  $\zeta$  increases, because there are an increasing number of oscillatory cancellations. Thus, direct summation of  $f(t)$  leads to unacceptable difference-of-large-number cancellation errors. Previous workers have dealt with this problem by first integrating over each cycle or half-cycle and then applying various acceleration tricks to the sequence of subintegrals. These procedures require the evaluation of a large number of integrals and do not generally permit the use of the special properties which the sum  $F(\zeta, t)$  is shown below to exhibit.

Cancellation errors can be minimized by rewriting Eq. (4) in the form,

$$I(\zeta) = \int_0^{2\pi/\zeta} \cos \zeta t \, dt \left[ (F(\zeta, t) - F(\zeta, 0)) + \frac{\zeta t}{2\pi} \left( F(\zeta, 0) - F\left(\zeta, \frac{2\pi}{\zeta}\right) \right) \right], \quad (5)$$

which is allowed because the constant and linear terms which have been added to Eq. (5) both integrate to zero against the cosine. This error-reducing "orthogonalization" is next extended to the individual terms. In actual numerical calculations, the sum function  $F$  should be defined as

$$F(\zeta, t) \equiv \sum_{j=0}^{j \max} \left[ \left( f\left(t + \frac{2\pi j}{\zeta}\right) - f\left(\frac{2\pi j}{\zeta}\right) \right) + \frac{\zeta t}{2\pi} \left( f\left(\frac{2\pi j}{\zeta}\right) - f\left(\frac{2\pi(j+1)}{\zeta}\right) \right) \right]. \quad (6)$$

There is enough local cancellation in Eq. (6) so that the sums can be performed with sufficient accuracy before including the basic  $\cos \zeta t$  term and before performing any numerical integrations over half- or whole-cycles. The technique of summing first is in marked contrast to the methods discussed in the literature, for example, by Hurwitz and Zweifel [4] and Alaylioglu, Evans, and Hyslop [9].

The sum  $F(\zeta, t)$  from Eq. (2) or Eq. (6) can be expressed as a Fourier series,

$$F(\zeta, t) \equiv \sum_{k=0}^{\infty} [A_k \cos k\zeta t + B_k \sin k\zeta t], \quad (7)$$

so that the integral in Eq. (4) reduces to

$$I(\zeta) = (\pi/\zeta) A_1 . \tag{8}$$

In general, the coefficients  $\{A_k\}$  and  $\{B_k\}$  may be complex. However, without loss of generality we can assume that  $f(t)$ , and hence  $F(\zeta, t)$ , is real so that  $\{A_k\}$  and  $\{B_k\}$  are real sequences. Using the Fourier integral transformation,

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(\omega) e^{-i\omega t} d\omega,$$

$F(\zeta, t)$  can be written as

$$F(\zeta, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(\omega) d\omega \sum_{j=0}^{\infty} e^{-i\omega t} e^{-2\pi i \omega j / \zeta} e^{-\beta j}, \tag{9}$$

where the convergence factor  $e^{-\beta j}$  has been inserted to determine the position of certain poles which will appear relative to the path of integration. Later we will let  $\beta \rightarrow 0$  when the limit is unambiguous. The sum on  $j$  can now be performed giving

$$F(\zeta, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\tilde{f}(\omega) d\omega e^{-i\omega t}}{(1 - e^{-2\pi i \omega / \zeta} e^{-\beta})}. \tag{10}$$

To find the coefficients  $\{A_k\}$  and  $\{B_k\}$  and thus  $I(\zeta)$  in particular, we multiply both Eq. (7) and Eq. (10) by  $e^{ik\zeta t}$ , integrate from  $t = 0$  to  $t = (2\pi/\zeta)$ , and find that

$$\frac{\pi}{\zeta} (A_k + iB_k) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\tilde{f}(\omega) d\omega}{(\omega - k\zeta)} \frac{(e^{-2\pi i \omega / \zeta} - 1)}{(e^{-(2\pi i \omega / \zeta) - \beta} - 1)}. \tag{11}$$

The poles of the integrand lie above the real axis at  $\omega = l\zeta + (i\zeta\beta/2\pi)$  for  $l = 0, \pm 2, \text{ etc.}$  There is no pole at  $\omega = k\zeta$  if  $\beta > 0$ . When  $\omega \neq k\zeta$  and  $\beta \rightarrow 0$  the exponential terms in the numerator and denominator become equal and cancel. When  $\omega = k\zeta$ , the zero of  $(\omega - k\zeta)$  cancels against the zero in the numerator. Thus the only pole of concern lies at  $\omega = k\zeta + (i\zeta\beta/2\pi)$  and Eq. (11) becomes

$$\frac{\pi}{\zeta} (A_k + iB_k) = \frac{1}{2\pi i} \lim_{\beta \rightarrow 0} \int_{-\infty}^{\infty} \frac{\tilde{f}(\omega) d\omega}{(\omega - k(i\zeta\beta/2\pi))}. \tag{12}$$

Using the definition of the principal part integral Eq. (12) becomes,

$$\frac{\pi}{\zeta} (A_k + iB_k) = \tilde{f}(k\zeta) + \frac{1}{2\pi i} P \int_{-\infty}^{\infty} \frac{\tilde{f}(\omega) d\omega}{(\omega - k\zeta)}. \tag{13}$$

If  $f(t)$  is even in addition to being real,  $\tilde{f}(\omega)$  must also be even and real. Then the principal part integral contributes only to the sine coefficients  $B_k$ , which integrate

to zero against  $\cos \zeta t$  in Eq. (4). Thus, Eq. (13) shows that the Fourier coefficients of the even part of the sum  $F(\zeta, t)$ ,

$$F^e(\zeta, t) \equiv (1/2) \left[ F(\zeta, t) + F\left(\zeta, \frac{2\pi}{\zeta} - t\right) \right], \quad (14)$$

are simply

$$A_k = (\zeta/\pi) \tilde{f}(k\zeta). \quad (15)$$

The power of the method becomes apparent when one tries to evaluate  $I(\zeta)$  for large  $\zeta$ . In this case  $F^e(\zeta, t)$  has the exceedingly simple and accurate approximation

$$F^e(\zeta, t) = A_0 + A_1 \cos \zeta t. \quad (16)$$

In fact, when  $\tilde{f}(k\zeta)$  decays exponentially with increasing  $k$ , evaluating  $F^e(\zeta, t)$  at only two points in  $0 \leq t \leq 2\pi/\zeta$  suffices to give the coefficient  $A_0$  which integrates to zero against  $\cos \zeta t$  and  $A_1$  which gives the desired integral by Eq. (8).

When  $\zeta$  is so small that  $F^e(\zeta, 0)$  and  $F^e(\zeta, (\pi/\zeta))$  are not adequate to find  $A_1$  with sufficient accuracy from Eq. (16), more points are needed in each cycle because  $A_2, A_3, \dots$  also contribute. The best generalization is to evaluate  $F^e(\zeta, t)$  at  $N + 1$  equally spaced points on  $0 \leq t \leq \pi/\zeta$ . Then  $I(\zeta)$  is found by a finite discrete Fourier cosine transform of the form

$$I(\zeta) = \frac{\pi}{N\zeta} \sum_{l=0}^{2N-1} \cos \frac{\pi l}{N} F^e\left(\zeta, \frac{\pi l}{N\zeta}\right). \quad (17)$$

The error here is then determined by the size of the Fourier coefficient which is the first alias of the desired mode  $k = 1$ . When  $N = 1$  the largest error term is  $\tilde{f}(3\zeta)$ . In general the error term from aliasing is  $\tilde{f}(2N\zeta + \zeta)$ , which is indistinguishable from  $\tilde{f}(\zeta)$  at the  $N + 1$  values of  $t$  in the interval  $0$  to  $\pi/\zeta$ . Here  $\tilde{f}(2N\zeta)$  is indistinguishable from the constant term on the grid of  $N + 1$  points spanning the half-cycle, but integrates to zero so does not contribute to the error. Since the points of evaluation of  $f$  are equally spaced, the same  $f$  evaluations could be used for several values of  $\zeta$ . Furthermore, as in the case of the Bessel functions, recursion relations and multiple-angle formulae can be used to significantly reduce the number of transcendental function subroutine calls.

### III. EXAMPLES

The method is now demonstrated on two examples, one which can be integrated analytically and the Bessel function  $K_{it}(x)$ , whose evaluation originally motivated this work. The results in each case will be compared with summation of the half-

cycle integrals and with Shanks acceleration applied to partial sums of the half-cycle integrals [9, 10]. In each of these comparison cases, Gaussian integration with 15-digit coefficients [17] is used to evaluate each of the half-cycle integrals. Comparison cases are run with equal numbers of function evaluations across a whole-cycle of  $\cos \zeta t$ .

We do not provide comparisons with any direct quadrature methods which do not recognize the essential periodicity of the oscillatory portion of the integrand. The evidence is overwhelming that such approaches are inadequate. Nor do we attempt to compare with all possible choices of half- or whole-cycle quadrature formulae or with the spectrum of acceleration techniques. We have chosen a good representative of each. Rather, in these examples we wish to demonstrate the advantage which can be gained by noting the analytic simplification which our equivalent "orthogonalized" integrand undergoes in just the limit which gives the usual numerical approaches the most difficulty.

The first example has a closed form

$$I_1(\zeta, x) = \int_0^\infty \frac{\cos \zeta t}{\cosh xt} dt = \frac{\pi}{2x \cosh(\pi\zeta/2x)}, \quad (20)$$

and the test is run with  $x = 2$ ,  $\zeta = 4$ . These values provide a case where  $f(t) = 1/\cosh xt$  decreases smoothly and appreciably in the first few cycles and hence where acceleration of the half-cycle partial integrals is expected to pay the largest dividends. At the same time the relatively small value of  $\zeta$  means that the orthogonalized Fourier method should not be maximally efficient. Several function evaluations per half-cycle are required to extract  $A_1$  with sufficient accuracy from other low-order harmonics. Table I displays the results of this test. The 1-point Gaussian results always evaluate the integrand at the zero of the term  $\cos \zeta t$  and hence the  $2N = 2$  results are meaningless for both the direct sum of the 1-point Gaussian integrals and the Shanks acceleration of those results. The  $N = 1$  orthogonalized Fourier result is accurate to two figures (the correct digits are indicated by the underscore beneath each result) but the  $N = 2$  result shows no improvement over this  $N = 1$  result. The results are identical because the evaluation of  $F(\zeta, (\pi/2\zeta))$  and  $F(\zeta, (3\pi/2\zeta))$  occurs at zeroes of  $\cos \zeta t$  and hence adds no information to the finite discrete transform being performed.

In this first test, the Shanks acceleration result was achieved using roughly half as many cycles of the cosine. Therefore, it is nominally twice as efficient as the other methods for a given number of evaluation points per cycle. Thus the result for  $2N = 12$  by the Shanks acceleration took roughly the same amount of computation and gives roughly the same accuracy as the  $2N = 6$  result by the orthogonalized Fourier method. Therefore, even in this relatively small- $\zeta$  case, the orthogonalized Fourier method is at least as accurate per function evaluation as the accelerated method. Furthermore, it is easier to apply.

TABLE I

$$\text{First Test Problem } \int_0^{\infty} \frac{\cos \zeta t}{\cosh xt} dt.$$

Evaluations of $f$ Per Cycle ( $2N$ )	$N$ -Point Gaussian $\frac{1}{2}$ Cycle Integrals	Shanks Acceleration	Orthogonalized Fourier
2	$\sim 0.0$	$\sim 0.0$	<u>.0678807375</u>
4	.0839745904	.083745919	<u>.0678807375</u>
6	.0662966642	.0662966655	<u>.0677539750</u>
8	.0678104294	.0678104307	<u>.0677537382</u>
10	.0677536908	.0677536921	<u>.0677537378</u>
12	.0677536123	.0677536136	<u>.0677537378</u>
14	.0677537442	.0677537456	<u>.0677537378</u>
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty = \text{exact}$	<u>.0677537778</u> ...	<u>.0677537378</u> ...	<u>.0677537378</u> ...

In this test  $\zeta = 4$  and  $x = 2$ . This integral does not oscillate and hence nominally favors the usual acceleration methods. The significant figures are underlined.

TABLE II

$$\text{Second Test Problem } \int_0^{\infty} e^{-x \cosh t} \cos \zeta t dt.$$

Evaluations of $f$ Per Cycle ( $2N$ )	$N$ -Point Gaussian $\frac{1}{2}$ Cycle Integrals	Shanks Acceleration	Orthogonalized Fourier
2	$\sim 0.0$	$\sim 0.0$	<u><math>7.553054 \times 10^{-28}</math></u>
4	$9.370454 \times 10^{-28}$	$9.37045 \times 10^{-28}$	<u>7.553054</u>
6	<u>7.383455</u>	<u>7.383455</u>	<u>7.553053</u>
8	<u>7.561115</u>	<u>7.561115</u>	<u>7.553060</u>
10	<u>7.552814</u>	<u>7.552814</u>	<u>7.553056</u>
12	<u>7.553059</u>	<u>7.553059</u>	<u>7.553052</u>
14	<u>7.553052</u>	<u>7.553052</u>	<u>7.553050</u>
$\vdots$	$\vdots$	$\vdots$	$\vdots$
converged result	<u>7.553050</u> ...	<u>7.553050</u> ...	<u>7.553050</u> ...

Modified Bessel Function  $K_{\zeta}(x)$  with  $x = 40$ ,  $\zeta = 39$ . Here so many cycles contribute that the acceleration advantage is only about 10% and the orthogonalized Fourier method is about 5 or 6 times more efficient than the other two methods.

The second test problem,

$$K_{it}(x) \equiv \int_0^{\infty} e^{-x \cosh t} \cos \zeta t \, dt, \quad (21)$$

is the modified Bessel function of imaginary order. In Table II, the results are shown for  $\zeta = 39$  and  $x = 40$ , the limit where  $\zeta$  is large and our method is expected to work best. Note that at most only one extra digit of precision is obtained by going from 2 points per cycle in the orthogonalized Fourier method to 14-points per cycle. This is so because round-off accuracy is obtained by the  $2N = 2$  result. By contrast, the 12- and 14-point formulae are required by the other two methods to obtain even comparable accuracy. This is clearly an efficiency increase of at least a factor of 6. Furthermore, the acceleration advantage is less than 10% in this problem. Shanks acceleration brings virtually no gain over summing the half-cycle integrals directly because in either case so many cycles of  $\cos \zeta t$  are required that a small reduction in the number makes no appreciable difference. The major gain, as demonstrated by the use of the orthogonalized Fourier method, comes from reducing the number of evaluation points per cycle to as small a number as possible.

*Note added in proof.* In practical usage the accuracy of our method can be estimated by comparing the size of the integrand  $f(t)$  near  $t = 0$  with the size of the expected answer. When oscillatory cancellation is expected to reduce the integrand by a factor even smaller than the machine round off limit, the numerical value obtained for the integral is suspect.

#### ACKNOWLEDGMENT

The authors wish to acknowledge helpful conversations with Dr. T. P. Coffey and Dr. R. L. Pexton.

#### REFERENCES

1. L. N. G. FILON, *Proc. Roy. Soc. (London)*, **49** (1928), 38.
2. W. W. CLENDENIN, *Numer. Math.* **8** (1966), 422.
3. E. A. FLINN, *J. Assoc. Comput. Mach.*, **7** (1960), 181.
4. H. HURWITZ AND P. F. ZWEIFEL, *M.T.A.C.* **10** (1956), 140.
5. H. HURWITZ, R. A. PFEIFER, AND P. F. ZWEIFEL, *M.T.A.C.* **13** (1959), 87.
6. A. SAENGER, *J. Math. Anal. Appl.* **8** (1964), 1.
7. G. DEBALBINE AND J. N. FRANKLIN, *Math. Comp.* **20** (1966), 570.
8. I. M. LONGMAN, *Math. Comp.* **14** (1960), 53.
9. A. ALAYLIOGLU, G. A. EVANS, AND J. HYSLOP, *J. Comp. Phys.* **13** (1973), 433.
10. D. SHANKS, *J. Math. Phys.* **34** (1955), 1.
11. E. ORAN AND J. DAVIS, *J. App. Phys.* **45** (1974), 2480.



12. S. LUKE, "Determination of Potential Curves from Spectral Data," M. S. thesis, University of Maryland, 1964.
13. D. HUNTER, *Math. Comp.* **18** (1964), 123.
14. S. P. MORGAN, "Tables of Bessel Functions of Imaginary Order and Imaginary Argument," California Institute of Technology, 1947.
15. S. LUKE AND S. WEISSMAN, "Bessel Functions of Imaginary Order and Imaginary Argument," University of Maryland, Institute for Molecular Physics, copies available from U.S. Department of Commerce, Office of Technical Services, Washington, D.C.
16. J. P. BORIS AND E. S. ORAN, NRL Memorandum Report 2925, Sept. 1974.
17. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," p. 887, Dover Publications, Inc., New York, 1965.

RECEIVED: November 11, 1974.

JAY P. BORIS  
ELAINE S. ORAN  
*Naval Research Laboratory*  
*Washington, D. C.*