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Algebraic approximations to some integrals in optics

B T N Evans and G R Fournier
Defense Research Establishment Valcartier, Courcelette, Quebec G0A 1R0, Canada

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Abstract. A method is described for obtaining algebraic approximations to certain integrals that appears to be independent of known methods, such as Taylor, orthonormal functions, Laplace's method, etc. It resembles the numerical technique of product integration. Often the solutions are globally valid over the full range of each parameter. In some cases a trade-off can be performed between the accuracy and the functional complexity of the solution.

As examples, specific integrals for estimating extinction from aerosols are resolved. These analytical solutions are applicable to scattering from spheres, spheroids, discs and infinite cylinders.

1. Introduction

There are some areas in physics where an analytic approximation to an integral is highly desirable even though it is inexact. This is particularly true when the physical theory is known to be only an approximation itself. A striking example is integrals that occur in the Fresnel–Huygens or Kirchhoff form of scalar diffraction theory which is applicable to both optics and acoustics. Aerosol scattering problems provide another example. In order to retain at least one of the following an approximate analytic solution is needed: physical insight, correct asymptotic behaviour, computational speed and/or computational robustness.

This paper describes a method for obtaining algebraic approximations to certain integrals in optics. It resembles, but is different from, an analytic version of product integration [1].

For practical purposes, an analytic solution will mean that the result of integration must be represented in terms of combinations of the elementary and special functions of mathematical physics.

The integrals that can be approximated by this method are the same as those found in integral tables but the arguments of some of the functions in the kernel are much more complicated. As will be shown, the main limitation of the technique is that there is no *á priori* error estimation.

2. Method

This section gives the general mathematical framework required to implement the integration technique.

2.1. Outline of concept

Suppose one has the following integral to perform:

$$I = \int_a^b g(\lambda_i, h(\eta_j, x))\, f(\sigma_k, x)\, \mathrm{d}x \tag{1}$$

where g, h and f are any continuously differentiable functions and λ_i, η_j and σ_k are parameters independent of x whose domain can cover, in general, the complex plane. In order to refer to the whole set of parameters, define $\wp = \{\lambda_i, \eta_j, \sigma_k\}$. As it stands, (1) is a general integral with a function that has a potentially very complicated argument $h(\eta_j, x)$. Most integrals that have analytic solutions have simple arguments. The following method extends the list of analytically soluble integrals to a list that includes analytically approximated integrals.

Begin by assuming that a function $u(q_l, h)$ can be found such that

$$\int_{h(\eta_j,a)}^{h(\eta_j,y)} u(q_l, h)\, \mathrm{d}h \approx \int_a^y f(\sigma_k, x)\, \mathrm{d}x \tag{2}$$

is an acceptable approximation valid over the range of integration. Here y ranges between a and b, and the q_l are n fitting parameters. The number of fitting parameters n will generally depend on the functional form chosen for u. Applying Leibniz's theorem for differentiation of an integral on (2):

$$\frac{\mathrm{d}}{\mathrm{d}y} \int_{h(\eta_j,a)}^{h(\eta_j,y)} u(q_l, h)\, \mathrm{d}h \approx \frac{\mathrm{d}}{\mathrm{d}y} \int_a^y f(\sigma_k, x)\, \mathrm{d}x$$

which gives

$$u(q_l, h(y))\, \mathrm{d}h \approx f(\sigma_k, y)\, \mathrm{d}y. \tag{3}$$

Multiplying each side of (3) by $g(h)$ and integrating we get

$$I \approx \int_\alpha^\beta g(h)\, u(h)\, \mathrm{d}h \tag{4}$$

where $\alpha = h(\eta_j, a)$ and $\beta = h(\eta_j, b)$ to simplify the notation. Whether (2) is an acceptable approximation will depend on the desired accuracy of (4).

It is required that (4) be analytically integrable. It is often preferable, but not necessary, that both the integrals in (2) should also be analytically integrable. It is clear that when approximation (2) is exact this procedure is just a variable substitution.

Equation (2) can be further generalized to

$$\int_\alpha^\beta \sum_k a_k\, u_k(q_{lk}, h)\, \mathrm{d}h \approx \int_a^y f(\sigma_k, x)\, \mathrm{d}x \tag{5}$$

with a_k weighting constants, keeping in mind that for each k

$$\int_\alpha^\beta g(h)\, u_k(h)\, \mathrm{d}h \tag{6}$$

must be analytically integrable. Thus for each function, u_k, that satisfies the integrability conditions in (6), an additional functional form is found that may improve the approximation in (5). This concept will be made clearer by an outline of some possible procedures and several examples taken from actual physical problems.

2.2. *Outline of a procedure*

The following subsections outline a procedure for implementing the previous concept.

2.2.1. *Finding candidate* u. In deriving a practical procedure for implementing this method, it is useful to prune the set of possible forms of u. The strongest constraint is the integrability condition (4) or (5). One way of determining part of the allowed set of functional forms for u is by looking up a table of definite integrals that contain products of g and other functions. A more general way is to consider the small list of general integrals [2–5]. This list can be used to survey rapidly almost all known analytic definite integrals. Although these integrals are complicated, they, at the very least, serve as indicators as to the existence of possible forms of u. Examples from this list, two of which will be used, are given below.

$$\int_0^1 x^{\rho-1}(1-x)^{\beta-\nu-u}\,{}_2F_1(-u,\beta;\nu;x)\,G^{m,n}_{p,q}\left(z\,x^s\middle|\begin{matrix}a_1, & \ldots, & a_p\\ b_1, & \ldots, & b_q\end{matrix}\right)\mathrm{d}x$$
$$= \frac{\Gamma(\nu)\Gamma(\beta+1-\nu)s^{u+\nu-\beta-1}}{\Gamma(\nu+u)}$$
$$\times\, G^{m+s,n+s}_{p+2s,q+2s}\left(z\middle|\begin{matrix}g_s, & a_1, & \ldots, & a_p, & h_s\\ i_s, & b_1, & \ldots, & b_q, & j_s\end{matrix}\right) \tag{7}$$

$$\int_1^\infty x^{-\rho}(x-1)^{\sigma}\,{}_2F_1(\kappa+\sigma-\rho,\lambda+\sigma-\rho;\sigma;1-x)\,G^{m,n}_{p,q}\left(zx\middle|\begin{matrix}a_1, & \ldots, & a_p\\ b_1, & \ldots, & b_q\end{matrix}\right)\mathrm{d}x$$
$$=\Gamma(\sigma)G^{m+2,n}_{p+2,q+2}\left(z\middle|\begin{matrix}a_1, & \ldots, & a_p, & \kappa+\sigma-\rho, & \rho\\ \kappa, & \lambda, & b_1, & \ldots, & b_q\end{matrix}\right) \tag{8}$$

$$\int_0^1 x^{\sigma-1}(1-x)^{\rho-1}F^{A:B;B'}_{C:D;D'}\left(\begin{matrix}(a): & (b); & (b')\\ (c): & (d); & (d')\end{matrix}\middle|\alpha x^m(1-x)^n,\beta x^m(1-x)^n\right)\mathrm{d}x$$
$$=\frac{\Gamma(\sigma)\Gamma(\rho)}{\Gamma(\sigma+\rho)}F^{A+m+n:B;B'}_{C+m+n:D;D'}$$
$$\times\left(\begin{matrix}(a), & \dfrac{\sigma}{m}, & \ldots, & \dfrac{\sigma+m-1}{m}, & \dfrac{\rho}{n}, & \ldots,\\ (c), & \dfrac{\sigma+\rho}{m+n}, & \ldots, & \ldots, & \ldots, & \ldots,\end{matrix}\right.$$
$$\left.\begin{matrix}\dfrac{\rho+n-1}{n} & : & (b); & (b')\\ \dfrac{\sigma+\rho+m+n-1}{m+n} & : & (d); & (d')\end{matrix}\middle|\frac{m^m\alpha}{(m+n)^{m+n}},\frac{n^n\beta}{(m+n)^{m+n}}\right). \tag{9}$$

Equations (7) and (9) are examples of general Euler-type integrals. In (7), ${}_2F_1$ is the Gauss hypergeometric function and $G^{m,n}_{p,q}$ is Meijer's G-function. In (9), $F^{A:B;B'}_{C:D;D'}$ is a Kampé de Fériet function. This double variable hypergeometric function and its properties are discussed at length in [6] and, more recently, in [5]. One very important property of the Kampé de Fériet functions, that will be used in an example, occurs when C and A are both zero in which case they become just the product of two generalized hypergeometric functions of a single variable:

$$F^{0:B;B'}_{0:D;D'}\left(\begin{matrix}(a): & (b); & (b')\\ (c): & (d); & (d')\end{matrix}\middle| x, y\right) = {}_BF_D\left(\begin{matrix}(b)\\(d)\end{matrix}\middle| x\right) {}_{B'}F_{D'}\left(\begin{matrix}(b')\\(d')\end{matrix}\middle| y\right). \tag{10}$$

Equation (8) is a general Weyl integral over the product of a Gauss hypergeometric function and a Meijer's G-function. The detailed conditions of validity for these integrals will not be stated here so as not to sidetrack the main issues. They can, however, be found in the cited references.

With these integrals the functions g and u plus the appropriate integral transform can be identified. Hence g or u could be either a Meijer's G-function, a generalized hypergeometric function, simple functions (such as x^ρ, $(1-x)^\mu$, e^x or $\sin(x)$), etc. Thus most functions occurring in mathematical physics are covered.

Additional qualitative considerations of the functional form of the right-hand side of (2) can further reduce the set of candidate forms for u. Some of the more obvious ones are the monotonicity, curvature and asymptotic behaviour in both large and small limits. A more subtle condition is the weighting provided by g in (4).

2.2.2. Obtaining the fitting parameters q_l. The fitting parameters, q_l (in general, but not always, functions of $\wp$, a and b), in (2) are obtained by some appropriate minimizing procedure that reduces the error in the approximation (4). This can be stated in one form as

$$\mathrm{Min}\left|\int_a^b\left\{\int_{h(\eta_j,a)}^{h(\eta_j,y)} g(h)\,u(q_l,h)\,\mathrm{d}h - \int_a^y g(h(x))\,f(x)\,\mathrm{d}x\right\}\mathrm{d}y\right| \tag{11}$$

where the Min is understood to be performed for a particular set of $\wp$. The process is repeated over the parametric space of interest in $\wp$. If the level of error is not satisfactory, another candidate form for u must be tried either in (2) or (5). Note that fitting of a_k is also required in the latter case.

Possible minimizing strategies could include numerical methods such as quasi-Newton, conjugate gradient or simplex, etc. These methods initially do not produce analytic expressions of q_l in terms of h, $\wp$, a and b. However, provided that the dependency is not too complicated, acceptable functional approximations may be found.

This process is complicated, can be computationally demanding and could, ultimately, be intractable. However, the examples in the next section show that often the situation can be considerably simplified by relaxing the constraint equation (11). Indeed it will be shown that even a trial and error method for finding u can often suffice. The constraint condition (11) is also reduced by first assuming that g is a constant, and then fitting at only a small set of points, y_l, equal to the number of fitting parameters n. Thus (11) becomes

$$\left|\int_{h(\eta_j,a)}^{h(\eta_j,y_l)} u(q_l,h)\,\mathrm{d}h - \int_a^{y_l} f(x)\,\mathrm{d}x\right| = 0 \qquad l = 1,2,\ldots,n. \tag{12}$$

The function g is only peripherally considered when choosing y_l and u. As will be shown by examples, (12) can sometimes be solved analytically, i.e. q_l in terms of h,

$\wp$, a and b. This simplified procedure has been shown to work for functions with simple forms such as monotonic ones, whose curvatures are easily modelled.

Equation (12) can be restated as an interpolation of $f(x)\,\mathrm{d}x$ by $u(h)\,\mathrm{d}h$ at n points y_l. At this point the procedure is similar to an analytic version of product integration [1, p 74]. Two significant differences are: (1) that $f(x)\,\mathrm{d}x$ is being interpolated instead of $f(x)$; and (2) h is not a simple power of x. These two differences have made all our attempts to perform a general error analysis of limited value. For example, in performing the standard procedure [7], the upper bound to the error ϵ is

$$\epsilon \leqslant \left\| u(h) - \frac{f(h^{-1})}{h'(h^{-1})} \right\| \int_{h(a)}^{h(b)} g(h)\,\mathrm{d}h. \tag{13}$$

In order for this upper bound to be useful the inverse function h^{-1} must exist over the range $[a, b]$ and the first term in (13) cannot have a singularity. Since the nature of h is unknown *a priori* and hence u is also unknown, no error scaling can be found. Each case must be evaluated individually using (13) or some other, specific method.

3. Examples

In this section several applications of the method to various integrals occurring in optical scattering theory are given. None of these can be transformed into integrals that have closed form solutions in terms of special functions. Moreover, since the parameters in each kernel can arbitrarily take on values from 0 to ∞, Taylor series expansions and asymptotic methods such as Laplace's or steepest descents will not work because of convergence problems. Since part of the kernel has a complicated argument, any expansion in sets of orthogonal functions will also involve this argument and hence will most likely make any possible solution undesirable. In all three cases, the solution obtained is valid globally over the complete range of each parameter in $\wp$. This last point will be illustrated by tables.

3.1. Example 1

This occurs in the study of scalar scattering from randomly oriented infinite aspect discs [8] (normal incidence is treated in [9], p 97).

$$Q_{\mathrm{d}} = 2(1 - \mathrm{Re}(I_{\mathrm{d}})) \qquad \text{with} \qquad I_{\mathrm{d}} = \int_0^1 \mathrm{e}^{-\omega(x)}\,\mathrm{d}x \tag{14}$$

where $\omega(x) = 2\mathrm{i}s[(m^2 - x)^{1/2} - (1 - x)^{1/2}]$, s is the particle size parameter, a real number varying between 0 and ∞, and m is the refractive index and is hence complex with $\mathrm{Re}(m)$ varying between 1 and ∞ and $\mathrm{Im}(m)$ varying between 0 and $-\infty$. Hence the magnitude of $\omega(x)$ varies from 0 to ∞ as well.

Following the notation of the previous section, $h(\eta_1, \eta_2, x) = \omega$, $g(h) = \mathrm{e}^{-h}$, $f(x) = 1$, $a = 0$, and $b = 1$. The parameters are clearly $\eta_1 = s$ and $\eta_2 = m$ and thus $\wp = \{\eta_1, \eta_2\}$.

The functional form of u is constrained by the integrability condition (4). As $g(h) = \mathrm{e}^{-h}$, the simplest non-trivial possible forms of $u(h)$ are limited to $c\mathrm{e}^{-dh}$ or $1/(h+c)^d$ where c and d are constants. The term 'simplest' is defined here by the order of the hypergeometric function used. For these forms e^h is a ${}_0F_0$ and $1/(h+c)$ is a ${}_1F_0$, all other hypergeometric functions are much more complicated in their behaviour, computation and in the integrals that would result from this procedure. Of the two forms identified earlier, ce^{-dh} gives rise to a set of transcendental equations that needs to be solved in order to obtain c and d. Hence first choose the form $1/(h+c)^d$, which produces readily solvable equations. Later, a second approximation using the form ce^{-dh} will be derived.

Example 1(a) (first approximation). The form $1/(h+c)^d$ gives the approximation of I in terms of exponential integrals of order d.

Let

$$J(y_l) \equiv \int_0^{y_l} f(x)\,\mathrm{d}x = y_l. \tag{15}$$

Since, over the range of physical interest $\mathrm{Re}(m) > 1$, h is a simply behaved function of y_l, there is a simple transformation relating h to J. Here, this transformation u can be of the form stated earlier. Thus we have

$$\int u(h)\,\mathrm{d}h \propto \int \frac{\mathrm{d}h}{(h+c)^d} \propto \frac{1}{(h+c)^{(d-1)}}. \tag{16}$$

It is empirically found that $d = 2$ is a reasonably good approximation to J. Furthermore since this form allows a maximum of three fitting parameters, $n = 3$.

Thus

$$J(y_l) = y_l \approx \frac{q_1}{h(y_l) + q_2} + q_3 \qquad l = 1,2,3. \tag{17}$$

This set of equations can be expressed as three linear equations which are readily solved for q_l. The values of y_l were chosen so that the equations are simple, i.e. $y_1 = 0$, $y_2 = 1/2$ and $y_3 = 1$. Other sets of y_l could be used achieving a slightly better approximation at the expense of algebraic complexity. With the chosen set of y_l, the solution to (17) is

$$\begin{aligned} q_1 &= -(h(0) + q_2)q_3 \\ q_2 &= \frac{h(0)h(1/2) - 2h(0)h(1) + h(1/2)h(1)}{h(0) - 2h(1/2) + h(1)} \\ q_3 &= \frac{h(1) + q_2}{h(1) - h(0)}. \end{aligned} \tag{18}$$

Here the notation for $h(\eta_1, \eta_2, y_l)$ is simplified to $h(y_l)$ for clarity.

Substituting these equations into (4):

$$\begin{aligned} I_\mathrm{d} &\approx -q_1 \int_{h(0)}^{h(1)} \frac{\mathrm{e}^{-h}}{(h+q_2)^2}\,\mathrm{d}h \\ &= q_1 \mathrm{e}^{q_2} \left[\frac{E_2(h(1) + q_2)}{h(1) + q_2} - \frac{E_2(h(0) + q_2)}{h(0) + q_2} \right]. \end{aligned} \tag{19}$$

Note that E_2 is the second-order exponential integral. Thus the integral (14) has been approximated as the difference of two second-order exponential integrals.

Table 1(*a*) presents a comparison between the exact numerical calculation of I_d and the approximation (19).

As seen in table 1(*a*), when the magnitude of I_d is significant the percentage error is relatively small. However, when the magnitude of I_d approaches 0 the percentage error can be quite large. The latter effect is due to an error in the phase of the approximation with respect to the exact solution. This effect will occur when the approximation does not have the same zero crossings as the exact integral. This applies to any approximation technique and is therefore not specific to the present procedure. Note that where the approximation is matched at a zero, i.e. at infinite refractive index, the percentage error is small. Evidently matching one or more zeros of the integral could be a useful criterion in the choice of an adequate form of h. However, in the present case the quantity of physical interest is Q_d and thus, whenever I_d is small, the percentage error in Q_d will also be small. For example, for the worst case in table 1(*a*), $m = 2.0$ and $s = 5$, where the error in I_d is 103.7%, the corresponding percentage error in Q_d is only 11.0%. As the next approximation gives simpler and more accurate we will postpone the discussion of an error bound.

Example 1(b) (second approximation). Again let

$$J(y_l) = y_l$$

as in (15) but now let $u(h) = q_2 e^{q_1 h}$. Here $d \equiv q_1$ and $c \equiv q_2$. Hence

$$\int_{h(0)}^{h(y)} u(h)\,dh = \frac{q_2}{q_1}\left[e^{q_1 h(y)} - e^{q_1 h(0)}\right]. \tag{20}$$

In (20) there are two unknowns and thus two equations or fitting points in the range $0 \leqslant y \leqslant 1$ are needed. Call these two fitting points $y1$ and $y2$. Elimination of q_2 results in the following transcendental equation:

$$\frac{y1}{y2} = \frac{e^{q_1(h(y1)-h(0))} - 1}{e^{q_1(h(y2)-h(0))} - 1}. \tag{21}$$

Newton's method of successive approximations can be used to approximate q_1 starting with q_1 as $m \to 1$. Taking $y1 = 1$ and $y2 = 1/2$, as $m \to 1$, choose $e^{q_1(h(1)-h(0))} \to 0$, and $e^{q_1(h(1/2)-h(0))} \to 1/2$. The latter is readily solved giving

$$\lim_{m\to 1} q_1 = \frac{-\ln 2}{h(1/2) - h(0)}. \tag{22}$$

This result is completely consistent with (21) as $m \to 1$. Using this as a first guess in Newton's method and iterating once:

$$q_1 \approx \frac{1}{h(1/2) - h(0)}\left[\frac{1}{2^v - v/(1-2^{-v})} - \ln 2\right] \qquad \text{with } v \equiv \frac{h(1) - h(0)}{h(1/2) - h(0)}. \tag{23}$$

This can be simplified without introducing any serious error

$$q_1 \approx \frac{1}{h(1/2) - h(0)}\left[\frac{1}{2^v - v} - \ln 2\right]. \tag{24}$$

Table 1. Error tables for examples 1(*a*) and 1(*b*).

Example 1(*a*)

m	s	Exact	Approximation	Error (%)
1.1	0.001	1−0.000312902i	1−0.000331086i	0,5.8
1.1	0.01	0.999994−0.00313015i	0.999993−0.00331084i	0.0001,5.8
1.1	0.1	0.999439−0.0312943i	0.999337−0.0330977i	0.01,5.8
1.1	1	0.944813−0.305286i	0.935227−0.320415i	1.0,5.0
1.1	2	0.790095−0.566587i	0.758557−0.581541i	4.0,2.6
1.1	5	0.0551996−0.849220i	0.0305116−0.781481i	44.7,8.0
1.1	10	−0.592805−0.237394i	−0.540190−0.272222i	8.9,14.7
1.1	50	0.0609117+0.197822i	0.0487599+0.217617i	19.9,10.0
1.1	100	−0.0911145−0.0580755i	−0.0989528−0.0729561i	8.6,25.6
1.5	1	0.258516−0.932335i	0.226920−0.925756i	12.2,0.7
1.5	2	−0.743586−0.465533i	−0.719633−0.407902i	3.2,12.4
1.5	5	0.490254+0.09049i	0.416438+0.162019i	15.1,79.0
1.5	10	0.0836259+0.269668i	0.0418624+0.276025i	49.9,2.4
1.5	50	0.0192536−0.0568162i	0.0215849−0.0637607i	12.1,12.2
1.5	100	0.0160325−0.0253829i	0.0183567−0.0307823i	14.5,21.3
1.5−0.01i	1	0.25309−0.911135i	0.222336−0.90455i	12.2,.72
1.5−0.01i	10	0.065439+0.220519i	0.0320381+0.226246i	51.0,2.6
1.5−0.01i	100	0.00221063−0.00340189i	0.00259562−0.00402052i	17.4,18.2
1.5−0.1i	1	0.207354−0.741218i	0.183119−0.734624i	11.7,.89
1.5−0.1i	10	0.00677562+0.0353941i	0.00220001+0.0368946i	67.5,4.2
1.5−1i	1	0.0183699−0.107124i	0.0152086−0.014582i	17.2,2.4
2.0	1	−0.700659−0.641335i	−0.706793−0.603780i	0.88,5.9
2.0	2	0.0469974+0.813015i	0.0734549+0.743366i	56.3,8.6
2.0	5	0.0958382+0.345685i	−0.00351873+0.373174i	96.3,8.0
2.0	10	−0.158222−0.109586i	−0.164505−0.162528i	4.0,48.3
2.0	50	0.0216164−0.0338167i	0.0250502−0.0426432i	15.9,26.1
2.0	100	0.0175966−0.00939819i	0.0225043−0.00950006i	27.9,1.1
35−35i	0.001	0.930190−0.0639669i	0.930189−0.0640105i	0.0001,.068
35−35i	0.01	0.384032−0.314763i	0.383882−0.314941i	0.04,.042
35−35i	0.05	−0.0289054+0.00866923i	−0.0288829+0.00873602i	0.08,.77
35−35i	0.09	0.00182362+0.000190088i	0.00182381+0.000182345i	0.01,4.1

Example 1(*b*)

m	s	Exact	Approximation	Error (%)
1.1	0.001	1−0.000312902i	1−0.000301928i	0,3.5
1.1	0.01	0.999994−0.00313015i	0.999995−0.00301927i	0.0001,3.5
1.1	0.1	0.999439−0.0312943i	0.999494−0.0301864i	0.0055,3.5
1.1	1	0.944813−0.305286i	0.950086−0.295589i	0.56,3.2
1.1	2	0.790095−0.566587i	0.808331−0.55474i	2.3,2.1
1.1	5	0.0551996−0.849220i	0.0858266−0.887196i	55.5,4.5
1.1	10	−0.592805−0.237394i	−0.657304−0.235561i	10.9,.79
1.1	50	0.0609117+0.197822i	0.0716946+0.177654i	17.7,10.2
1.1	100	−0.0911145−0.0580755i	−0.0844268−0.0481207i	7.3,17.1
1.5	1	0.258516−0.932335i	0.250508−0.930355i	3.1,0.21
1.5	2	−0.743586−0.465533i	−0.736335−0.452007i	1.0,2.9
1.5	5	0.490254+0.09049i	0.484817+0.113791i	1.1,25.7
1.5	10	0.0836259+0.269668i	0.0820465+0.263631i	1.9,2.2
1.5	50	0.0192536−0.0568162i	0.0170664−0.0555991i	11.4,2.1
1.5	100	0.0160325−0.0253829i	0.0152596−0.0257732i	4.8,1.5
1.5−0.01i	1	0.25309−0.911135i	0.245337−0.908895i	3.1,.25
1.5−0.01i	10	0.065439+0.220519i	0.0644749+0.216257i	1.5,1.9
1.5−0.01i	100	0.00221063−0.00340189i	0.00213159−0.00341096i	3.6,0.3

Table 1. (continued)

m	s	Exact	Approximation	Error (%)
1.5−0.1i	1	0.207354−0.741218i	0.201352−0.737172i	2.9,.5
1.5−0.1i	10	0.00677562+0.0353941i	0.00691929+0.035498i	2.1,0.3
1.5−1i	1	0.0183699−0.107124i	0.0168085−0.104787i	8.5,2.2
2.0	1	−0.700659−0.641335i	−0.703720−0.622919i	0.44,2.9
2.0	2	0.0469974+0.813015i	0.0589671+0.779809i	25.5,4.1
2.0	5	0.0958382+0.345685i	0.0569472+0.369546i	40.6,6.9
2.0	10	−0.158222−0.109586i	−0.164528−0.128163i	4.0,17.0
2.0	50	0.0216164−0.0338167i	0.0213706−0.0369586i	1.1,9.3
2.0	100	0.0175966−0.00939819i	0.0190871−0.00888136i	8.5,5.5
35−35i	0.001	0.930190−0.0639669i	0.930188−0.0639992i	0.0002,.050
35−35i	0.01	0.384032−0.314763i	0.383921−0.314895i	0.029,.042
35−35i	0.05	−0.0289054+0.00866923i	−0.0288888+0.00871867i	0.057,.57
35−35i	0.09	0.00182362+0.000190088i	0.00182374+0.00018435i	0.0066,3.0

Equation (24) has a worst error throughout the complex plane of 0.65% (which occurs as $m \to \infty$). The other fitting parameter q_2 is easily expressed in terms of q_1:

$$q_2 = \frac{q_1 e^{-q_1 h(0)}}{e^{q_1(h(1)-h(0))} - 1}. \tag{25}$$

With q_1 as in (24) and q_2 as in (25) the final result is

$$I_d \approx \int_{h(0)}^{h(1)} e^{-h} q_2 e^{q_1 h}\, dh = \frac{q_2}{q_1 - 1}\left[e^{h(1)(q_1-1)} - e^{h(0)(q_1-1)}\right]. \tag{26}$$

Table 1(b) is similar to table 1(a) but with approximation (26) replacing approximation (19).

The numerical values in table 1(b) behave in a similar fashion to those in table 1(a). Hence large percentage errors occur near the zeros of I_d and the worst error in the table is at $m = 2.0$ and $s = 5$. But table 1(b) shows that (26), even though it is simpler, is almost always a better approximation to I_d than (19). This simpler result was obtained at the cost of having to analyse a transcendental equation (21). This was relatively simple in the present case but may not always be so.

Using (13) and series expansions of (14) and (26), the behaviour of the error in this approximation can be explored. After some straightforward algebra, the absolute error, ϵ, can be shown to scale as follows:

$$\epsilon \propto \left[e^{2is\sqrt{2(m-1)}} - 1\right]/s \to 0 \qquad m \to 1$$

$$[e^{2is} - 1]/s \qquad m \to \infty$$

$$s\left[\sqrt{m^2-1} - (m-1)\right] \qquad s \to 0$$

$$e^{-2ish(1)}[e^{-2is(h(0)-h(1))} - 1]/s \to 0 \qquad s \to \infty.$$

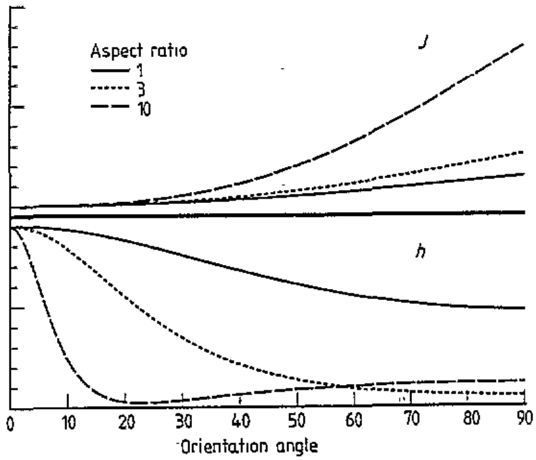

Figure 1. A plot of $h(\theta)$ and $J(\theta)$ against θ for various values of r (example 2).

3.2. *Example 2*

The integral in this example is taken from [8] and [10]. As in the previous example, it occurs in the scalar theory of electromagnetic and acoustic scattering. This integral accounts for the effect of edge scattering from randomly oriented prolate spheroids of arbitrary aspect ratio.

$$I_e = \int_0^{\pi/2} P\sin(\theta)\exp(-c_0(r/Ps)^{2/3}{}_2F_1[-\tfrac{2}{3},\tfrac{1}{2};1;1-(1/P^2)])\,d\theta \tag{27}$$

where s, r and c_0 are constants and $P = [\cos^2(\theta) + r^2\sin^2(\theta)]^{1/2}$. For this case r, the aspect ratio, can vary from 1 to ∞, s, again the size parameter, can vary from 0 to ∞ and the Fock constant, $c_0 \approx 1$.

Identify h with ${}_2F_1[-\frac{2}{3},\frac{1}{2};1;1-(1/P^2)]/P^{2/3}$, $g(\lambda_1,h)$ with $e^{\lambda_1 h}$, f with $P\sin(\theta)$, $a = 0$ and $b = \pi/2$. For the parameters, $\lambda_1 = c_0(r/s)^{2/3}$, and $\eta_1 = \sigma_1 = r$. Thus $\wp = \{\lambda_1, \eta_1\}$.

Let

$$\begin{aligned} J(y_l) &= \int_0^{y_l} P\sin(\theta)\,d\theta \\ &= \frac{r}{2}\left[\sqrt{1-\epsilon^2} + \frac{\sin^{-1}(\epsilon)}{\epsilon}\right] \\ &\quad - \frac{r}{2}\left[\cos(y_l)\sqrt{1-\epsilon^2\cos^2(y_l)} + \frac{\sin^{-1}(\epsilon\cos(y_l))}{\epsilon}\right] \end{aligned}$$

and

$$\epsilon^2 = 1 - 1/r^2. \tag{28}$$

Figure 1 is a plot of $h(\theta)$ and $J(\theta)$ against θ for various values of r. These curves are very similar and it is evident that there should be a simple transformation that would take one function into the other.

Empirically $d = 2$ is a reasonably good approximation to the curvature of J for the same functional form for u as in example 1(a). As before, this form gives the maximum number of three fitting parameters, i.e. $n = 3$. Thus, again,

$$J(y_l) \approx \frac{q_1}{h(y_l) + q_2} + q_3 \qquad l = 1, 2, 3. \tag{29}$$

As before, the values of y_l were chosen to keep the equations simple, i.e. $y_1 = 0$, $y_2 = \pi/4$ and $y_3 = \pi/2$. With the chosen set of y_l and using the fact that $h(0) = 1$, the solution to (29) is

$$\begin{aligned} q_1 &= \gamma q_3[J(\pi/2) - q3] \\ q_2 &= \gamma q_3 - h(\pi/2) \\ q_3 &= \frac{h(\pi/2) - h(\pi/4)}{\gamma + [1 - h(\pi/4)]/J(\pi/4)} \\ \gamma &= \frac{h(\pi/2) - 1}{J(\pi/2)}. \end{aligned} \tag{30}$$

Substituting these equations into (4),

$$\begin{aligned} I_e &\approx q_1 \int_\alpha^\beta \frac{e^{-\lambda_1 h}}{(h + q_2)^2}\, dh \\ &= e^{\lambda_1 q_2} q_1 \left[\frac{E_2(\lambda_1 \alpha)}{\alpha} - \frac{E_2(\lambda_1 \beta)}{\beta}\right] \end{aligned} \tag{31}$$

with $\alpha \equiv h(0) = 1$ and $\beta \equiv h(\pi/2)$. Table 2 presents the error between the exact numerically calculated value of I_e and (31) for a wide range of r and s values.

For an aspect ratio of 1, the approximation is equal to I_e exactly for any size parameter s. The error is greatest for a given r when s is small. This is once again due to the presence of a zero in the integral for $s = 0$. The approximation is exact (i.e. equal to 0) for $s = 0$, however the asymptotic behaviour as s approaches 0 is not quite correct. This is not important for the physical problem of edge scattering since the real quantity of interest is related to $2 - I_e(s)/I_e(\infty)$.

A proper discussion of an error bound to this example is of limited use since the inverse of h must be obtained numerically.

3.3. Example 3

This example occurred in the study of scattering from randomly oriented infinite cylinders ([8, 9, p 313, 11, 12, p 290]). The quantity of physical interest in cylindrical scattering theory is Q_c, the extinction efficiency and is given by

$$Q_c = 4\mathrm{Re}\,(I_c^2 + iI_c^1)\,. \tag{32}$$

$$I_c^1 = \int_0^{\pi/2} H_1(w)\sin^2(\theta)\, d\theta \tag{33}$$

$$I_c^2 = \int_0^{\pi/2} J_1(w)\sin^2(\theta)\, d\theta. \tag{34}$$

where H_1 is the first-order Struve function, J_1 is the first-order Bessel function and $w = 2s[(m^2-\cos^2(\theta))^{1/2}-\sin(\theta)]$. The size parameter s can vary from 0 to ∞, Re(m) can vary from 1 to ∞, and Im(m) from 0 to $-\infty$. Again m is the index of refraction.

In integral (33) $h = w/2s$, $g(\lambda_1, h) = H_1(\lambda_1 h)$, $f(\theta) = \sin^2(\theta)$, $a = 0$, and $b = \pi/2$. The parameters are $\lambda_1 = 2s$ and $\eta_1 = m$. Thus $\wp = \{\lambda_1, \eta_1\}$. Again the integrability condition (4) must be satisfied. Since $g(\lambda_1, h) = H_1(\lambda_1 h) = {}_1F_2[1; 3/2, 5/2; -\lambda_1^2 h^2/4]$, (33) can be transformed into an integral of a form similar to (9). Considering (10), the hypergeometric representation of H_1 as given earlier and in (9), then the choices for u will be 'restricted' to a general hypergeometric ${}_pF_q$. However, since attention must be given to the computational feasibility of the solution, only the lowest order hypergeometric functions should be considered. Note also that the exponent of the variable h in the chosen hypergeometric function must be 2 in accordance with (9).

Let

$$J(y_l) = \int_0^{y_l} \sin^2(\theta)\,\mathrm{d}\theta = \tfrac{1}{2}y_l - \tfrac{1}{2}\cos(y_l)\sin(y_l). \tag{35}$$

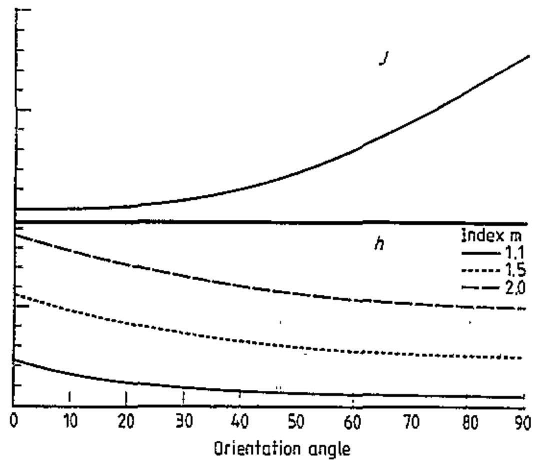

Figure 2. A plot of $h(\theta)$ and $J(\theta)$ against θ (example 3) I_d and the approximation (19).

Figure 2 is a plot of $h(\theta)$ and $J(\theta)$ against θ. Again as in the previous example, these curves are similar in that they are both monotonic with gentle curvature. Given the restrictions placed on u as detailed earlier, the simplest hypergeometric function that can be used is ${}_0F_0[;ch^2] = \mathrm{e}^{ch^2}$. In this case the approximation to J would be

$$J(y_l) \approx q_1 \mathrm{Erf}[q_2 h(y_l)] + q_3 \qquad l = 1, 2, 3. \tag{36}$$

Table 2. Error table for example 2.

Aspect ratio	Size parameter	Exact	Approximation	Error(%)
1	b	I_e	I_e	0
1.25	0.01	3.65592×10^{-9}	3.10578×10^{-9}	15.05
1.25	0.1	0.0153844	0.0149671	2.71
1.25	1	0.456008	0.453797	0.48
1.25	2	0.645879	0.643957	0.30
1.25	5	0.847290	0.845950	0.16
1.25	10	0.954779	0.953836	0.10
1.25	100	1.12007	1.11984	0.02
1.5	0.01	1.92704×10^{-8}	1.57466×10^{-8}	18.29
1.5	0.1	0.0230733	0.0222162	3.71
1.5	1	0.549222	0.545706	0.64
1.5	2	0.764053	0.761085	0.39
1.5	5	0.989166	0.987146	0.20
1.5	10	1.10846	1.10705	0.13
1.5	100	1.29101	1.29067	0.03
2.0	0.01	1.45147×10^{-7}	1.20570×10^{-7}	16.9
2.0	0.1	0.0419768	0.0404307	3.68
2.0	1	0.745312	0.740096	0.70
2.0	2	1.01026	1.00589	0.43
2.0	5	1.28302	1.28007	0.23
2.0	10	1.42612	1.42407	0.14
2.0	100	1.64362	1.64311	0.03
5.0	0.01	3.89743×10^{-6}	3.61508×10^{-6}	7.24
5.0	0.1	0.385611	0.380045	1.44
5.0	1	1.97382	1.95165	1.12
5.0	2	2.55329	2.53113	0.87
5.0	5	3.12749	3.10992	0.56
5.0	10	3.42199	3.40885	0.38
5.0	100	3.8627	3.85911	0.09
10	0.01	1.22907×10^{-5}	1.17944×10^{-5}	4.04
10	0.1	0.385611	0.380045	1.44
10	1	4.02320	3.96007	1.57
10	2	5.14791	5.08044	1.31
10	5	6.24900	6.19179	0.92
10	10	6.80926	6.76488	0.65
10	100	7.64262	7.62982	0.17
100	0.01	0.00014741	0.000144273	2.12
100	0.1	4.03452	3.97989	1.35
100	1	40.6192	39.7725	2.08
100	2	51.7342	50.7669	1.87
100	5	62.5487	61.6353	1.46
100	10	68.0260	67.2530	1.14
100	100	76.1406	75.8643	0.36
10^4	0.01	0.0147756	0.014492	1.92
10^4	1	4062.54	3974.18	2.17
10^4	100	7613.79	7576.89	0.48
10^5	0.01	0.147756	0.144931	1.91
10^5	100	76137.9	75764.8	0.49
10^6	0.01	1.47756	1.44923	1.92
10^6	100	761379.	757639.	0.49

Choosing $y_1 = 0$, $y_2 = 1$ and $y_3 = \pi/2$ and solving for the fitting parameters:

$$q_1 = \frac{-\pi/4}{\mathrm{Erf}[q_2 h(0)] - \mathrm{Erf}[q_2 h(\pi/2)]}$$
$$q_3 = -q_1 \mathrm{Erf}[q_2 h(0)] \tag{37}$$

and q_2 is the root of

$$\frac{\mathrm{Erf}[q_2 h(0)] - \mathrm{Erf}[q_2 h(1)]}{\mathrm{Erf}[q_2 h(0)] - \mathrm{Erf}[q_2 h(\pi/2)]} = \frac{4}{\pi} J(1). \tag{38}$$

In this situation we cannot solve for one of the fitting parameters, q_2 explicitly. The solution of (38) must, therefore, be approximated by some simple analytic function. This can be done by replacing the Erf functions in (38) with their first-order asymptotic expansion. This is justified since it can be shown that $q_2 h(y_l)$ is always greater than 1.49. Doing this, the limiting function, both for large and small Abs$(m-1)$, is

$$q_2 = \sqrt{\frac{1}{h^2(\pi/2) - h^2(1)} \ln\left[\frac{4J(1)h(1)}{\pi h(\pi/2)}\right]}. \tag{39}$$

Since the asymptotic expansion has the worst error for small Abs$(m-1)$, all other values of m will produce a better approximation. When this approximation is used an error of 1% or less is introduced in the calculation.

Applying the method to (33) with this information:

$$\begin{aligned} I_c^1 &\approx \frac{-2q_1 q_2}{\sqrt{\pi}} \int_{h(0)}^{h(\pi/2)} H_1(\lambda_1 h) \mathrm{e}^{-q_2^2 h^2} \, \mathrm{d}h \\ &= \frac{-4 q_1 q_2 \lambda_1^2}{3\pi^{3/2}} \int_{h(0)}^{h(\pi/2)} h^2 {}_1\mathrm{F}_2\left(\begin{matrix} 1 \\ 3/2, \quad 5/2 \end{matrix}\middle| -\frac{\lambda_1^2 h^2}{4}\right) {}_0\mathrm{F}_0(-q_2^2 h^2) \, \mathrm{d}h \\ &= \frac{4 q_1 q_2 \lambda_1^2}{9\pi^{3/2}} \Bigg\{ h^3(0) \mathrm{F}^{1:1;0}_{1:2;0}\left[\begin{matrix} 3/2: & 1; & \\ 5/2: & 3/2, & 5/2; \end{matrix}\middle| \frac{-\lambda_1^2 h^2(0)}{4}, -q_2^2 h^2(0)\right] \\ &\quad - h^3(\pi/2) \mathrm{F}^{1:1;0}_{1:2;0}\left[\begin{matrix} 3/2: & 1; & \\ 5/2: & 3/2, & 5/2; \end{matrix}\middle| \frac{-\lambda_1^2 h^2(\pi/2)}{4}, -q_2^2 h^2(\pi/2)\right] \Bigg\} \end{aligned} \tag{40}$$

where in the last equation the Kampé de Fériet functions have been reduced from $\mathrm{F}^{2:1;0}_{2:2;0}$ to $\mathrm{F}^{1:1;0}_{1:2;0}$ since a set of coefficients coincided.

With the same substitutions used to obtain the solution to (33), equation (34) becomes

$$\begin{aligned} I_c^2 &\approx \frac{2q_1 q_2}{\sqrt{\pi}} \int_{h(0)}^{h(\pi/2)} J_1(\lambda_1 h)\, e^{-q_2^2 h^2} \, \mathrm{d}h \\ &= \frac{2 q_1 q_2}{\lambda_1 \sqrt{\pi}} \Bigg\{ \mathrm{e}^{-q_2^2 h^2(0)} \left[U_2\left(\frac{\mathrm{i}\lambda_1^2}{2q_2^2}, \lambda_1 h(0)\right) - \mathrm{i} U_1\left(\frac{\mathrm{i}\lambda_1^2}{2q_2^2}, \lambda_1 h(0)\right)\right] \\ &\quad - \mathrm{e}^{-q_2^2 h^2(\pi/2)} \left[U_2\left(\frac{\mathrm{i}\lambda_1^2}{2q_2^2}, \lambda_1 h\left(\frac{\pi}{2}\right)\right) - \mathrm{i} U_1\left(\frac{\mathrm{i}\lambda_1^2}{2q_2^2}, \lambda_1 h\left(\frac{\pi}{2}\right)\right)\right] \Bigg\} \end{aligned} \tag{41}$$

where U_1 and U_2 are Lommel functions of two variables [13, 14].

Schemes for evaluating Kampé de Fériet and Lommel functions are given in [16]. These algorithms are derived from the concepts found in [5, 13, 15, 16].

It may seem that I_c^1 and I_c^2 are more easily computed by numerical integration of (33) and (34) than by using approximations (40) and (41). However, (32) requires the calculation of the Struve function and Bessel functions at arbitrary complex values for every point considered in the numerical integration scheme. In contrast (40) and (41) requires the evaluation of, at most, 30 integer-order Bessel and exponential integral functions. In practice, the approximations are orders of magnitude faster than the numerical calculation.

Table 3. Error table for Q_c.

m	s	Exact	Approximation	Error (%)
1.1−0.1i	0.5	0.1831792	0.1779059	2.9
1.1−0.1i	1	0.3648979	0.3534534	3.1
1.1−0.1i	5	1.476016	1.452150	1.6
1.3−0.01i	0.01	0.0003780	0.0003735	1.2
1.3−0.01i	0.1	0.0067400	0.0064846	3.8
1.3−0.01i	0.5	0.0980497	0.0923592	5.8
1.3−0.01i	1	0.345219	0.325103	5.8
1.3−i	0.5	1.138432	1.136944	0.1
1.3−i	1	1.627256	1.624300	0.2
1.3−i	5	1.987548	1.987380	0.008
1.5−0.01i	0.01	0.0004215	0.0004172	1.0
1.5−0.01i	0.1	0.011543	0.011174	3.3
1.5−0.01i	0.5	0.224886	0.215881	4.0
1.5−0.01i	1	0.801148	0.773416	3.5
1.5−0.01i	10	2.369586	2.364842	0.2
1.5−0.1i	0.5	0.351618	0.343325	2.4
1.5−0.1i	1	0.954629	0.931818	2.4
1.5−0.1i	5	2.09136	2.07990	0.5
1.5−i	0.5	1.184728	1.142128	3.6
1.5−i	1	1.700268	1.696536	0.2
2.0−0.1i	0.5	0.8229108	0.8112036	1.4
2.0−0.1i	1	2.192642	2.177689	0.7

Table 3 is a table of representative errors of Q_c. Note that Q_c approaches 2 for large s and any m, as predicted by Babinet's principle of diffraction from large objects.

4. Integrals involving the exponential function

This section indicates how this integration technique allows for a trade-off between the complexity of the special function used and the accuracy of the solution. Since several of the examples shown in the last section involve integrals over the exponential function of a complicated argument, this form of integral will be used to demonstrate the trade-off. (It is not coincidental that integrals over the exponential function are common since they are specific cases of general diffraction-type integrals.)

Consider the integral

$$I = \int_a^b e^{h(x)} f(x)\, dx. \tag{42}$$

The technique then requires

$$I \approx \int_{h(a)}^{h(b)} e^h u(h)\, dh. \tag{43}$$

If one chooses the form of $u(h)$ to be a polynomial of h with integer powers, the resulting approximation to I will be in terms of a sum of exponential integrals. Thus

$$I \approx \int_{h(a)}^{h(b)} e^h \sum_{k=-n}^{m} a_k h^k\, dh = \sum_{k=-n}^{m} a_k \left(\frac{E_{-k}[h(a)]}{h^{-k-1}(a)} - \frac{E_{-k}[h(b)]}{h^{-k-1}(b)} \right) \tag{44}$$

where m and n are any positive integers or zero. Choosing $u(h)$ to be a polynomial of h with rational, real or complex powers, then the approximation becomes a series of incomplete gamma functions. Hence,

$$\begin{aligned} I &\approx \int_{h(a)}^{h(b)} e^h \sum_{k=-n}^{m} a_k h^{\mu(k)}\, dh \\ &= \sum_{k=-n}^{m} a_k \left(\Gamma[\mu(k)+1, h(a)] - \Gamma[\mu(k)+1, h(b)]\right) \\ &\quad h(a) \text{ and } h(b) \neq 0 \\ &= \sum_{k=0}^{m} a_k (\gamma[\mu(k)+1, h(b)] - \gamma[\mu(k)+1, h(a)]) \\ &\quad \mathrm{Re}[\mu(k)] + 1 > 0. \end{aligned} \tag{45}$$

Clearly, as one increases the number of terms in the polynomial representation of $u(h)$, the accuracy of the solution will be improved at the cost of adding additional terms. This allows for balancing solution complexity against accuracy.

5. Conclusions and discussion

A method for obtaining an analytic approximation to integrals that may have complicated functions in their kernels was developed. Several examples from physical optics were given. The technique sometimes produces a compact form that is more easily calculable. It allows the approximation of integrals for which standard approaches fail. There is also the possibility of trade-offs between functional complexity of the solution and accuracy. The solutions are often globally valid over the full range of each parameter.

As the technique is quite general, error bound estimation is difficult and further work is needed. Currently, the only useful approach is case by case.

Not all of these advantages may occur when using the technique. When compact forms can be achieved not only can the integral then be rapidly computed but considerable gains in physical insight can follow. Having the ability to compute rapidly, even approximately, difficult integrals is a fundamental requirement in design and inverse problems where parameters have to be varied over large ranges and statistics established for the sensitivity of the results.

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