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NUMERICAL CALCULATION OF SINGULAR INTEGRALS RELATED TO HANKEL TRANSFORM

F. FEUILLEBOIS
Laboratoire d'Aérothermique, C.N.R.S.,
4 ter, Route Des Gardes Meudon, France F - 92190

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Abstract—The singular integral $S = \int_0^\infty f(x)e^{-x}J_0(\omega x)\,dx$, related to the Hankel transform of order 0, is calculated numerically by using an integral expression for the Bessel function of order zero, J_0. With the assumptions that the function $f(x)$ is bounded and is analytic in some complex domain, the double integral obtained in this way is calculated by a combination of changes of variables and Gauss methods using Laguerre, Chebyshev and Legendre polynomials. The singular integral $S' = \int_0^\infty f(x)e^{-x}J_1(\omega x)\,dx$ is derived from S. The subroutines written in FORTRAN run very fast on a personal computer and give a relative precision better than 5×10^{-6}.

1. INTRODUCTION

The Fourier transform of a function $f(R_1, R_2)$ is defined as:

$$\hat{f}(\lambda_1, \lambda_2) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(R_1, R_2)e^{i(\lambda_1 R_1 + \lambda_2 R_2)}\,dR_1\,dR_2. \tag{1}$$

Let now $g(\rho)$, with $\rho = \sqrt{R_1^2 + R_2^2}$ be a function which is invariant by rotation around the origin. The Fourier transform of g is

$$\hat{g}(\lambda) = \int_0^\infty g(\rho)J_0(\lambda\rho)\rho\,d\rho \tag{2}$$

where $\lambda = \sqrt{\lambda_1^2 + \lambda_2^2}$ and J_0 is the Bessel function of order 0. The transformation defined by equation (2) is also called the Hankel transform of order 0. The inverse transform has exactly the same form.

In some applications, the function g may decrease exponentially. Consider the model integral:

$$S = \int_0^\infty f(x)e^{-x}J_0(\omega x)\,dx \tag{3}$$

which is to be calculated numerically. $f(x)$ is assumed to be bounded. Because of the oscillation of the Bessel function J_0 together with the exponential decay, classical numerical techniques like, e.g., Romberg's [4] are inefficient especially for large ω.

The same problem arises for the integral

$$S' = \int_0^\infty f(x)e^{-x}J_1(\omega x)\,dx \tag{4}$$

where J_1 is the Bessel function of order 1 and $f(x)$ is assumed to be bounded.

In section 2, some prerequisite integrals will be considered. Then in section 3, we will present a method in which the integral (3) will be transformed to a double integral using an integral expression for the Bessel function of order zero. Although this approach does not appear a priori as the most straightforward one, it is proved to be efficient for the numerical calculation. The example in which $f(x) = 1$ is calculated numerically and the results are shown and compared to the exact result.The calculation of the integral (4) simply uses the derivative of (3) with respect to ω. It is presented in section 4. The example in which $f(x) = 1$ is also considered for this integral and the numerical result is compared to the exact one.

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2. SOME PREREQUISITE INTEGRALS

Integrals like

$$\int_a^b f(x)\,dx \tag{5}$$

$$\int_0^\infty f(x)e^{-x}\,dx \tag{6}$$

$$\int_{-1}^1 f(x)(1-t^2)^{-1/2}\,dx \tag{7}$$

can be calculated by using classical Gaussian quadrature formulae, viz. Gauss-Legendre for (5), Gauss-Laguerre for (6) and Gauss-Chebyshev for (7). These formulae are given in classical handbooks [1,3,4].

Consider now an integral which has a behaviour similar to (3) at infinity, that is an exponential decay together with an oscillation:

$$\int_0^\infty f(x)e^{-x}\cos\omega x\,dx. \tag{8}$$

Like for (3), classical numerical techniques are inefficient especially for large ω. However, for the integral in (8), a simple change of variables is sufficient to obtain an efficient integration technique as we will see now.

The integral (8) is the real part of the integral

$$J = \int_0^\infty f(x)e^{-(1-i\omega)x}\,dx. \tag{9}$$

Let

$$z = (1-i\omega)x. \tag{10}$$

Then (9) becomes

$$J = \frac{1}{1-i\omega}\int_L f\left(\frac{z}{1-i\omega}\right)e^{-z}\,dz. \tag{11}$$

where L is a half straight line in the complex plane (see figure 1); the argument of the current point of this line is $\arctan(-\omega)$.

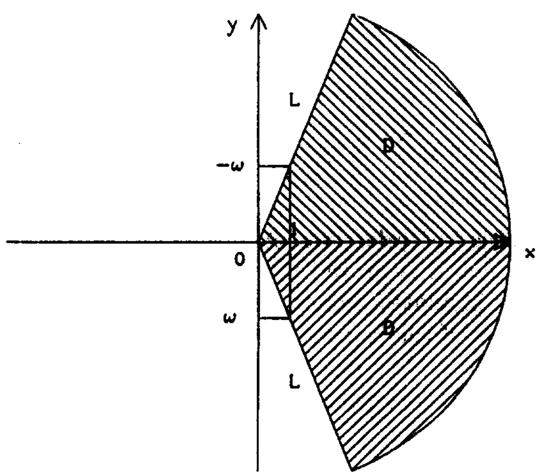

Figure 1: Domains in the complex plane.

Consider the domain D in the complex plane limited by the line L, the positive part Ox of the real axis, and the line at infinity. Let C be the integration contour around D. If the function $f(\frac{z}{1-i\omega})$ is analytic in D, then by Cauchy's theorem

$$\frac{1}{1-i\omega}\int_C f(\frac{z}{1-i\omega})e^{-z}\,dz = 0. \tag{12}$$

$f(\frac{z}{1-i\omega})$ is analytic in D, provided $f(z)$ is assumed to be analytic in D', which is the domain bounded by the positive real axis Ox, the half straight line L' with argument $\arctan\omega$, and the line at infinity (see Figure 1).

With this assumption, and since the part of the contour at infinity gives a zero contribution to the integral in (12), there is only an integral on L and an integral on Ox (with the negative sign) in (12). Then J, equation (11), can be obtained from an integration on Ox:

$$J = \frac{1}{1-i\omega}\int_0^\infty f(\frac{z}{1-i\omega})e^{-z}\,dz. \tag{13}$$

The calculation of J may be done numerically in FORTRAN using the complex variables and the classical Gauss-Laguerre formulae for an integral of the type (6). The real part of (9), that is (8), is then obtained together with the imaginary part, that is:

$$\int_0^\infty f(x)e^{-x}\sin\omega x\,dx. \tag{14}$$

A FORTRAN subroutine named QCEXP performs these calculations[1]. As an example, the following integrals were calculated numerically:

$$\int_0^\infty xe^{-x}\cos(1000x)\,dx = -0.999997000027\times 10^{-6} \tag{15}$$

$$\int_0^\infty xe^{-x}\sin(1000x)\,dx = 0.1999996000051\times 10^{-8} \tag{16}$$

the exact results being respectively

$$-0.999997000005\times 10^{-6}$$

and

$$0.1999996000006\times 10^{-8}.$$

This shows the excellent precision obtained even for large ω. The calculation time is very short as with all Gauss' type methods, and the program runs easily on a personal computer.

3. CALCULATION OF THE INTEGRAL INVOLVING THE BESSEL FUNCTION OF ORDER 0

Consider now the integral S, equation (3). The Bessel function of order 0, J_0 can be written as an integral, after [2, formula 8, page 953]:

$$J_0(z) = \frac{1}{\pi}\int_{-1}^{1}(1-t^2)^{-1/2}\cos zt\,dt. \tag{17}$$

Then the expression (3) for S may be rewritten as:

$$S = \int_{-1}^{1}(1-t^2)^{-1/2}g_0(t)\,dt \tag{18}$$

[1] All the FORTRAN subroutines quoted in this article are available directly from the author upon request.

where

$$g_0(t) = \frac{1}{\pi} \int_0^\infty f(x) e^{-x} \cos(\omega x t)\, dx. \quad (19)$$

Since g_0 is even in t, and alternative expression for (18) is

$$S = 2 \int_0^1 (1 - t^2)^{-1/2} g_0(t)\, dt. \quad (20)$$

The numerical method follows. The function g_0, equation (19), is calculated using the method of section 2 for the integral (8). Then the integral in equation (18) is calculated using the classical Gauss-Chebyshev quadrature formulae as for integral (7). This method works well numerically for values of $|\omega|$ up to order of unity; as an example, we calculated the following numerical value for $\omega = 1$:

$$\int_0^\infty e^{-x} J_0(x)\, dx = 0.707106781193 \quad (21)$$

whereas the exact result is $1/\sqrt{2} = 0.707106781186$.

However, for large values of $|\omega|$, the Gauss-Chebyshev quadrature method is not appropriate, because g_0 has a peak around 0 which becomes sharp when $|\omega|$ becomes large. This is better seen on an example. From [2], page 707, we know the exact result:

$$\int_0^\infty e^{-x} J_0(\omega x)\, dx = (1 + \omega^2)^{-1/2}. \quad (22)$$

In order to recover this result numerically using the above method, we calculate first the integral (19)

$$g_0(t) = \frac{1}{\pi} \int_0^\infty e^{-x} \cos(\omega x t)\, dx. \quad (23)$$

The exact result is

$$g_0(t) = \frac{1}{\pi(1 + \omega^2 t^2)}. \quad (24)$$

This function, which is to be integrated between -1 and 1, has a sharp peak in $t = 0$ for large ω (see Figure 2).

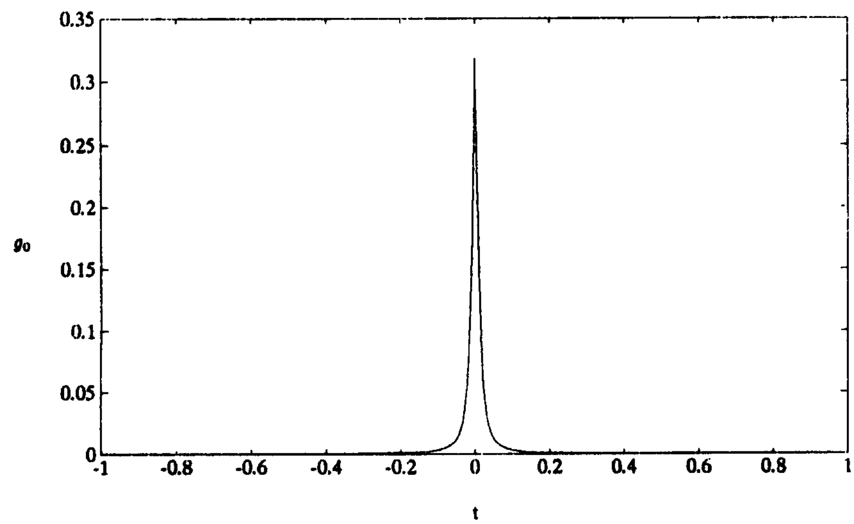

Figure 2: Function $g_0(t)$ for $\omega = 100$.

Using the result (24) for $f(x) = 1$, let in the general case of an arbitrary $f(x)$

$$h_0(t) = \pi(1 + \omega^2 t^2) g_0(t) \tag{25}$$

so that the integral (20) to be calculated becomes

$$S = 2\int_0^1 \frac{1}{\pi}(1-t^2)^{-1/2} h_0(t) \frac{dt}{1+\omega^2 t^2}. \tag{26}$$

The peak of the integrand occurs for small t. Using the ideas of the method of matched asymptotic expansions, we write the integral in (26) as a sum of two terms, an "inner" one and an "outer" one:

$$S = 2\left(\int_0^\epsilon + \int_\epsilon^1\right) \tag{27}$$

where ϵ is a number such that:

$$1 \ll \epsilon^{-1} \ll |\omega|. \tag{28}$$

Let $y = \frac{1}{\omega}\arctan\omega t$ in the first integral, and $t = \sin\theta$ in the second integral; then

$$S = 2(S_1 + S_2) \tag{29}$$

where

$$S_1 = \int_0^{\frac{1}{\omega}\arctan\omega\epsilon} f_1(y)\,dy \tag{30}$$

with

$$f_1(y) = \frac{1}{\pi}\left(1 - \frac{\tan^2\omega y}{\omega^2}\right)^{-1/2} h_0\left(\frac{\tan\omega y}{\omega}\right) \tag{31}$$

and

$$S_2 = \int_{\arcsin\epsilon}^{\pi/2} f_2(\theta)\,d\theta \tag{32}$$

with

$$f_2(\theta) = \frac{h_0(\sin\theta)}{\pi(1+\omega^2\sin^2\theta)}. \tag{33}$$

Since $f_1(y)$ and $f_2(\theta)$ are regular, the standard Gauss-Legendre formulae can be used to calculate numerically the integrals S_1 and S_2. The size ϵ of the matching region can be adjusted at will provided the condition (28) is satisfied. We found by trial that, for $f(x) = 1$, the best compromise to obtain the best precision for all $|\omega| > 1$ is

$$\epsilon = |\omega|^{-1/3}. \tag{34}$$

We have seen that the method using the classical Gauss-Chebyshev quadrature formulae works well for values of $|\omega|$ up to order of unity, and that the method we have just exposed is more adapted for large values of $|\omega|$. The value ω_1 of $|\omega|$ at which one should switch from one method to the other was searched by trial. It was found that the best precision on the results is obtained for $\omega_1 = 1.5$.

A FORTRAN subroutine name QJ0EX performs these calculations. Note that the function $f(x)$ should in general be declared complex, since QCEXP is used in the course of the calculation. As an example, the integral

$$\int_0^\infty e^{-x} J_0(\omega x)\,dx$$

was calculated and compared to the exact result (22) for several values of ω. The results are shown in Table 1.

The relative difference between the numerically calculated integral and the exact result is less than 5×10^{-6} for all values of ω. Actually, the precision 5×10^{-6} is obtained around $\omega = 10^6$ but the typical precision is more often of the order of 10^{-8} or less. The calculation time is very short since only Gauss' type methods are used, and the program runs easily on a personal computer.

Table 1
Calculation of $\int_0^\infty e^{-x} J_0(\omega x)\,dx$ for various values of ω. Note that there is a switch from one method to the other at $\omega = 1.5$.

ω	Numerical Result	Exact Result
1	0.7071067811935	0.7071067811865
1.5	0.5547001896635	0.5547001962252
1.5001	0.5546745924751	0.5546745955967
10^6	$0.9999953118850 \times 10^{-6}$	$0.9999999999995 \times 10^{-6}$
10^{12}	$0.9999999914673 \times 10^{-12}$	$1.0000000000000 \times 10^{-12}$

4. CALCULATION OF THE INTEGRAL INVOLVING THE BESSEL FUNCTION OF ORDER 1

Consider now the integral involving J_1, equation (4). A possible approach is, like in section 3, to use an integral relation for J_1 ([2], formula 8, page 953):

$$J_1(z) = \frac{z}{\pi} \int_{-1}^{1} (1-t^2)^{1/2} \cos zt\, dt. \tag{35}$$

Then the expression for S' in (4) is written:

$$S' = \int_{-1}^{1} (1-t^2)^{1/2} g_1(t)\, dt \tag{36}$$

where

$$g_1(t) = \frac{\omega}{\pi} \int_0^\infty f(x) x e^{-x} \cos(\omega x t)\, dx. \tag{37}$$

and we proceed like in section 2. However, for large $|\omega|$, g_1 has a sharp peak in $t = 0$ and varies rapidly around $t = 0$. This may be seen on an example. We know from [2], page 707, the exact result:

$$\int_0^\infty e^{-x} J_1(\omega x)\, dx = \frac{\sqrt{1+\omega^2} - 1}{\omega\sqrt{1+\omega^2}}. \tag{38}$$

In order to recover this result numerically, we calculate first the integral (37)

$$g_1(t) = \frac{\omega}{\pi} \int_0^\infty x e^{-x} \cos(\omega x t)\, dx. \tag{39}$$

The exact result is

$$g_1(t) = \frac{\omega(1-\omega^2 t^2)}{\pi(1+\omega^2 t^2)^2}. \tag{40}$$

This function which is to be integrated between -1 and 1 varies rapidly around $t = 0$ for large $|\omega|$ (see Figure 3).

Moreover, it happens to have a positive and a negative part, the integrals of which are of the same order of magnitude. We then have to subtract two quantities of the same order and the resulting precision is poor. Note that the same problem would arise when calculating (3) with $f(x) = x$. This is the reason why we assumed $f(x)$ to be bounded.

For these reasons, we consider an alternate method to calculate the integral in (4). Using the classical property for the Bessel functions

$$J_1(\omega x) = -\frac{1}{\omega} \frac{dJ_0(\omega x)}{dx} \tag{41}$$

we integrate (4) by parts and obtain

$$\begin{aligned} S' = &-\frac{1}{\omega} \int_0^\infty f(x) e^{-x} J_0(\omega x)\, dx \\ &+\frac{1}{\omega} \int_0^\infty f'(x) e^{-x} J_0(\omega x)\, dx \end{aligned} \tag{42}$$

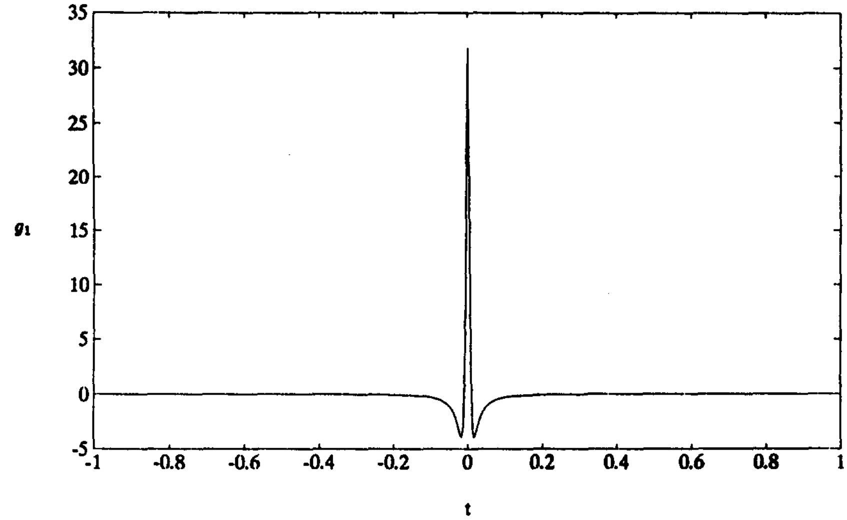

Figure 3: Function $g_1(t)$ for $\omega = 100$.

This equation may be written in a more concise notation:

$$S'[f] = \frac{S[f'] - S[f]}{\omega}. \tag{43}$$

A FORTRAN subroutine named QJ1EX uses this equation to call the subroutine QJ0EX. Note that here the function f and its derivative f' should be supplied. Both functions should be declared as complex, because the subroutine QCEXP is used in the course of the calculation. As an example the integral

$$\int_0^\infty e^{-x} J_1(\omega x)\, dx$$

was calculated and compared to the exact result (38) for several values of ω. The results are shown in table 2. Since the main calculations are done with QJ0EX, the remarks concerning the precision and calculation time are the same as in the preceding section.

Table 2
Calculation of $\int_0^\infty e^{-x} J_1(\omega x)\, dx$ for various values of ω.
Note that there is a switch from one method to the other at $\omega = 1.5$.

ω	Numerical Result	Exact Result
1	-0.7071067811935	-0.7071067811865
1.5	-0.3698001264423	-0.3698001308168
1.5001	-0.3697584110893	-0.3697584131702
10^6	$-0.9999953118850 \times 10^{-12}$	$-0.9999999999995 \times 10^{-12}$
10^{12}	$-0.9999999914673 \times 10^{-24}$	$-1.0000000000000 \times 10^{-24}$

5. CONCLUSION

The singular integrals S, equation (3), related to Hankel transform and S', equation (4), are calculated numerically.

The integral S is calculated by using an integral expression (17) for the Bessel function of order zero, J_0. With the assumptions that the function $f(x)$ is bounded and is analytic in the complex domain D' (see figure 1), the double integral (18) (19) obtained in this way is calculated

(1) for $|\omega| \leq 1.5$ by Gauss-Laguerre and Gauss-Chebyshev formulae;
(2) for $|\omega| > 1.5$ by Gauss-Laguerre formulae, changes of variables, and Gauss-Legendre formulae.

The singular integral S', equation (4), is calculated in terms of integrals of the type S, equation (3): see equation (43).

The subroutines QJ0EX, to calculate (3), and QJ1EX, to calculate (4), are tested on example cases. They run very fast on a personal computer and give a relative precision better than 5×10^{-6} for all values of ω.

The method uses the integral in (8) as an intermediate step in the calculation. The possibility to calculate directly this integral together with the related integral in (14) is also provided with the subroutine QCEXP. The relative precision given by this subroutine is typically 5×10^{-11}.

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