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Numerical Fourier and Bessel Transforms in Logarithmic Variables*

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A method is described for the numerical calculation of Fourier transforms in variables that are the logarithms of the original variable and transform variable. The method involves only the application of two successive Fourier transforms and can also be applied to Bessel and spherical Bessel transforms. Numerical examples show that the method gives very accurate results up to large values of the transform variable.

1. INTRODUCTION

The purpose of this article is to describe a technique for calculating Fourier sine or cosine transforms, or Fourier-Bessel transforms, that may be very useful and convenient in many situations.

The basis of the method is the use of variables that are the logarithms of the original and transform variables. These variables are particularly appropriate in atomic physics calculations because for atoms of moderately large Z there are considerably different length scales in the problem. The length scale appropriate to the inner electrons is a_0/Z, where a_0 is the Bohr radius, whereas the length scale appropriate to the outer electrons is a_0. Similarly, in the transform variables, the wave number scales are Z/a_0 and $1/a_0$ respectively.

The problem then arises in carrying out a numerical integration that, if a small mesh suitable for the inner electrons is chosen, a prohibitively large number of points may be required for the outer electrons. For example, for $Z = 10$, choices of $\Delta r = 0.01$ (r being the original variable) and $r_{\max} = 5$, might be appropriate. Similarly, in k (the transform variable) choices of $\Delta k = 0.2$ and $k_{\max} = 100$ might be reasonable. It is seen that to use the same mesh for all the electrons, a prohibitively large number of operations ($\sim 500^2$) is required to calculate a single transform. This problem can be avoided by the use of logarithmic variables for which Δr and Δk increase linearly with r and k. For an example of such a calculation, for which logarithmic variables are appropriate we refer to a discussion by Green and Garvey [1] on atomic form factors.

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Although these considerations from atomic physics led to the development of the method, it should be of value in calculations in which frequent calculations of Fourier or Bessel transforms are required at many values (as contrasted to a single value) of the transform variable. In particular, the method uses two successive calculations of Fourier transforms. The fast Fourier transform technique [2] (FFT) can then be applied so that the computing time is proportional to $N \ln N$ rather than N^2. Furthermore, no calculations of Bessel functions are required for Bessel transforms.

The method will be described in Section 2. The results of some calculations of spherical Bessel transforms will be given in Section 3 and in Section 4 the method will be compared with other methods of doing related problems.

The use of logarithmic variables in transforms in which the kernel is a function of the product of the two variables has been proposed previously by Gardner, *et al.* [3] in a related context to solve the problem of decomposing a function that is a linear combination of decreasing exponentials. The Gardner method has been elaborated by Schlesinger [4], and Smith and Cohn-Sfetcu [5], and has been generalized to the problem of analyzing multicomponent signals by Cohn-Sfetcu, *et al.* [6, 7]. After this article was submitted for publication, the author received a preprint by Siegman [8] in which the application to the calculation of Bessel transforms (Eq. (18)) has been outlined.

2. Method

We are interested in integrals of the form

$$g(k) = \int_0^\infty f(r) \sin kr \, dr. \tag{1}$$

It will be assumed that $f(r) \to 0$ at least linearly as $r \to 0$ as is usually the case in practice. We put $r = e^\rho$, $k = e^\kappa$, $\hat{g}(\kappa) = g(e^\kappa)$, $\hat{f}(\rho) = f(e^\rho)$. Then Eq. (2.1) is

$$\hat{g}(\kappa) = \int_{-\infty}^\infty \sin(e^{\kappa+\rho}) \hat{f}(\rho) \, e^\rho \, d\rho. \tag{2}$$

It is seen that Eq. (2) is a convolution type integral and it is therefore natural to calculate it by Fourier transforms. To this end, we put

$$e^{\rho/2}\hat{f}(\rho) = \int_{-\infty}^\infty e^{-it\rho}\phi(t) \, dt, \tag{3a}$$

$$\phi(t) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{it\rho} e^{\rho/2}\hat{f}(\rho) \, d\rho, \tag{3b}$$

$$e^{\rho/2} \sin(e^\rho) = \int_{-\infty}^\infty e^{it\rho} M(t) \, dt, \tag{4a}$$

$$M(t) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{-it\rho} e^{\rho/2} \sin(e^\rho) \, d\rho. \tag{4b}$$

It is then readily found that

$$\hat{g}(\kappa) = 2\pi e^{-\kappa/2} \int_{-\infty}^{\infty} e^{i\kappa t} \phi(t)\, M(t)\, dt. \tag{5}$$

Therefore, it is seen that to calculate $\hat{g}(\kappa)$, it is necessary only to find the Fourier transform of $e^{\rho/2}\hat{f}(\rho)$, multiply it by $M(t)$, and transform back.

It is noticed that e^{ρ} has been factored between $\hat{f}(\rho)$ and $\sin(e^{\rho})$. This factorization is convenient, in that it turns out that $M(t)$ has constant modulus, but not essential for the method.

The function $M(t)$ is given by

$$\begin{aligned} M(t) &= \frac{1}{2\pi} \int_0^{\infty} r^{-1/2-it} \sin r\, dr \\ &= \frac{1}{2\pi} \Gamma(1/2 - it) \sin \frac{\pi}{2} (1/2 - it) \\ &= \frac{1}{2^{3/2}\pi} \Gamma(1/2 - it) \left[\cosh\left(\frac{\pi t}{2}\right) - i \sinh\left(\frac{\pi t}{2}\right)\right]. \end{aligned} \tag{6}$$

Since [9]

$$|\Gamma(1/2 - it)|^2 = \pi/\cosh \pi t,$$

$M(t)$ has constant modulus, and is given by

$$M(t) = (8\pi)^{-1/2} e^{i(\Phi_1 - \Phi_2)}, \tag{7}$$

where

$$\Phi_2(t) = \tan^{-1}(\tanh(\pi t/2)) \tag{8}$$

and $\Phi_1(t)$ is the argument of $\Gamma(1/2 - it)$. The latter is readily calculated by expressing $\Gamma(1/2 - it)$ in terms of $\Gamma(n + 1/2 - it)$ and using the known asymptotic behavior of the Γ function [9]. The result is

$$\begin{aligned} \Phi_1(t) &= \operatorname{Im}[\ln \Gamma(1/2 - it)] \\ &= \lim_{n\to\infty} \left\{ \sum_{m=1}^{n} \tan^{-1}\left(\frac{2t}{2m-1}\right) - t \ln r + t - n\phi \right. \\ &\quad \left. + \frac{\sin \phi}{12r} - \frac{\sin(3\phi)}{360r^3} + \frac{\sin(5\phi)}{1260r^5} \cdots \right\}, \end{aligned} \tag{9}$$

where

$$\phi = \tan^{-1}[2t/(2n+1)], \qquad r = [(n + \tfrac{1}{2})^2 + t^2]^{1/2}.$$

The choice of n is dictated only by the requirement that the asymptotic expansion of the Γ function be valid. It was found that choosing $n = 10$, and retaining the terms given in (9), gave results for $\Phi_1(t)$ correct to ten decimal places. Greater accuracy could be readily obtained by using double-precision arithmetic and retaining the next few terms in the asymptotic expansion.

We note that if $f(r)$ is real, Eq. (5) can be written

$$\hat{g}(\kappa) = 4\pi e^{-\kappa/2} \operatorname{Re} \int_{-\infty}^{\infty} e^{i\kappa t} \phi(t)\, M(t)\, dt. \tag{10}$$

Further, if a cosine transform is required, it is obtained by changing the sign of $\sinh(\pi t/2)$ in (6) or replacing Φ_2 by $-\Phi_2$.

Integrals of the form

$$g_l(k) = \int_0^{\infty} j_l(kr) f(r) r^2\, dr \tag{11}$$

are also frequently required. There is a certain degree of arbitrariness in performing the integral since various powers of r can be factored out of $j_l(kr)$. It is convenient for this reason to write the integral as

$$g_l(k) = k^{m-1} \int_0^{\infty} (kr)^{1-m} j_l(kr)\, r^{m+1} f(r)\, dr, \tag{12}$$

where $m = 0, 1, \ldots, l$.

Proceeding as before, we find that

$$\hat{g}_l(\kappa) = 2\pi e^{(m-3/2)\kappa} \int_{-\infty}^{\infty} e^{i\kappa t} M_{l,m}(t)\, \phi_m(t)\, dt, \tag{13}$$

where

$$\phi_m(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{it\rho} e^{(m+3/2)\rho} f(e^{\rho})\, d\rho, \tag{14}$$

$$M_{l,m}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-it\rho} e^{(3/2-m)\rho} j_l(e^{\rho})\, d\rho \tag{15}$$

$$= \frac{1}{2\pi} \int_0^{\infty} r^{1/2-m-it} j_l(r)\, dr. \tag{16}$$

This integral can be evaluated by using identities for spherical Bessel functions, and it is found that

$$M_{l,m}(t) = (8\pi)^{-1/2} \prod_{j=1}^{p} (j - \tfrac{1}{2} - it) \prod_{j=1}^{l} (2j - l + m - \tfrac{1}{2} + it)^{-1}$$

$$\times \left[\cos\left(\frac{p\pi}{2}\right) e^{i(\Phi_1 - \Phi_2)} + \sin\left(\frac{p\pi}{2}\right) e^{i(\Phi_1 + \Phi_2)}\right], \tag{17}$$

where $p = l - m$ and Φ_1 and Φ_2 are given in Eqs. (8) and (9).

Bessel transforms of the form

$$g_n(k) = \int_0^\infty J_n(kr) f(r) r \, dr \tag{18}$$

can also be calculated by the above methods. Proceeding as before, we find

$$\hat{g}_n(\kappa) = 2\pi e^{(\mu-1)\kappa} \int_{-\infty}^{\infty} e^{i\kappa t} Q_{n,\mu}(t) \, \phi_\mu(t) \, dt, \tag{19}$$

where

$$\phi_\mu(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{it\rho} e^{(1+\mu)\rho} f(e^\rho) \, d\rho, \tag{20}$$

$$Q_{n,\mu}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-it\rho} e^{(1-\mu)\rho} J_n(e^\rho) \, d\rho, \tag{21}$$

and μ is an arbitrary number such that $-\frac{1}{2} < \mu < n + 1$. The integral in Eq. (21) can be calculated as [9]

$$\begin{aligned} Q_{n,\mu}(\kappa) &= \frac{1}{2\pi} \int_0^\infty r^{-\mu-it} J_n(r) \, dr \\ &= \frac{1}{2\pi} 2^{-\mu-it} \frac{\Gamma((n - \mu - it + 1)/2)}{\Gamma((n + \mu + it + 1)/2)} . \end{aligned} \tag{22}$$

If n is a nonnegative integer, and μ has been chosen so that $n - \mu$ is even, this can be written

$$\begin{aligned} Q_{n,\mu}(t) = \frac{1}{2\pi} 2^{-it} &\frac{(n - \mu - 1 - it)(n - \mu - 3 - it) \cdots (1 - it)}{(n + \mu - 1 + it)(n + \mu - 3 + it) \cdots (1 + it)} \\ &\times \frac{\Gamma((1 - it)/2)}{\Gamma((1 + it)/2)} . \end{aligned} \tag{23}$$

The factor $\Gamma((1 - it)/2)/\Gamma((1 + it)/2)$ has unit modulus, and its phase is given by $2\,\Phi_2(t/2)$ where Φ_2 is given in Eq. (9).

In certain calculations the integral

$$g_l(k, k') = \int_0^\infty j_l(kr) \, j_l(k'r) f(r) \, r^2 \, dr \tag{24}$$

may be required. This can be calculated using Eqs. (11)–(15) for spherical Bessel transforms, provided $M_{l,m}(t)$ is replaced by

$$M_{l,m}(t, \lambda) = \frac{1}{2\pi} \int_0^\infty r^{1/2-m-it} j_l(r) \, j_l(\lambda r) \, dr, \tag{25}$$

where $\lambda = k'/k$. It can be assumed that $\lambda \leqslant 1$.

The integral in Eq. (25) is a Weber–Schafheitlin integral and can be written as

$$M_{l,m}(t, \lambda) = (4\lambda^{1/2}2^{y})^{-1} \frac{\Gamma(l + 1 - y/2)}{\Gamma(1/2 + y/2)} (1 - \lambda^2)^{(y-1)/2} P^{-l-1/2}_{(y-1)/2}\left(\frac{1 + \lambda^2}{1 - \lambda^2}\right),$$

where $y = m + \frac{1}{2} + it$. It can then be verified that the $M_{l,m}$ satisfy the following recurrence relation in l:

$$\lambda(2l - y)\, M_{l-1,m} - (2l + 1)(1 + \lambda^2)\, M_{l,m} + \lambda(2l + 2 + y)\, M_{l+1,m} = 0. \quad (26)$$

The values of $M_{l,m}(t, \lambda)$ can be calculated for arbitrary l by combining Eq. (26) with the special cases [9]

$$M_{0,m}(t, \lambda) = (4\pi\lambda y)^{-1}\, \Gamma(1 - y) \cos(\pi y/2)[(1 + \lambda)^{y} - (1 - \lambda)^{y}], \quad (27)$$

$$M_{-1,m}(t, \lambda) = -(4\pi\lambda y)^{-1}\, \Gamma(1 - y) \cos(\pi y/2)[(1 + \lambda)^{y} + (1 - \lambda)^{y}]. \quad (28)$$

The function

$$\Gamma(1 - y) \cos(\pi y/2) = \Gamma(-m + \tfrac{1}{2} - it) \sin[(\pi/2)(m + it)]/2^{1/2} \quad (29)$$

can be readily expressed in terms of $\Phi_1(t)$ and $\Phi_2(t)$ in Eqs. (8) and (9).

3. Numerical Examples

The method that has been described seems to be sufficiently complicated mathematically that it is difficult to give a detailed error analysis of it. It has therefore been applied to some specific examples to try to understand the best way to implement it.

The problem is essentially to calculate the two Fourier transforms. It is necessary to choose an integration scheme, and parameters $\Delta\rho$, N_ρ, Δt, N_t which describe the meshes in the ρ and t integrations. The use of the FFT appears to be so attractive that methods assuming uniform meshes in ρ and t have been considered primarily. If the FFT is used, the mesh parameters are constrained by $N_\rho = N_t = N$ and $\Delta\rho\, \Delta t = 2\pi/N$. Also $\Delta\kappa = \Delta\rho$ and $N_\kappa = N_\rho$. The Fourier transforms may then also be calculated at extraneous large and small values of κ that are of no practical interest, and for which the results are inaccurate.

Preliminary calculations were made for $f(r) = e^{-r}$ using the trapezoidal rule, Simpson's rule, and Filon's method to carry out the numerical integrations of Eqs. (3b) and (5). Another method [10] that has been tried is to expand the given function in a Chebyshev series and sum the Fourier transforms of each term in the series. In the example considered the trapezoidal rule yielded the most accurate results so it was used in further calculations. It may be noted that for the integrals being considered, which essentially vanish at the end points, the trapezoidal rule is a fourth-order

method. The Chebyshev expansion method, using 41 data points, was found to be less accurate than the trapezoidal rule using 65 data points, and failed altogether using 65 data points in single-precision arithmetic. This method therefore seems to be not too useful for the present calculation, although it is probably feasible to subdivide the entire interval and use a lower-order version of the method on the subintervals.

It was found empirically that a ratio $\Delta t/\Delta\rho \sim 2$ seemed to give the most accurate results in the case considered.

The transform $\phi(t)$, when calculated numerically by the trapezoidal rule, satisfies the identity $\phi(T - t) = \phi(t)^*$ where $T = N\Delta t = 2\pi/\Delta\rho$. This implies that the values of $\phi(t)$ for $t > T/2$ must be spurious and therefore the t integration was cut off at $t = T/2$. The integration in Eq. (5) is then over the Nyquist interval $(-T/2, T/2)$.

The calculations described were made on a computer with a 14 decimal digit word length.

The method has been applied to calculate the spherical Bessel transforms of Eq. (11) for the function

$$f(r) = e^{-r} \tag{30}$$

for various l values. For $l = 0$, this reduces to the sine transform of $r\,e^{-r}$.

The analytic results have been calculated as follows. If we define

$$I_{l,m}(Z) = \int_0^\infty e^{-Zr} j_l(r)\, r^m\, dr \tag{31}$$

it can be shown that

$$I_{l,l+1} = \frac{2l}{1 + Z^2}\, I_{l-1,l}\,,$$

$$I_{l,l} = (2l - 1)\, I_{l-1,l-1} - Z I_{l-1,l}\,,$$

$$I_{l,m} = \frac{(1 + Z^2)\, I_{l,m+2} - 2Z(m + 1)\, I_{l,m+1}}{(l - m)(l + m + 1)}\,.$$

These identities, together with

$$I_{0,0} = \tan^{-1}(1/Z), \qquad I_{0,1} = (1 + Z^2)^{-1}$$

permit the recursive calculation of $I_{l,l}$ and $I_{l,l+1}$, and hence of $I_{l,2}$. The desired result is then $k^{-3} I_{l,2}(Z/k)$.

The results for $l = 0$ are shown in Table 1. In one case the calculation was done with $N = 64$, $\Delta\rho = 0.2$, $-10 \leqslant \rho \leqslant 2.6$. Then $\Delta t \approx 0.5$ and $t_{\max} \approx 16$. The results were calculated for $-3 \leqslant \kappa \leqslant 9.6$, $\Delta\kappa = 0.2$, but are invalid for $\kappa > \sim 4$. It is seen that the results are valid to 5 or 6 significant figures for $\kappa < 0$ and to 6 or better decimal places for $\kappa > 0$. The calculation was repeated with $N = 256$, $\Delta\rho = 0.1$, $-18 \leqslant \rho \leqslant 7.5$. Then $\Delta t \approx 0.25$ and $t_{\max} \approx 32$. The results were calculated for

TABLE I

Spherical Bessel Transforms of e^{-r} with $l = 0$, Showing the Analytic Results, and the Results for Two Numerical Calculations

κ	k	Analytic	$N = 64$ $\Delta\rho = 0.2$ $\rho_{\min} = -10$	$N = 256$ $\Delta\rho = 0.1$ $\rho_{\min} = -18$
−3	0.0498	1.990121735	1.990068	1.990121735
−2	0.1353	1.928702168	1.928672	1.928702168
−1	0.3679	1.551606985	1.5516106	1.551606985
0	1.0	0.5	0.50000072	0.5000000000
1	2.7183	(−2)2.841867324	(−2)2.8418736	(−2)2.841867324
2	7.3891	(−4)6.470074976	(−4)6.470077	(−4)6.470074975
3	20.086	(−5)1.222773055	(−5)1.22380	(−5)1.222773055
4	54.598	(−7)2.249194200	(−7)2.341	(−7)2.249194200
5	148.41	(−9)4.12193297	(−8)1.33	(−9)4.12193301
6	403.43	(−11)7.5501763	(−9)9.26	(−11)7.5501805

TABLE II

Spherical Bessel Transforms of e^{-r} with $l = 10$ in the Same Cases as Table I

κ	Analytic	$N = 64$ $\Delta\rho = 0.2$ $\rho_{\min} = -10$	$N = 256$ $\Delta\rho = 0.1$ $\rho_{\min} = -18$
−2	(−11)6.6825	(−5)7.51	(−11)6.7203
−1	(−7)9.5245197	(−6)5.882	(−7)9.5245214
0	(−3)1.933805884	(−3)1.9364	(−3)1.933805886
1	(−2)4.379309023	(−2)4.3793135	(−2)4.379309023
2	(−2)2.559147429	(−2)2.559146481	(−2)2.559147429
3	(−3)3.129977969	(−3)3.129979318	(−3)3.129977969
4	(−4)2.161750217	(−4)2.161749257	(−4)2.161750217
5	(−5)1.213305819	(−5)1.213303907	(−5)1.213305819
6	(−7)6.312462077	(−7)6.31256	(−7)6.312462077

$-7 \leqslant \kappa \leqslant 18.5$ but are shown only for $-3 \leqslant \kappa \leqslant 6$. It is seen that they are valid to 10 significant figures for $\kappa < 0$ and better than 10 decimal places for $\kappa > 0$.

The results of the same calculations in the case $l = 10$ are shown in Table II. It is seen that they are again accurate to about 6 and 10 decimal places, respectively, with the accuracy improving for large κ. The relative inaccuracy at small κ is not too

TABLE III

Spherical Bessel Transform of e^{-r} with $l = 10$, Calculated with $m = 10$

κ	Analytic	$N = 64$ $\Delta\rho = 0.2$ $\rho_{\min} = -7$	$N = 256$ $\Delta\rho = 0.1$ $\rho_{\min} = -7$
−3	(−15)3.228247340	(−15)3.2282466	(−15)3.228247340
−2	(−11)6.682441388	(−11)6.682441833	(−11)6.682441389
−1	(−7)9.524519666	(−7)9.52451957	(−7)9.524519666
0	(−3)1.933805884	(−3)1.933806187	(−3)1.933805884
1	(−2)4.379309023	(−2)4.37958	(−2)4.379309015
2	(−2)2.559147429	0.10513	(−2)2.559147098

troublesome since if one were interested in extreme accuracy for $\kappa \ll 0$ one would use a more standard quadrature rule because the slow oscillation of the integrand would cause no difficulty. The accuracy at small κ can be improved, however, at the expense of the results for large κ, by choosing a larger value of m to perform the calculation. The results of such a calculation, with $l = m = 10$ are given in Table III. It is seen that for $\kappa < 0$, the results of the two calculations are accurate to better than 8 and 12 decimal places, respectively.

The reason for the dependency of the accuracy on the choice of m is clearly the factor $e^{m\kappa}$ in Eq. (13). In order to obtain high accuracy, $e^{m\kappa}$ should be small so that the integral in (13) is large; this is achieved with $m = l$ for $\kappa \ll 0$ and $m = 0$ for $\kappa \gg 0$.

The method was also applied to the spherical Bessel transform of

$$f(r) = (1 + r^2)^{-1} \tag{32}$$

TABLE IV

Spherical Bessel Transform of $(1 + r^2)^{-1}$, $l = 0$, Calculated with $\Delta\rho = 0.1$, $N = 256$, $\rho_{\min} = -7$

κ	Analytic	Numerical
−3	30.0179530	30.0179596
−2	10.1375609	10.1375633
−1	2.9556047	2.9556054
0	0.57786367	0.57786385
1	(−2)3.8132089	(−2)3.8132129
2	(−4)1.31373	(−4)1.31382
3	(−10)1.48	(−9)3.41

in the case $l = 0$. The result in this case is

$$g(k) = \pi/2\, e^{-k}/k. \tag{33}$$

This is a difficult case because of the very slow decrease of the integrand ($\sim r^{-1}$) at large r. Because of the necessity of maintaining a large range in ρ, the calculation was only done for $\Delta\rho = 0.1$, $N = 256$, $\rho_{\min} = -7$. The results are given in Table IV and are seen to be accurate to only about 7 decimal places for $\kappa > 0$ and 7 significant figures for $\kappa < 0$. If one were confronted with this difficult long-range behavior in practice, however, one would try to extract the long-range part and perform the integration analytically.

Another example that has been considered is the spherical Bessel transform of

$$f(r) = (1 + r^2)^{-3} \tag{34}$$

in the case $l = 0$. In this case the result is given by

$$g(k) = (\pi/16)(1 + y)\, e^{-y}. \tag{35}$$

The results are given in Table V and are seen to be accurate to at least 10 decimal places in the more accurate calculation.

TABLE V

Spherical Bessel transform of $(1 + r^2)^{-3}$ for $l = 0$

κ	Analytic	$N = 64$ $\Delta\rho = 0.2$ $\rho_{\min} = -10$	$N = 256$ $\Delta\rho = 0.1$ $\rho_{\min} = -18$
−3	0.1961141183	0.196036	0.1961141183
−2	0.1947056966	0.194684	0.1947056966
−1	0.1859129752	0.185912595	0.1859129752
0	0.1444659187	0.14446637	0.1444659187
1	(−2)4.817673854	(−2)4.8176766	(−2)4.817673854
2	(−3)1.017927151	(−3)1.0179235	(−3)1.017927151
3	(−9)7.833876174	(−9)9.2879	(−9)7.8338745

In general, the choice of intervals for the ρ and t integrations and the choice of $\Delta\rho$ and Δt must be dictated by the particular problem. One must choose $\rho_{\min}$ and $\rho_{\max}$ so that the ρ integrand is acceptably small at the ends of the interval. This will approach zero very rapidly as $\rho \to \infty$ unless $f(r)$ is of very long range, e.g., $f(r) \sim r^{-1}$, and the choice of $\rho_{\max}$ need present no difficulty. The choice of $\rho_{\min}$ may give a slight problem in the case $f(0) \neq 0$. In this case, it may be desirable to subtract a function whose

transform is known, e.g., $f(0)\ e^{-\alpha r}$, to improve the rate at which the integrand approaches zero as $\rho \to -\infty$.

The choice of $\Delta\rho$ is dictated, qualitatively, by the "smoothness" of $f(r)$ with an ill-behaved function requiring a small $\Delta\rho$. The FFT is most effectively implemented if $\Delta\rho = (\rho_{\max} - \rho_{\min})/2^n$, however.

The Nyquist interval $(-T/2,\ T/2)$, $T = 2\pi/\Delta\rho$, dictated by the use of the FFT is natural since the asymptotic behavior of $\phi(t)$ in Eqs. (3b), (14), and (20) is also governed by the smoothness of $f(r)$; if $f(r)$ is well behaved $\Delta\rho$ is not required to be too small, and $T = 2\pi/\Delta\rho$ need not be too large.

The choice of Δt in the t integration is dictated by the 'bandwidth' of the result $\hat{g}(\kappa)$; the FFT choice of $\Delta t = 2\pi/(N\Delta\rho)$ corresponds to $\hat{f}(\rho)$ and $\hat{g}(\kappa)$ having the same bandwidth. This is not unreasonable since κ and ρ are dimensionless variables, and it is also suggested by the convolution integral in Eq. (2).

4. Discussion

It is envisaged that the methods described in this article will be of considerable value in calculations in which large numbers of Fourier sine or cosine transforms, or Bessel, or spherical Bessel transforms are required for functions given either analytically or in tabular form. The latter possibility is important because other techniques, to be discussed, require analytic expressions for $f(r)$ or the values of $f(r)$ at special points. The method can therefore be applied if, for example, $f(r)$ is the numerical solution of a differential or integral equation.

It may be objected that the method assumes the evaluation of the function at the data points uniform in $\ln r$ rather than r. However, in many calculations, it can be arranged to use $\rho = \ln r$ as the variable throughout, and indeed, in many calculations, e.g., atomic structure calculations [11], ρ and κ are the natural variables to use.

In a large scale calculation it may be assumed that all the auxiliary quantities, i.e., trigonometric functions and $\Phi_1(t)$, $\Phi_2(t)$, are calculated and stored initially. The calculation of a transform is then reduced to the calculation of two Fourier transforms which may be carried out by FFT and require computing time proportional to $N \ln N$. There are also complex multiplications to be carried out that are proportional to N in number. This is comparable to the time that would be required by Filon's method, which could also be reduced to two applications of the FFT, one at the even, and one at the odd data points.

The principal difficulties in dealing with integrals such as those in Eqs. (1), (11), and (18) arise at large values of k for which the integrand oscillates rapidly and large cancellations occur. (As has been remarked, for small k the integral can be dealt with readily by classical methods.) A study of techniques for dealing with such integrals has recently been made by Blakemore, *et al.* [12] (to be referred to as BEH), who conclude that the optimum scheme is the partition-extrapolation method. In this method the integration is performed over successive half-cycles of the integrand using Gaussian integration for a trigonometric weight function and the resulting

integrals are summed using a technique for accelerating the convergence (ϵ-algorithm). Three of the examples (I_1, I_3, I_9) considered by BEH correspond to the examples considered here. The number of function evaluations required to obtain 9 figure accuracy in the result have been ascertained by BEH and been found to range from about 40 for e^{-r} to about 70 for $(1 + r^2)^{-3}$. This seems to be much better than the 64 function evaluations to obtain about 6 decimal accuracy and 256 evaluations to obtain about 10 decimal accuracy in the present scheme. The partition-extrapolation method suffers the drawback, however, that the points at which the function $f(r)$ is to be evaluated depend on the value of k and seems therefore not to be suitable if the function is given in tabular form or if the transform is required at many k values. The method also seems to be most directly applicable to trigonometric integrals for which the zeros of the integrand are immediately available. Another scheme considered by BEH, the Chebyshev expansion method [10], avoids the difficulty that the evaluation points depend on k, but also requires special evaluation points for $f(r)$. This method was found to be very effective in the example $f(r) = e^{-r}$ considered in Table I; it was found to yield accuracy comparable to the $N = 256$ calculation using only 41 data points on the interval $0 \leqslant r \leqslant 25$. It may be noted though that in a related calculation, to evaluate

$$\int_{-\infty}^{\infty} \exp(\tfrac{3}{2}\rho - e^{\rho})\, e^{it\rho}\, d\rho = \Gamma(\tfrac{3}{2} + it),$$

it was found to yield only about 5 figure accuracy using 41 data points on the interval $-15 \leqslant \rho \leqslant 3$.

The cutoff in the t integration at $t_{\max} = N\Delta t/2$ seems rather arbitrary and it might be though that the sharp cutoff would introduce some error and that the method could be improved by smoothing the cutoff. This was attempted by using the smoothing function $2(1 - \cos ht)/(ht)^2$ where $h = \Delta\rho$. This is not an arbitrary choice but is the factor that is obtained if a "lowest-order Filon's" calculation is made for the Fourier transform in ρ. By lowest order we mean that the function to be transformed is fitted by linear segments and the Fourier transform calculated analytically. The result of this smoothing procedure was a remarkable loss of accuracy, to about 1 %. It appears that it is important to use the trapezoidal rule in the integrations and to cut off the t integration in the way which was done.

It is not clear why this particular integration scheme is so effective, but two remarks may be of interest. The method that has been followed should be in principle exact for functions of the form

$$f_\alpha(r) = r^{-\frac{1}{2}+i\alpha}, \tag{36}$$

where $\alpha = 2\pi n/R$, $n = 0, \pm 1, \ldots \pm N/2$, $R = r_{\max} - r_{\min}$. The Fourier sine transform of $f_\alpha(r)$ is

$$g_\alpha(k) = 2\pi M(\alpha)^* k^{-\frac{1}{2}-i\alpha}. \tag{37}$$

The orthogonality condition,

$$\sum_{n=0}^{N-1} e^{2\pi mni/N} = N, \qquad m = 0, \pm N, \pm 2N, \ldots,$$
$$= 0, \qquad \text{otherwise}, \tag{38}$$

can be applied if the trapezoidal rule of integration is used and the result follows. The method should then of course also be exact for any linear combination of the function $f_\alpha(r)$. The second remark also stems from the orthogonality property of Eq. (38) and is that the numerical transform is in principle its own inverse (apart from the factor $\pi/2$) as is the exact sine transform. It has been confirmed numerically that the twice iterated sine transform is much more accurate than the single sine transform.

The present method would probably not be suitable for functions $f(r)$ which are themselves oscillatory. For example, it would not be reasonable to apply it to the case $f(r) = J_0(r)$ because of the linear increase of Δr which would obscure the oscillations. In this case, other methods would also run into difficulty. It is probably also not directly applicable to functions that are discontinuous or have discontinuous derivatives. In such a case an important feature of the Fourier transform is the long range oscillatory tail and this would be obscured by the linear increase of Δk.

It has been pointed out to the author by J. W. Cooley that even more efficient methods than the FFT exist for carrying out numerical convolutions such as Eq. (2) using number theoretic transforms [13]. The effectiveness of such methods would probably be limited, however, because functions of the form $\sin(e^\rho)$ would be treated numerically and the rapid oscillation at large ρ values would apparently limit the accuracy obtainable.

In conclusion, it is felt that the present method is attractive because it is simple to implement computationally, because it permits the use of the FFT, because it applies to functions given in tabular form and because it also applies to Bessel and spherical Bessel transforms. It is also invariant to changes in scale in the direct and transform variables, if the range of the ρ integration is chosen sufficiently liberally, which makes it valuable in atomic structure calculations.

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