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Evaluation of Fourier transforms by Gauss–Laguerre quadratures

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Abstract. Numerical schemes for the evaluation of Fourier transforms with Gauss–Laguerre quadratures are presented. These schemes which incorporate functional values at complex arguments are tested for efficacy and accuracy. We illustrate their effectiveness on a simple model system by computing the form factor and its Laplacian for the neon atom.

1. Introduction

The numerical evaluation of Fourier transforms is an important problem in many areas of physics and chemistry. This transform is usually approximated by some quadrature rule. However, due to the oscillatory behaviour of the integrand and the infinite range of the integral, extreme care must be exercised especially for larger values of the frequency. This may necessitate the use of a large number of functional evaluations in the particular quadrature scheme. Thus the computational burden is enhanced. In this article we study the convergence properties of methods which involve simple transformations into the complex plane, in order to assess the capability of these methods in producing accurate results for physically significant systems. These methods, which approximate the Fourier transform by the Laplace integral, seem to have been first suggested by Wong [1] (method I), and Feuillebois [2] has recently made these methods more specific (method II) for transforms of functions with an explicit exponential dependence. We will show how these methods may be adapted to be even more specific (method III) for functions with exponential *behaviour*. We illustrate these points with our example of the computation of atomic form factors. Note that atomic units of length a_0 (Bohr) ($= 0.529177 \times 10^{-10}$ m) are used throughout this article. The values of the momentum transfer are therefore given in units of a_0^{-1} ($= 1.889727 \times 10^{10}$ m^{-1}).

2. Methodology

Let us consider the Fourier transform

$$F(k) = \int_0^\infty g(r)f(r)e^{ikr}\,dr. \tag{1}$$

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Feuillebois [2] has recently shown that for $g(r) = e^{-r}$ and the change of variable $z = (1 - ik)r$ (equation (1)) may be expressed as

$$F(k) = \frac{1}{1 - ik} \int_0^\infty f\left(\frac{z}{1 - ik}\right) e^{-z}\, dz \tag{2}$$

provided that $f(z/(1-ik))$ is analytic in the respective complex domain. The integral in equation (2) is ideally suited for integration with a Gauss–Laguerre quadrature since the factor e^{-z} is included in the weights. Thus, equation (2) may be approximated by

$$F(k) = \frac{1}{1 - ik} \sum_{j=1}^{N} f\left(\frac{z_j}{1 - ik}\right) w_j + E_N(f) \tag{3}$$

where z_j, w_j are the abscissae and weights of the N-order Gauss–Laguerre rule and E_N is the error in the quadrature approximation. These rules may be constructed from the corresponding Laguerre polynomials which are orthogonal with respect to the weight function e^{-z} [3] (method II).

On the other hand Wong [1] has shown that for $g(r) = r^m$, with $m > -1$, and the change of variable $z = -ikr$, the transform may be expressed as

$$F(k) = \left(\frac{i}{k}\right)^{m+1} \int_0^\infty f\left(\frac{iz}{k}\right) z^m e^{-z}\, dz. \tag{4}$$

The integral in equation (4) may be approximated with a *generalized* Gauss–Laguerre quadrature

$$F(k) = \left(\frac{i}{k}\right)^{m+1} \sum_{j=1}^{N} f\left(\frac{iz_j}{k}\right) w_j + E_N(f) \tag{5}$$

where z_j, w_j are now the abscissae and weights of *generalized* Gauss–Laguerre quadratures, i.e. obtained from the orthogonal polynomials with weight function $z^m e^{-z}$ and E_N is the corresponding error term (method I).

If one combines these two methods and further considers $g(r) = r^m e^{-\alpha r}$, where α is a positive real parameter and imposes the variable change $z = (\alpha - ik)r$, one arrives at the relationship

$$F(k) = \left(\frac{1}{\alpha - ik}\right)^{m+1} \int_0^\infty f\left(\frac{z}{\alpha - ik}\right) z^m e^{-z}\, dz \tag{6}$$

which may be treated with *generalized* Gauss–Laguerre quadratures as in the case of equation (5), i.e.

$$F(k) = \left(\frac{1}{\alpha - ik}\right)^{m+1} \sum_{j=1}^{N} f\left(\frac{z_j}{\alpha - ik}\right) w_j + E_N(f) \tag{7}$$

where z_j, w_j are the abscissae and weights of the corresponding N-order *generalized* Gauss–Laguerre quadrature (method III).

The atomic form factor, $F(k)$, is one of the most important quantities in experimental structure determination and can be obtained from elastic x-ray and electron scattering experiments [4]. It may be expressed as

$$F(k) = 4\pi \int_0^\infty r^2 \rho(r) \frac{\sin(kr)}{kr} \, dr \tag{8}$$

where $\rho(r)$ is the spherically averaged one electron density. Equation (8) may be re-formulated as

$$F(k) = \frac{4\pi}{k} \mathrm{Im} \left\{ \int_0^\infty r\rho(r) e^{ikr} \, dr \right\}. \tag{9}$$

Thus we may utilize equation (9) to compute atomic form factors via the three methods we have discussed. For method I, $g(r) = r$, thus we may utilize equation (5) with $f(z) = \rho(z)$, and use the *generalized* Gauss–Laguerre quadratures with $m = 1$. It is known [5] that Gauss–Laguerre quadratures may be used to integrate functions over the interval $[0,\infty]$, which have no explicit exponential character, but which possess a general exponential type behaviour,

$$\int_0^\infty f(x) \, dx = \sum_{j=1}^{N} h(x_j) w_j + E_N(h) \tag{10}$$

where $h(x)$ is defined as $f(x)e^x$, and x_j, w_j are the abscissae and weights of the corresponding quadratures. This technique has in fact been recently used for the evaluation of some integrals over $[0,\infty]$ arising in density functional theory [6]. It has also been used in the numerical determination of the *generalized* Fermi–Dirac integrals arising in astrophysical phenomena [7]. Since the density has an exponential type behaviour we may employ this technique in methods II and III. Thus we use $z\rho(z)e^z$ in equation (3) and $\rho(z)e^{\alpha z}$ in equation (7).

As a second test we compute $\nabla^2 F(k)$, the Laplacian of the form factor. This function has recently been shown to be able to extract salient information from atomic form factors, and is defined as [8]

$$\nabla^2 F(k) = \frac{4\pi}{k} \int_0^\infty r^3 \rho(r) \sin(kr) \, dr. \tag{11}$$

Thus $\nabla^2 F(k)$ may be computed by taking the imaginary part of the results of the three methods of Fourier integration in a manner analagous to the one for $F(k)$, with the exception that $m = 3$ for $\nabla^2 F(k)$ in the corresponding *generalized* Gauss–Laguerre quadratures.

3. Results and discussion

We have computed the atomic form factor of neon using the three methods with a variety of different orders of Gauss–Laguerre and *generalized* Gauss–Laguerre quadratures. The charge density used in equations (3), (5) and (7) were computed from the near Hartree–Fock wavefunction of Clementi and Roetti [9]. We chose to study form

factors since analytical formulae are readily available [10] (and references therein). Thus this test system provides us with an effective means of judging the performance of the quadratures. We treat the results obtained from the analytical formulae as *exact* in order to compute the relative error of the quadratures. All computations were performed in double precision on a SUN 3/50 computer which yields about fifteen figures of accuracy. Our quadrature formulae were checked to be accurate to fourteen figures. The computations for methods I, II and III were done in double precision complex arithmetic.

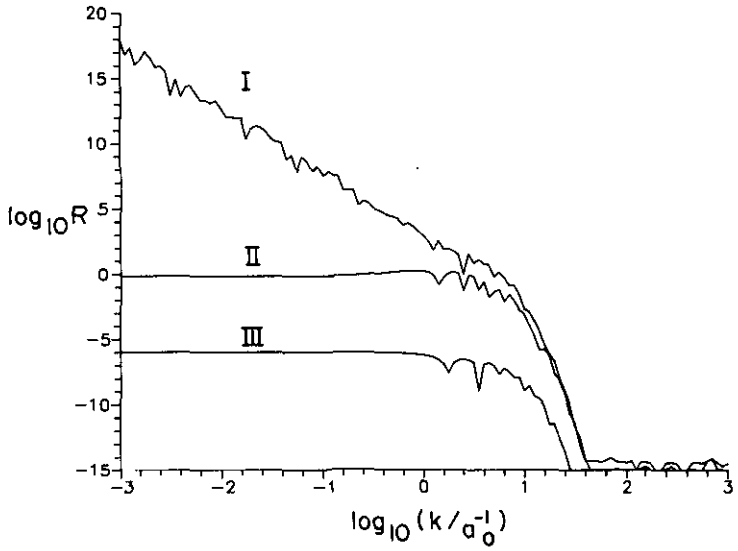

Figure 1. *Plot of the relative error, R,* in the neon form factor as a function of k for the three different methods using 16 point Gauss–Laguerre quadratures. Note that in this and the following figures we have included fifteen significant figures although our quadratures are good to fourteen figures.

In figure 1 we study the performance of the respective methods at 120 equally spaced values of $\log_{10} k$. We used the 16 point Gauss–Laguerre and the *generalized* Gauss–Laguerre (with $m = 1$) quadratures for this study. The value of the real parameter, α, in method III was arbitrarily chosen to be seven since the normalization condition of $F(0) = N$ (the number of electrons), was quite closely met for this value as k approached zero. The results show that method III is by far the best for the presented range of k. However, the other two methods are seen to exhibit similar performances between the first and second orders of magnitude of k. What is perhaps most interesting is that all of these methods perform better for larger values of k, precisely where problems are encountered in the conventional treatments due to the highly oscillatory nature of the integrand. On the other hand, only method III offers any reasonable accuracy at small k. The reader must be reminded that we are using a relatively small (16 point) quadrature, i.e. even greater accuracy should be converged upon with a larger order quadrature. We illustrate this fact in figure 2 for $k = 1\ a_0^{-1}$ and $k = 10\ a_0^{-1}$ We used 2, 4, 6, 8, 12, 16, 24 and 32 point quadratures in this study. We observe that at least for method III one may obtain higher accuracy by increasing the order of quadrature. Indeed, for $k = 1\ a_0^{-1}$, a 32 point quadrature will yield a result very close to the maximum accuracy possible. This is not true

for methods I and II as very little accuracy is gained by increasing the order which possibly indicates that the results are very near the threshold of best possible accuracy for the respective methods and this value of k. For $k = 10\ a_0^{-1}$, the accuracy does improve with increasing order of quadrature for all three methods, with method II yielding better results than method I.

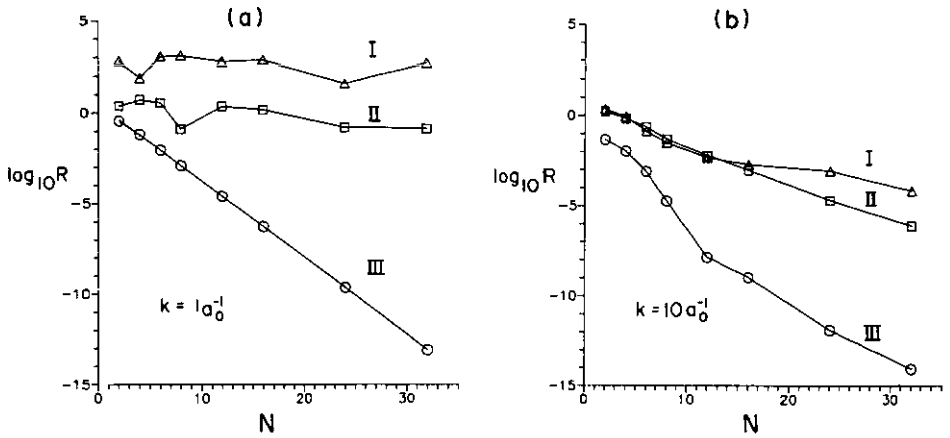

Figure 2. Convergence study of the quality of quadrature approximations to the neon form factor obtained from the three methods as a function of the order of quadrature for (*a*) $k = 1\ a_0^{-1}$ and (*b*) $k = 10\ a_0^{-1}$.

Figures 1 and 2 have established that method III is by far superior for a greater range of k. However, central to this method is the choice of the parameter α. Thus we need to study the performance of the method with different values of this parameter. This information is presented in figure 3. Two points should be immediately obvious: First, the quality of the result is quite dependent on the choice of α. Second, since the curves for different values of α cross, it would seem that the optimum choice of α depends on which region of k one is interested in, i.e. there is no α which is universally the best for the whole range of k. However a judicious choice of α as illustrated by the plot will yield good results. If the normalization is known, one might suggest a procedure which chooses α so that as k gets small, the value of $F(k)$ approaches the normalization $F(0)$.

Lastly, we have performed an analagous analysis on $\nabla^2 F(k)$ and we present the results in table 1 for the 16 point quadratures. Although all three methods are seen to perform similarly for large k, this is not true for small k. Method III is clearly superior although the differences between it and the other two methods are less pronounced than in the case of the form factor.

4. Conclusions

We have presented an extension of powerful and simple methods for the numerical evaluation of Fourier transforms and have illustrated this by computing the atomic form factor and the Laplacian of the form factor for neon, from the charge density. This method is generally applicable to the extent that it may be used whenever the function to be transformed has an exponential type behaviour. The only restriction

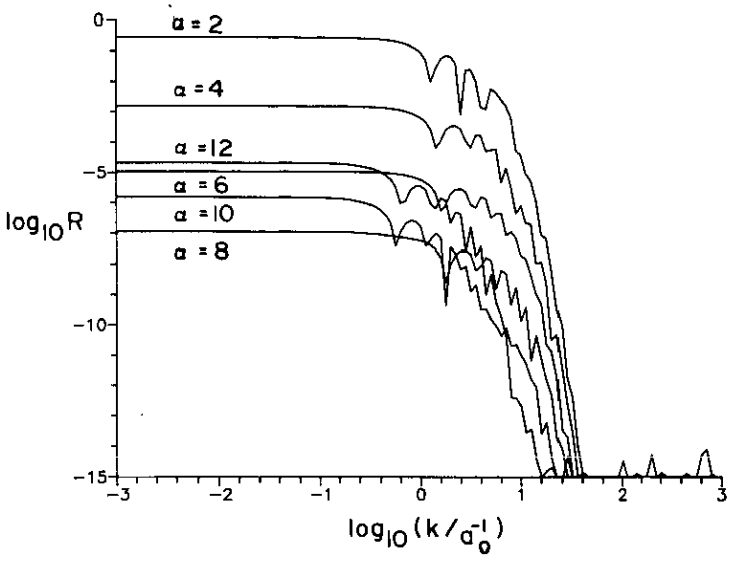

Figure 3. A study of the error obtained from the use of different values of α in method III, as a function of k, for the neon form factor. The 16 point Gauss–Laguerre quadratures were used.

Table 1. The logarithm of the relative error† in $\nabla^2 F(k)$ with the use of the 16 point Gauss–Laguerre quadratures at various k values for the three different methods.

k/a_0^{-1}	Method III	Method II	Method I
0.001	−6.672	−1.670	24.879
0.010	−6.672	−1.670	17.642
0.100	−6.678	−1.750	10.905
1.000	−6.826	−1.350	3.228
10.00	−7.848	−1.447	−0.418
100.0	−14.185	−15.000	−14.185
1000	−14.268	−15.000	−14.268

† Note that the logarithms of all relative errors with an absolute value $\leqslant 10^{-15}$ are reported as −15.000.

is that the function must be analytic in the complex domain and be readily evaluated at complex arguments.

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