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NOTE

Spherical Bessel Transforms

A method for the calculation of spherical Bessel transforms is presented which requires the evaluation of two numerical integrals, one of which is a fast Fourier (sine) transform, without the explicit use of the Bessel functions. With emphasis on transforms of relatively high order, the procedure is shown to have a practical and accurate application in the calculation of radial momentum-space wave functions from the corresponding position-space functions. Examples used are high angular momentum states of the hydrogen atom and rovibrational states of the diatomic molecule RbCs. © 1993 Academic Press, Inc.

1. INTRODUCTION

Computational methods for evaluating integral transforms are required in a variety of applications in chemistry, physics, and engineering [1]. In this contribution to the subject, we are concerned with the problem of computing radial momentum-space wave functions for central potentials through the spherical Bessel transform of the corresponding function obtained by solving the appropriate radial Schroedinger equation in position space. The need for fast, efficient, and accurate algorithms for this purpose has arisen, for example, in the description of atomic and molecular stationary states in momentum space [2] and in the larger problem of simulating wave-packet propagation on potential surfaces [3]. Notable among the existing methods is that of Talman [4], which converts the problem to the evaluation of two Fourier transforms by use of logarithmic spatial and momentum variables. It is therefore restricted to applications where such grids are suitable; it is not recommended for very oscillatory functions, and it appears to be most useful for transforms of low order. (These conditions are usually met in atomic structure calculations.) Other specialized methods have been presented by Sommer and Zabolitsky [5] and by Puoskari [6]. Our approach was developed as part of an investigation of the momentum-space characteristics of rovibrational states and Franck–Condon transitions of diatomic molecules [7, 8], for which linear grids are appropriate and transforms of relatively high order are sometimes needed. As outlined below, the method is closely related to one used by Sun *et al.* [9] in close coupling-wave packet calculations on atom–diatom collisions, but it is different in essential details. The following section shows how the problem of generating the spherical Bessel functions and the associated integral transform is replaced by two numerical integrals, one of which is amenable to FFT methods and the other requires some straightforward complex algebra and a standard quadrature formula. The remaining section presents some numerical examples of high-order transforms for large angular momentum states of the hydrogen atom and the molecule RbCs, followed by a short discussion.

2. METHOD

The radial wave functions of a central potential in position and momentum spaces, $R_{n,l}(r)$ and $\tilde{R}_{n,l}(p)$, are related by the spherical Bessel transform

$$\tilde{R}_{n,l}(p) = (2/\pi\hbar)^{1/2} \int_0^\infty (pr/\hbar)\, j_l(pr/\hbar)\, R_{n,l}(r)\, dr \qquad (1)$$

and the analogous inverse relation, where $j_l(z) = (\pi/2z)^{1/2} J_{l+1/2}(z)$ is the spherical Bessel function of order l (the angular momentum quantum number of the state) [8]. Similar to the procedure of Ref. [9], the first step of the method is insertion of unity in the form $(pr/\hbar)^l e^{-\alpha(pr/\hbar)}(pr/\hbar)^{-l} e^{\alpha(pr/\hbar)}$ into the integrand of Eq. (1), such that

$$\tilde{R}_{n,l}(p) = \hbar^{-1/2} \int_0^\infty [(pr/\hbar)^{l+1/2} e^{-\alpha(pr/\hbar)} J_{l+1/2}(pr/\hbar)] \times [(pr/\hbar)^{-l} e^{\alpha(pr/\hbar)} R_{n,l}(r)]\, dr \qquad (2)$$

where α is a dimensionless parameter; followed by definition of two functions of a dimensionless transform variable x, $A_l(x)$ and $B_{n,l}(x, p)$, through the relations

$$(pr/\hbar)^{l+1/2} e^{-\alpha(pr/\hbar)} J_{k+1/2}(pr/\hbar) = \int_0^\infty \sin(xpr/\hbar)\, A_l(x)\, dx \qquad (3)$$

and

$$(pr/\hbar)^{-l} e^{\alpha(pr/\hbar)} R_{n,l}(r) = (2p/\pi\hbar^{1/2}) \int_0^\infty \sin(xpr/\hbar)\, B_{n,l}(x, p)\, dx. \qquad (4)$$

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Inversion of Eqs. (3) and (4) with aid of the relation

$$\int_0^\infty \sin(xpr/\hbar)\sin(x'pr/\hbar)\,dr = (\pi\hbar/2p)\,\delta(x-x') \tag{5}$$

gives

$$A_l(x) = (2p/\pi\hbar)\int_0^\infty \sin(xpr/\hbar)(pr/\hbar)^{l+1/2} \times e^{-\alpha(pr/\hbar)} J_{l+1/2}(pr/\hbar)\,dr \tag{6}$$

$$= (2/\pi)^{3/2}\,2^l l!\,\mathrm{Im}[(\lambda+x)(\lambda^*-x)]^{-(l+1)}, \tag{7}$$

where $\lambda = 1 + i\alpha$ and

$$B_{n,l}(x,p) = \hbar^{-1/2}\int_0^\infty \sin(xpr/\hbar)(pr/\hbar)^{-l}\,e^{\alpha(pr/\hbar)} R_{n,l}(r)\,dr. \tag{8}$$

The analytical form expressed by (Eq. (7) was derived with the help of an integral discussed by Watson [10].

In terms of the functions $A_l(x)$ and $B_{n,l}(x, p)$, the spherical Bessel transform expressed by Eq. (1) is given by

$$\tilde{R}_{n,l}(p) = \int_0^\infty A_l(x)\,B_{n,l}(x,p)\,dx. \tag{9}$$

While the notation used in this work is appropriate for transformations of radial wave functions between position and momentum spaces, the procedure is applicable to any spherical Bessel function transform, given that various forms of the integrals can be written by factoring powers of the transform variables from the integrands. Equation (9) is the working relation of our method, but it is also worth noting the equivalent form

$$\tilde{R}_{n,l}(p) = (2/\pi)^{3/2}\,2^{l-1} l!\,\mathrm{Im} \times \int_{-\infty}^{+\infty} \frac{B_{n,l}(x,p)}{[(\lambda+x)(\lambda^*-x)]^{l+1}}\,dx, \tag{10}$$

which we have found useful for deriving the transforms of elementary functions via the residue theorem.

A Fortran program was written using the FFT algorithms of Ref. [11] for the evaluation of Eq. (8) and Simpson's $\frac{1}{3}$-rule for the evaluation of Eq. (9). For a given value of the momentum, the FFT returns the values $B_{n,l}(x_k, p)$ at the points

$$x_k = k(\pi/pN\,\delta r) \tag{11}$$

for $k = 1, 2, \ldots, N$, where N (a power of 2) is the order of the FFT and δr is the interval on the linear grid of the spatial function ($r_j = r_0 + j\,\delta r$, with $j = 0, 1, \ldots, N_r$). Zero-filling was used to extend a function being transformed if its tabulated values have decayed to zero and $N_r < N$. As the above relations indicate, the approximate quadrature of Eq. (9) requires a grid-size $\delta x = \pi/pN\,\delta r$ and the calculation of the quantities $A_l(x_k)$ at the grid points. The choice of the parameter α is an ambiguous step in implementing the method, and it was made by trial-and-error. This was not difficult because a particular calculation was reproduced with a range of values, but it was usually not possible to span the full range of a transformed function with the same value.

For comparison, a second Fortran program was written which calculates $\tilde{R}_{n,l}(p)$ directly from Eq. (1) by Simpson's $\frac{1}{3}$-rule, with the spherical Bessel functions generated by the standard method of backwards iteration of the recurrence relation [12]. Calculations were very time-consuming by this method if the program called a subroutine to give $j_l(z)$ with arbitrary order and argument, so we used a procedure which presupposes a uniform sequence of arguments $z_i = i\,\delta z$ with $i = 1, 2, \ldots, M$. Beginning with z_1, j_l is calculated by iterating backwards, using orders $l+1$ and $l+2$ and, again, using orders $l+2$ and $l+3$. If the two results differ within a specified tolerance, then the procedure is continued until the required accuracy is obtained on comparing the results using orders $l+m-1$ and $l+m$, and $l+m$ and $l+m+1$. In general, the value of m that passes the tolerance test at one point in the sequence is passed on to begin the backwards recurrence at the next point. The efficiency of this scheme is reflected in the slow increase of m across the sequence.

3. NUMERICAL EXAMPLES AND DISCUSSION

As a simple test of the above method, we used it to calculate the momentum-space wave function for the state of the hydrogen atom with the highest angular momentum ($l = n-1$) within a particular level in its spectrum, for which [13] (atomic units have been used in all examples)

$$R_{n,n-1}(r) = \frac{(2r/n)^n}{n[(2n-1)!]^{1/2}}\,e^{-r/n} \tag{12}$$

and

$$\tilde{R}_{n,n-1}(p) = [2/\pi(2n-1)!]^{1/2}\,n!\,\frac{(4np)^n}{[1+(np)^2]^{n+1}}. \tag{13}$$

The function $B_{n,n-1}(x,p)$ derived from Eqs. (8) and (12) can be shown by elementary methods to be given by the expression

$$B_{n,n-1}(x,p) = \frac{(2/np)^{n+1}}{[(2n-1)!]^{1/2}}\,\frac{(1/np-\alpha)x}{[(1/np-\alpha)^2+x^2]^2}. \tag{14}$$

TABLE I

Test on $l = n - 1$ States of the Hydrogen Atom

n	r_0	δr	N_r	N	Relative error
20	0	25	60	64	3.85(−4)
20	0	25	60	128	1.48(−12)
40	0	75	70	128	2.40(−12)
60	0	125	80	128	3.95(−12)
80	3000	175	90	128	3.61(−12)
100	7000	250	100	128	3.65(−11)
100	7000	250	100	256	2.23(−11)
100	7000	250	100	512	5.75(−11)

It is worth noting that Eq. (13) is obtained from Eqs. (10) and (14) by determining the residue of a single pole of order 2 at $z = i(1/np - \alpha)$ arising from $B_{n,n-1}(z, p)$. The poles of order n arising from $A_{n-1}(x)$ can be avoided.

Results for calculations at $p_{\max} = [n(n+2)]^{-1/2}$, the momentum at the peak of $\tilde{R}_{n,n-1}(p)$, are given in Table I. It was found to be necessary to make α depend on momentum, with the form $\alpha = c/np$ and $c = 0.80$ giving good results. The relative error is with respect to the exact value given by Eq. (13) and the figure in brackets is an exponent of 10. Calculations of accuracy comparable to the 128-point transform were obtained by the direct method with very similar cpu requirements. Table I illustrates the viability of the alternate method for high-order transforms of relatively simple functions.

A much more demanding test of the method was conducted by calculating the momentum-space wave functions for various rovibrational states of the diatomic molecule (RbCs. The functions $R_{n,l}(r)$ were obtained by Numerov integration of the radial Schroedinger equation [8] using Rydberg–Klein–Rees (RKR) potentials for several electronic states of this molecule [14]. Figure 1 and Table II illustrate some calculations on the ($n = 10$, $l = 40$) and ($n = 52$, $l = 104$) states of the ground electronic configuration, which are exhibited simply to demonstrate the capabilities of the method. The latter is the final state of a prominant line in the laser-induced fluorescence spectrum from an excited $^1\Pi$ electronic configuration [14]. The main result of this test is that the 4096-point transform is comparable to the direct method in speed and accuracy for functions of the degree of complexity illustrated in the figure.

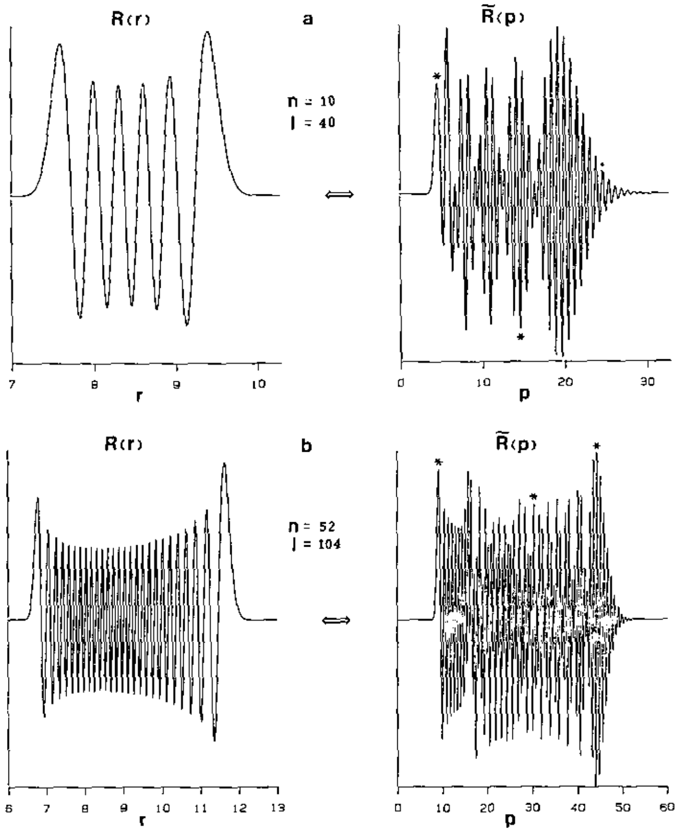

FIG. 1. Position and momentum radial wave functions for rovibrational states of $X^1\Sigma^+$ RbCs: (a) state $n = 10$, $l = 40$; (b) state $n = 52$, $l = 104$. The calculations listed in Table II correspond to the peaks marked with asterisks.

TABLE II

Test on Rovibrational States of the RbCs Molecule

n	l	δr	p	α	N	$\tilde{R}_{n,l}(p)$
10	40	0.01	4.60	2.00	1024	0.3264665071
10	40	0.01	4.60	2.00	2048	0.3263464483
10	40	0.01	4.60	2.00	4096	0.3262864768
10	40	0.01	4.60	2.00	8192	0.3262864768
10	40	0.01	4.60	Direct method		0.3262864764
10	40	0.01	14.6	0.50	1024	−0.3927153898
10	40	0.01	14.6	0.50	2048	−0.3924207248
10	40	0.01	14.6	0.50	4096	−0.3923763821
10	40	0.01	14.6	0.50	8192	−0.3923763821
10	40	0.01	14.6	Direct method		−0.3923763820
10	40	0.01	24.6	0.30	1024	0.06597106988
10	40	0.01	24.6	0.30	2048	0.06597616904
10	40	0.01	24.6	0.30	4096	0.06597641777
10	40	0.01	24.6	0.30	8192	0.06597641777
10	40	0.01	24.6	Direct method		0.06597641753
52	104	0.01	9.20	2.00	2048	-1.0×10^4
52	104	0.01	9.20	2.00	4096	0.3390849297
52	104	0.01	9.20	2.00	8192	0.3390849296
52	104	0.01	9.20	Direct method		0.3390849290
52	104	0.01	30.4	0.50	2048	−11.6
52	104	0.01	30.4	0.50	4096	0.2600477135
52	104	0.01	30.4	0.50	8192	0.2600477135
52	104	0.01	30.4	Direct method		0.2600477140
52	104	0.01	44.4	0.30	2048	0.3728258015
52	104	0.01	44.4	0.30	4096	0.3733731879
52	104	0.01	44.4	0.30	8192	0.3733731879
52	104	0.01	44.4	Direct method		0.3733731375

The main condition for obtaining an accurate result is that $\delta x = \pi / pN\, \delta r$ must be small enough, and it is interesting to note that increasing N beyond what is needed to ensure that this is the case does not improve the accuracy. This relation also suggests, and the data in Table II show, that the accuracy of a transform of lower N improves with increasing momentum.

In summary, the results presented above show that the FFT-based procedure for computing spherical Bessel transforms, without the explicit calculation of the Bessel functions, is a stable, efficient, and accurate algorithm applicable to both simple and highly oscillatory functions and to transforms of high order. This new scheme is practical and easy to program, and our current implementation of it is comparable in most respects to the method based on backwards recurrence if the latter is programmed efficiently. We have shown that a good way to do this is to pass on the order of the Bessel function needed to initiate the recurrence from one point on the integration grid to the next. The two methods are then similar in their cpu requirements, but the FFT-based method includes the parameter α, the choice of which, although not difficult, is an added complication.

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