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Numerical Evaluation of Spherical Bessel Transforms via Fast Fourier Transforms

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1. INTRODUCTION

The purpose of this article is to describe a new fast Fourier transform (FFT) method for calculating spherical Bessel transforms. The method is based on an expansion representation of the spherical Bessel functions in terms of sine and cosine trigonometric functions, multiplied by polynomials in inverse powers of the argument of the Bessel function [1]. The method should be of value in algorithms in which frequent calculations of spherical Bessel transforms are required at many values of the transform variables, which is frequently the situation in time-dependent scattering calculations. The method makes use of FFTs for which the computing time for each transform scales as $N \log_2(N)$, where N is the number of quadrature points, rather than the N^2 scaling of ordinary numerical quadratures. Also, the explicit evaluation of the spherical Bessel functions is not required in the method. The method differs from that given in the work of J. D. Talman [2, 3] and A. E. Siegmon [4]. In the work of Talman [2, 3] and Siegman [4], a change to logarithmic variables is required to recast the integral transform as a convolution integral, which is then evaluated by FFT procedures. However, as pointed out by Talman, this makes the step size Δr increase proportionally with r and renders the method unsuitable for functions of an oscillatory nature. In particular, the oscillatory nature of the function is lost in the increasing mesh intervals. In essence, the Talman–Siegman method is excellent for bound state wave functions, but it is not suitable for scattering state wave functions [2–4]. This in fact has been our experience and has led us to propose the present method.

In Section 2 the method is described. The numerical tests and results for a central potential scattering problem are briefly summarized in Section 3.

2. METHOD

We are interested in evaluating spherical Bessel transforms of the form

$$g(k) = \int_0^\infty dr r^2 j_l(kr)\, f(r) \tag{1}$$

and the inverse transform

$$f(r) = \frac{2}{\pi} \int_0^\infty dk k^2 j_l(kr)\, g(k), \tag{2}$$

where $j_l(kr)$ is the usual regular spherical Bessel function [1] of integer order, l.

The expansion representation of the spherical Bessel functions is given by [1]

$$\begin{aligned} j_l(kr) = \frac{1}{kr}\Bigg[& \sin(kr - l\pi/2) \\ & \times \sum_{s=0}^{[l/2]} (-1)^s (l+2s)!/(2s)!\,(2kr)^{2s}\,(l-2s)! \\ & + \cos(kr - l\pi/2) \\ & \times \sum_{s=0}^{[l-1/2]} (-1)^s (l+2s+1)!/(2s+1)! \\ & \times (2kr)^{2s+1}\,(l-2s-1)!\Bigg], \end{aligned} \tag{3}$$

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where $[l/2]$ denotes the largest integer less than or equal to $l/2$. The spherical Bessel transform is then computed via fast sine and cosine transforms of the individual terms in the summations. The number of sine transforms is $[l/2]+1$ and the number of cosine transforms is $[(l-1)/2]+1$ which gives a total of $l+1$ transforms. This gives a method which scales, in principle, as $(l+1)\,N\log_2 N$ compared to the N^2 scaling for simple quadratures. Therefore, this expansion method should be more efficient than simple quadrature up to l's of the order of $N/\log_2 N$.

In the implementation of Eq. (3), care must be exercised in obtaining results for values of kr much less than one. As the value of l increases, the finite precision of the computer causes difficulties because the $(kr)^l$ behavior of the $j_l(kr)$ results in Eq. (3) from a delicate cancellation between the portion of the right-hand side of Eq. (3) containing $\sin(kr-l\pi/2)$, and that containing $\cos(kr-l\pi/2)$. As kr decreases, the terms containing higher inverse powers of kr overwhelm all other terms and the result is instability. We remedied this problem for scattering by setting the value of $j_l(kr)$ to zero for $kr \ll 1$. This does not affect the results and leads to a completely stable algorithm. We note that in addition to the fact that $j_l(kr)$, $l>0$, tends to zero as kr becomes small, so also does the wave function for the lth partial wave. Of course, a more precise procedure can be used on a Taylor series representation of the Bessel function at small kr values. This involves more computational effort than our procedure of simply setting the value to zero, an effort which is not justified for our calculations. We note that while the problem of precision in the expansion of Eq. (3) for small kr becomes more significant as l increases, the replacement of $j_l(kr)$ by zero becomes more accurate in this situation.

3. EXAMPLE APPLICATION

This method has been applied to a central potential scattering problem [6, 7]. The tangent of the phase shifts was calculated and accuracy of results and computation times were verified by comparison with those obtained using standard trapezoidal quadrature and a time independent variable phase method [8].

TABLE I

Numerical Run Parameters

Variable	Description	Value
t_{max}	Maximum propagation time	10.0
Δt	Time step	0.005
μ	Reduced mass	1.0
δ	Width of driver packet	0.4
r_0	Initial center of packet in r-space	9.0
k_0	Initial center of packet in k-space	9.0
r_{max}	Maximum value of r-grid	62.71
N	Number of grid points	256, 512
$\Delta r(N=256)$	r-grid step size	0.245
$\Delta r(N=512)$	r-grid step size	0.123
Δk	k-grid step size	0.05
$k_{max}(N=256)$	Maximum value of k-grid	12.8
$k_{max}(N=512)$	Maximum value of k-grid	25.6

The scattering calculation involves solving the time-dependent Lippmann–Schwinger equation for the evolution of a wavepacket describing the scattering of a structureless particle by a spherically symmetric potential, V. The partial wave decomposition is employed, leading to the separate propagation of wavepackets describing the various orbital angular momenta making up the total wavepacket. The propagation equation is given by

$$\begin{aligned}\langle k, l|\,\Psi_l(n\tau)\rangle = [1+i\tau\hbar k^2/4\mu]^{-1}\,\frac{2}{\pi}\\ \times\int_0^\infty dr r^2 e^{-iV(r)\,n\tau/\hbar} j_l(kr)\\ \times\left\{\left(-\frac{i\tau}{\hbar}\right)\sum_{j=0}^{n-1} w_j e^{iV(r)\,j\tau/\hbar}\right.\\ \times\int_0^\infty dk' k'^2(\hbar^2 k'^2/2\mu)\, j_l(k'r)\\ \left.\times\langle k', l|\,\Psi_l(j\tau)\rangle + \langle r|\,\Psi_l(0)\rangle\right\},\end{aligned} \tag{4}$$

where $j_l(kr)$ is a spherical Bessel function, $\langle k, l|\,\Psi_l(n\tau)\rangle$ is the time dependent scattering wave function in k-space, $\langle r|\,\Psi_l(0)\rangle$ is the initial wave function in r-space which we chose as

$$\begin{aligned}\langle r|\,\Psi_l(0)\rangle = (2\pi\sigma^2)^{-1/4}\exp(-[r-r_0]^2/4\sigma^2)\\ \times\exp(-ik_0 r),\end{aligned} \tag{5}$$

and $V(r)$ is the model potential

$$V(r) = -\exp(-r). \tag{6}$$

The other parameters used in the calculation are given in Table I.

The tangent of the phase shift, $\tan(\eta)$, is related to the T-matrix by

$$\tan(\eta) = \frac{iT}{2-T}, \tag{7}$$

and the T-matrix elements are given by

$$T = \frac{4i}{hA(k)}\int_{-\infty}^{\infty} dt e^{iEt/\hbar}\int_0^\infty dr r^2 j_l(kr)\, V(r)\, \Psi_l(r,t), \tag{8}$$

where $A(k)$ is the initial wave packet in k-space.

Each of the calculations consisted of 2000 time step

iterations, and each iteration involves four spherical Bessel transforms. A forward and backward transform was carried out in Eq. (4) to obtain $\langle k, l|\, \Psi_l(n\tau)\rangle$. A third transform is used to transform $\langle k, l|\, \Psi_l(n\tau)\rangle$ to $\langle r|\, \Psi_l(n\tau)\rangle$, and finally the transform in Eq. (8) is carried out. The real and imaginary parts of the transformed function were computed separately, yielding a total of eight transforms performed per time step. Example results are shown in Table II.

The level of agreement among the methods is substantially better than that generally required in comparisons of different methods in scattering. A comparison (not shown) of the level of agreement between the time dependent results with 256 and 512 quadrature points using the expansion method, indicates that they are well converged. We note that the FFT is also based on a simple trapezoidal rule quadrature, so that one may wonder why the numerical results obtained by the PEM and TQM are not identical. They are, in fact, the same for most k and l values. However, the two methods *can* differ because they utilize different algorithms for computing the Bessel functions. Equation (3) is used for the PEM, while a standard recursion is used for the TQM. This difference is expected to be more noticeable for larger l values, and this is seen to be true for the results. However, in most cases, the PEM and TQM results agree more closely with each other than with the VPM results.

TABLE II

Comparison of Tangent Phase Shifts and CPU Times for Two Values of l with $N = 512$, $\Delta k = 0.05$, $\Delta r = 0.123$

		$l = 2$			
k	VPM	TQM CPUT: 15122	% diff	PEM 1889	% diff
2.0	0.2600	0.2597	1.15(−1)	0.2597	1.15(−1)
3.0	0.2288	0.2287	4.27(−2)	0.2287	4.37(−2)
4.0	0.1945	0.1946	5.14(−2)	0.1946	5.14(−2)
5.0	0.1668	0.1672	2.40(−1)	0.1672	2.40(−1)
6.0	0.1451	0.1459	5.51(−1)	0.1459	5.51(−1)
7.0	0.1279	0.1292	1.02	0.1292	1.02
8.0	0.1143	0.1158	1.31	0.1158	1.31
		$l = 8$			
k	VPM	TQM CPUT: 3537	% diff	PEM 2249	% diff
2.0	0.2027(−1)	0.2024(−1)	1.48(−1)	0.2024(−1)	1.48(−1)
3.0	0.4670(−1)	0.4670(−1)	0.00	0.4670(−1)	0.00
4.0	0.6358(−1)	0.6354(−1)	6.29(−2)	0.6354(−1)	6.29(−2)
5.0	0.7159(−1)	0.7166(−1)	9.78(−2)	0.7166(−1)	9.78(−2)
6.0	0.7425(−1)	0.7453(−1)	3.77(−1)	0.7453(−1)	3.77(−1)
7.0	0.7404(−1)	0.7452(−1)	6.48(−1)	0.7452(−1)	6.62(−1)
8.0	0.7229(−1)	0.7292(−1)	8.71(−1)	0.7291(−1)	8.58(−1)

Note. For the TQM and PEM results the percent difference from the VPM results are also given.

TABLE III

Theoretical versus Actual Speed Factor $(SF) = N/(l+1)\log_2 N$

Run	Theoretical SF	SF
$l = 2$, $N = 256$	10.7	4.0
$l = 8$, $N = 256$	3.6	1.4
$l = 2$, $N = 512$	19.0	8.0
$l = 8$, $N = 512$	6.3	2.7

Table II also compares the CPU times for the TQM and PEM, showing that the PEM does yield an enhancement of speed. The TQM scales as N^2, while PEM scales as $(l+1)\,N\log_2 N$. A theoretical speed factor SF is defined as the ratio of these scaling relations. Table III gives a comparison between this theoretical SF and the actual ratio of TQM to PEM CPU times. The reason the theoretical SF and actual SF do not agree is probably that the actual SF is computed using the CPU time for the total calculation, and includes other computations besides the Bessel transform. Thus, the ratio of actual CPU times should only become equal to SF if the Bessel transform dominates the calculation.

In conclusion, we do indeed find that the PEM yields a useful improvement over a straightforward TQM (Newton–Coates) evaluation of the spherical Bessel transform, at least for a significant range of orbital angular momenta and numbers of grid points. Because of the fundamental role played by such transforms in quantum scattering (i.e., any three dimensional, gas phase collision system will require the evaluation of spherical Bessel transforms in some way or another), it is worthwhile to search for new ways to calculate them.

Alternatively, one may seek to reformulate the scattering equations so as to enable one to directly employ FFTs in the propagation algorithm. We are pursuing both options in our research.

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