Journal of Computational Physics 355 (2018) 426–435

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Spherical Bessel transform via exponential sum approximation of spherical Bessel function

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A R T I C L E   I N F O

Article history:
Received 11 June 2017
Received in revised form 11 November 2017
Accepted 13 November 2017
Available online 20 November 2017

Keywords:
Hankel transform
Spherical Bessel transform
Bessel function
Oscillatory integrals
Balanced truncation method

A B S T R A C T

A new algorithm for numerical evaluation of spherical Bessel transform is proposed in this paper. In this method, the spherical Bessel function is approximately represented as an exponential sum with complex parameters. This is obtained by expressing an integral representation of spherical Bessel function in complex plane, and discretizing contour integrals along steepest descent paths and a contour path parallel to real axis using numerical quadrature rule with the double-exponential transformation. The number of terms in the expression is reduced using the modified balanced truncation method. The residual part of integrand is also expanded by exponential functions using Prony-like method. The spherical Bessel transform can be evaluated analytically on arbitrary points in half-open interval.

1. Introduction

In this paper, we consider the integrals transformation of a function $f(r)$ of the form,

$$\tilde{f}_l(k) = \int_0^\infty r^2 f(r) j_l(kr) dr \quad (k > 0), \tag{1}$$

where, $j_l(r)$ is the spherical Bessel function of the first kind of order l. The integral transformation (1) is referred as *a spherical Hankel* or *spherical Bessel transform* (SBT). The SBT appears when the Fourier transform of an angular momentum eigenfunction is considered. Let $\psi(\boldsymbol{r}) = f(r)Y_{lm}(\hat{\boldsymbol{r}})$, where $Y_{lm}(\hat{\boldsymbol{r}})$ is a spherical harmonic. Using the spherical wave expansion of plane wave,

$$e^{-i\boldsymbol{k}\cdot r} = \sum_{l=0}^{\infty} (-i)^l j_l(kr) Y_{lm}(\hat{\boldsymbol{k}}) Y_{lm}^*(\hat{\boldsymbol{r}}), \tag{2}$$

then, the Fourier transform of $\psi(\boldsymbol{r})$ can be written as

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https://doi.org/10.1016/j.jcp.2017.11.016
0021-9991/

$$\tilde{\psi}(\boldsymbol{k}) = \int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi(\boldsymbol{r})d\boldsymbol{r} = 4\pi(-i)^l \tilde{f}_l(k)Y_{lm}(\hat{\boldsymbol{k}}), \tag{3}$$

where $\tilde{f}_l(k)$ is expressed as SBT given in (1). Since the spherical Bessel function $j_l(r)$ is defined in terms of Bessel function $J_\nu(r)$ of half-integer order as,

$$j_l(r) = \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(r), \tag{4}$$

a SBT can be regarded as a special case of *a Hankel transform* (HT) defined as,

$$\tilde{g}(k) = \int_0^\infty r g(r) J_\nu(kr) dr \quad (k > 0). \tag{5}$$

Both HT and SBT are used in many field, including astronomy, optics, electromagnetics, seismology, and quantum mechanics. In particular, SBT is involved in the scattering in atomic or nuclear systems [1], and multi-center integrals arises in atomic and molecular integrals [2].

The straight forward evaluation of integral (1) using conventional numerical integration method, such as the Gauss–Laguerre rule, meets intractable difficulties when k becomes large, because the integrand is highly oscillatory. Several approaches to overcome the difficulty have been proposed. The most efficient approach is the fast SBT method, where the transform is made on a logarithmic mesh for both the r and k in conjunction with variable transformation [3–7]. The integration is performed by two successive application of the fast Fourier transform (FFT). One of the drawback of this approach is the use of logarithmic mesh that most of mesh points are concentrated close to the origin. The fast SBT algorithm on linearly spaced mesh has also developed, where the integral representation of the spherical Bessel function $j_l(r)$ in terms of the Legendre polynomial is used with variable transformation, and the integral is performed via FFT [8]. In these two methods, the values of integral (1) on the predefined mesh points (either logarithmic or linear mesh) can efficiently be evaluated in $O(N \log N)$ operations. On the other hand, an appropriate interpolation or extrapolation is necessary to obtain the integral value for arbitrary points other than the mesh points on real axis. The numerical method for SBT in another direction is to partition the integral (1) into the integrals over subintervals between the zeros of spherical Bessel functions. The integrals on subintervals form an alternating series and can be summed with acceleration method. The advantage of this approach is that one can control the accuracy by adjusting the quadrature points. The drawback is, however, that the computational cost is much higher than that of fast SBT, as the integration has to be performed each value of k. See ref. [9] for the detailed comparison of the performance between these two approaches. Alternative approach for HT using wavelets was also proposed [10,11]. But the method is for HT with integer order and hence it cannot be directly applied to evaluate SBT.

In this paper, a new method for numerical evaluation of SBT at arbitrary points in high accuracy is proposed. The basic idea behind is to fit the integrand $r^2 f(r)$ by sum of analytic functions so that the SBT in (1) can be obtained analytically. The HT algorithm with the similar mind has already reported, where the function $rg(r)$ in (5) is fitted by sum of exponential type functions [12,13]. In our approach, the oscillatory spherical Bessel kernel $j_l(kr)$ is also approximated by an exponential sum with complex parameters. This enable us to evaluate SBT analytically at arbitrary points in half-open interval. The advantage of the present method compared to those in refs. [12,13] is that $r^2 f(r)$ can be expanded by various kind of analytic functions, including algebraic functions, trigonometric functions, exponential functions and combinations of them, as long as $r^2 f(r)e^{-ar}$ can be integrated analytically.

This paper is organized as follows. The theoretical background for the approximation of spherical Bessel kernel via an exponential sum is explained in Sec. 2. The details of the numerical algorithm to obtain exponential sum approximation of spherical Bessel functions numerically is described in Sec. 3.1 and 3.2. The procedure to obtain exponential sum approximation of residual part $r^2 f(r)$ is briefly explained and some results of numerical tests are provided in Sec. 3.3.

2. Exponential sum approximation of spherical Bessel functions

In this section, we are considering the approximation of spherical Bessel kernel $j_l(r)$ by an exponential sum. Let $g(r)$ be a function of the form,

$$g(r) = \sum_{k=1}^{N} c_k e^{-a_k r} \quad (r \geq 0), \tag{6}$$

where $a_k \in \mathbb{C}$, $Re(a_k) > 0$ are distinct complex numbers, and $c_k \in \mathbb{C} \setminus \{0\}$. The function $g(r)$ is a smooth, exponentially decaying function, and it oscillates if $Im(a_k) \neq 0$. Our problem here is to find parameters a_k and c_k with small number of terms M, such that

$$\left| j_l(r) - g(r) \right| < \epsilon \quad (r \geq 0) \tag{7}$$

where $\epsilon > 0$ is a prescribed accuracy of the approximation.