JOURNAL OF COMPUTATIONAL PHYSICS 111, 256-259 (1994)

Numerical Evaluation of Spherical Bessel Functions of the First Kind

ALEKSANDER JABLONSKI

Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warszawa, Poland

Received November 4, 1992; revised July 20, 1993

Calculations of cross sections for elastic scattering of electrons require frequent evaluations of the spherical Bessel functions, $j_l(x)$ and $n_l(x)$, in a wide range of the argument x and the order l. It turns out that the usual algorithms providing the values of the spherical Bessel function of the first kind, $j_l(x)$, have a rather limited range of stability. It is shown that there is no algorithm implementing a single method which can be used in calculations associated with the theory of elastic scattering of electrons. An attempt is made to select different areas of stability from different algorithms in order to create a relatively fast and universal algorithm. © 1994 Academic Press, Inc.

1. INTRODUCTION

The reliable algorithms providing the values of the spherical Bessel functions in a wide range of the argument are required for calculations of parameters describing the phenomenon of electron elastic scattering on atomic potentials [1]. The Schrödinger equation for the elastic scattering event can be transformed into the set of the first-order differential equations which provide the consecutive phase shifts. An example of such a set is [1-3],

$$\delta_l'(r) = -\frac{1}{K}\frac{2m}{\hbar^2} V(r)[\hat{j}_l(Kr)\cos\delta_l(r) - \hat{n}_l(Kr)\sin\delta_l(r)]^2,$$
$$l = 0, 1, 2, \ldots \tag{1}$$

with the initial condition

$$\delta_l(0) = 0,$$

where $K = (2mE/\hbar^2)^{1/2}$ is the length of the wave vector, E is electron energy, m is the electron mass, $V(r)$ is the atomic potential, and r is the distance from the nucleus. The phase function $\delta_l(r)$ approaches the phase shift δ_l asymptotically:

$$\lim_{r\to\infty} \delta_l(r) = \delta_l.$$

The functions $\hat{j}_l(x)$ and $\hat{n}_l(x)$ are the independent solutions of the Riccati-Bessel equation and are related to the spherical Bessel functions, $j_l(x)$ and $n_l(x)$, according to

$$\hat{j}_l(x) = xj_l(x), \qquad \hat{n}_l(x) = xn_l(x).$$

There are other formulations of the scattering problem; however, they also require calculations of the spherical Bessel functions [1, Chaps. 17, 23]. Details concerning the respective algorithms can be found in more recent literature [2, 3]. Similarly, the Dirac equation for the scattering problem can be reduced to a set of the first-order differential equations, and the calculations of the relativistic phase shifts also require determination of the spherical Bessel functions [4, 5]. Calculations of accurate values of the function $n_l(x)$ is relatively easy since the recurrence relations are usually sufficient for this purpose. However, major problems are encountered in developing a universal and reliable algorithm for calculating the functions $j_l(x)$. These problems are considered in detail in the present work.

2. COMPUTATIONAL METHODS

The spherical Bessel functions, $j_l(x)$ and $n_l(x)$, are the independent solutions of the differential equation,

$$x^2\frac{d^2y}{dx^2} + 2x\frac{dy}{dx} + [x^2 - l(l+1)]\,y = 0, \qquad l = 0, 1, 2, \ldots. \tag{A1}$$

The function usually denoted by $j_l(x)$ is called the spherical Bessel function of the first kind. Let us compile and discuss different formulas and algorithms which may be used in calculation of the functions $j_l(x)$.

0021-9991/94 $6.00

2.1. *Series Expansion*

The series expansion has the form

$$j_l(x) = x^l \sum_{n=0}^{\infty} \frac{(-1)^n (x^2/2)^n}{n!\,(2l+2n+1)!!}$$
$$= \frac{x^l}{(2l+1)!!}\left[1 + \sum_{n=1}^{\infty} \frac{(-1)^n (x^2/2)^n}{n!\prod_{k=1}^{n}(2k+2l+1)}\right], \quad (2)$$

where the notation $i!!$, called a double factorial, denotes the product of all odd integers smaller than or equal to i. Equation (2) can be used in calculations of the spherical Bessel functions of the first kind for small values of argument, x.

2.2. *Ascending Recurrence*

A universal method for calculating the Bessel functions, as well as other special functions, involves the recurrence relations. However, such algorithms may be unstable in certain ranges of argument due to accumulation of rounding errors. This problem is addressed in an extensive review by Gautchi [6].

The recurrence relations for the spherical Bessel functions of the first kind are similar to the recurrence relations for other Bessel functions,

$$j_{l+1}(x) = \left(\frac{2l+1}{x}\right) j_l(x) - j_{l-1}(x). \quad (3)$$

The ascending recurrence can be started using the first two spherical Bessel functions

$$j_0(x) = \frac{\sin x}{x}, \qquad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}.$$

2.3. *Descending Recurrence*

The problems associated with error growth in calculations involving the recurrence relations can be avoided in some cases when the Miller algorithm is used, i.e., an algorithm in which calculations proceed in the direction of decreasing values of l [6]. Performance of such an algorithm applied in calculations of ordinary Bessel functions of integer order was discussed by Olver and Sookne [7]. Campbell [8] used the Miller algorithm in calculations of modified Bessel functions of the third kind. An algorithm involving descending recurrence was also recommended for calculations of the functions $j_l(x)$ [9]. We select an arbitrary value of the order $L > l$ and assume that

$$j_{L+1}(x) = F_{L+1} = 0$$
$$j_L(x) = F_L = 1.$$

Using the recurrence relations we obtain the series with descending order

$$F_{L-1}, F_{L-2}, \ldots, F_1, F_0.$$

On comparison of F_0 with the value of the $j_0(x)$ we obtain the proportionality factor p,

$$p = j_0(x)/F_0.$$

If the value of L is sufficiently large we have

$$j_l(x) = pF_l. \quad (4)$$

The Miller algorithm requires a proper choice of the value of L. The following arbitrary rule has been used in the present work

$$L = l + 100.$$

2.4. *Analytical Solution*

The solutions of the Bessel equation can be expressed analytically. The function $j_l(x)$ is given by

$$j_l(x) = \frac{1}{x}\left\{Q_l(x)\sin\left(x - \frac{l\pi}{2}\right) + R_l(x)\cos\left(x - \frac{l\pi}{2}\right)\right\}, \quad (5)$$

where

$$Q_l(x) = \sum_{n=0}^{[l/2]} (-1)^n \frac{(l+2n)!}{(2n)!\,(l-2n)!\,(2x)^{2n}}$$
$$R_l(x) = \sum_{n=0}^{[(l-1)/2]} (-1)^n \frac{(l+2n+1)!}{(2n+1)!\,(l-2n-1)!\,(2x)^{2n+1}}$$

and the square brackets denote the integer part of a given number.

2.5. *Phase and Amplitude Representation*

The spherical Bessel functions can be expressed in terms of the so-called amplitude and phase functions denoted by $D_l(x)$ and $\Delta_l(x)$, respectively [1, p. 200]. This representation is the basis for the most reliable and universal method to calculate the functions $j_l(x)$,

$$j_l(x) = \frac{1}{x} D_l(x) \sin \Delta_l(x), \quad (6)$$

where the amplitude function is calculated from

$$D_l^2(x) = \sum_{n=0}^{l} \frac{1}{x^{2n}} \frac{(l+n)!}{(l-n)!}\left[\frac{(2n-1)!!}{(2n)!!}\right] \quad (7)$$

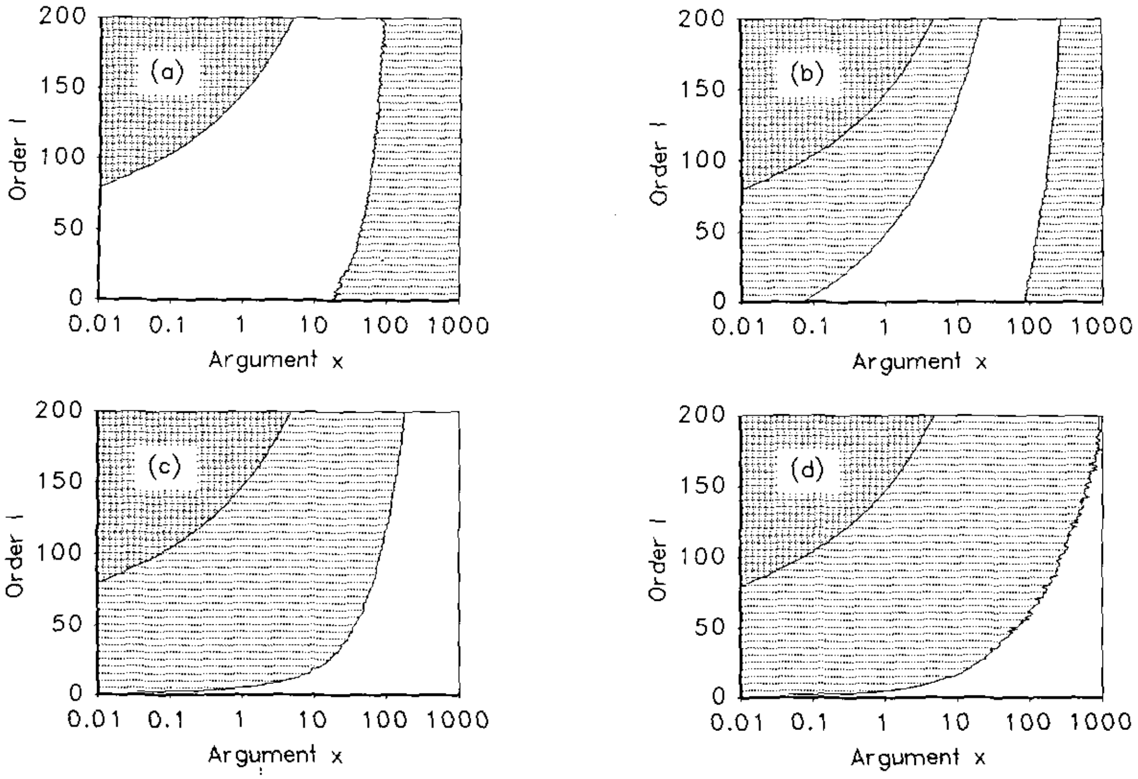

FIG. 1. Accuracy of different algorithms providing the spherical Bessel functions $j_l(x)$. Empty areas: accuracy of 10 decimal places or better; lined area: region of instability; crossed area: the values of the $j_l(x)$ is outside the range of real numbers (smaller than 10^{-300}): (a) series expansion; (b) descending recurrence; (c) ascending recurrence; (d) analytical solution.

and the phase function is defined by

$$\Delta_l(x) = \int_0^x \frac{1}{D_l^2(y)}\, dy. \tag{8}$$

Equations (6)–(8) can be used in a wide range of the argument x and the order l. However, the corresponding algorithm is very slow due to necessity of numerical integration of Eq. (8).

3. NUMERICAL RESULTS

All five algorithms based on Eqs. (2)–(6) were used in the present work in calculations of the functions $j_l(x)$. The argument x varied up to 1000 and the order l up to 200. Calculations were performed with an accuracy of 15 significant decimal places in the range from $\pm 10^{-300}$ to $\pm 10^{300}$, as ensured by the FORTRAN compiler. The phase and amplitude representation (Eq. (6)) provided the reference values of the $j_l(x)$ functions with accuracy of at least 10 significant decimal places. These values were used to check the performance of the other four much faster algorithms. Results of calculations are shown in Figs. 1a–d. The empty areas in these figures denote the range of values of the argument x and the order l for which the accuracy of the function $j_l(x)$ resulting from a given algorithm is equal to at least 10 decimal places. As one can see, none of the fast algorithms considered in the present work is universally valid. In all cases the area of stability of a given algorithm depends on both argument x and order l. The smallest area of stability is found for the analytical solution (Eq. (5)). This equation can be used only in cases when $l \ll x$. Sharafeddin *et al.* [10] mentioned that the algorithm involving Eq. (5) is not stable when the value of the argument is much smaller than unity. As shown in Fig. 1d, the range of stability seems to be much more limited.

We can note on close inspection of Figs. 1a–c that the areas of stability of the remaining three algorithms overlap (the series expansion algorithm and both algorithms involving recurrence). Thus, all three algorithms have to be used to construct the universal and relatively fast algorithm for calculating the functions $j_l(x)$. Figure 2 shows exemplary borders plotted in the middle of the overlapping stability areas. These curves are approximated by the polynomials

$$\ln x_a = a_1 l^3 + a_2 l^2 + a_3 l + a_4 \tag{9a}$$

$$\ln x_b = b_1 l^3 + b_2 l^2 + b_3 l + b_4. \tag{9b}$$

Values of coefficients a_i and b_i are listed in Table I.

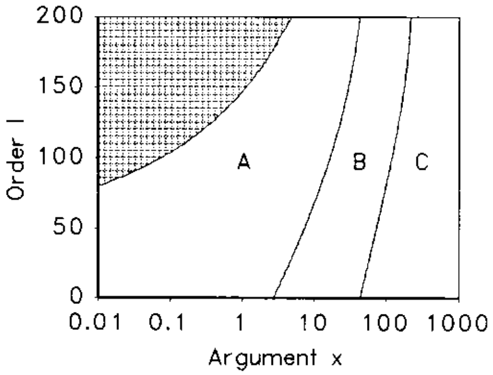

FIG. 2. Exemplary borders between regions of stability of selected algorithms used in construction of a universal algorithm: area A, series expansion; area B, descending recurrence; area C, ascending recurrence; border between areas A and B, Eq. (9a); border between areas B and C, Eq. (9b).

Eventually, the following rule is recommended in calculations of the function $j_l(x)$ for a given value of l and x:

if $\ln x < \ln x_a$ use the series expansion

if $\ln x_a < \ln x < \ln x_b$ use the descending recurrence

if $\ln x > \ln x_b$ use the ascending recurrence.

Availability of a fast and stable algorithm providing the values of the spherical Bessel functions of the first kind is crucial in calculations of the elastic scattering cross sections. The numerical integration of Eq. (1) requires frequent evaluations of the right-hand side containing the spherical Bessel functions, particularly when a reasonable accuracy is required. The use of Eqs. (6)–(8) in these calculations requires an unrealistic amount of computer time.

Let us consider now the range of the argument x and the order l associated with calculations of elastic electron scattering. It has been found that the number of phase shifts necessary for evaluation of the elastic scattering cross sections at energies up to 2 keV may reach 80 [2]. The number of phase shifts increases with energy, considerably exceeding 100 at energies reaching 10 keV. Consequently, reliable values of $j_l(x)$ up to such order l must result from a given algorithm. The argument $x = Kr$ ranges from very small values to a certain value Kr_0. The Thomas–Fermi–Dirac potential is frequently used to approximate the potential $V(r)$ in calculations of elastic scattering cross sections [2, 3]. This potential has a finite radius [11, 12] which may be assumed as the distance r_0. As follows from Eq. (1), the argument of the spherical Bessel functions is related to electron energy. Figure 3 shows this relation calculated at the distance r_0 for carbon and gold, i.e., for elements with low and high atomic numbers. On comparison with Figs. 1a–d and Fig. 2 one can see that, indeed, there is no universal algorithm for calculating the function $j_l(x)$ in the range of variation of the argument Kr. A somewhat simpler situation is in the case of relativistic calculations [2–5]. In that case, the functions $j_l(x)$ are determined only at the edge of the potential, r_0, i.e., along curves shown in Fig. 3. However, even in this case more than one algorithm has to be used to ensure high accuracy of the calculations.

TABLE I

The Fitted Coefficients a_i and b_i for the Polynomials (9a) and (9b) Approximating the Borders of Stability of Algorithms Used in Calculations of the Functions $j_l(x)$

Border between series expansion and the descending recurrence	Border between descending and ascending recurrence
$a_1 = -3.6693021 \times 10^{-8}$	$b_1 = -9.9921351 \times 10^{-8}$
$a_2 = -3.1745158 \times 10^{-5}$	$b_2 = 8.7822303 \times 10^{-6}$
$a_3 = 2.1567720 \times 10^{-2}$	$b_3 = 1.0238752 \times 10^{-2}$
$a_4 = 9.9123380 \times 10^{-1}$	$b_4 = 3.7588265$

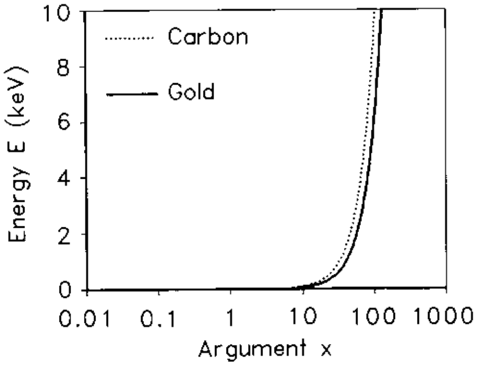

FIG. 3. Relation between the argument x and the electron energy at the edge of the Thomas–Fermi–Dirac potential for selected elements.

REFERENCES

1. F. Calogero, *Variable Phase Approach to Potential Scattering* (Academic Press, New York, 1967).
2. A. Jablonski, J. Gryko, J. Kraaer, and S. Tougaard, *Phys. Rev. B* **39**, 61 (1989).
3. A. Jablonski, *Phys. Rev. B* **43**, 7546 (1991).
4. S.-R. Lin, N. Sherman, and J. K. Percus, *Nucl. Phys.* **45**, 492 (1963).
5. P. J. Bunyan and J. K. Schonfelder, *Proc. Phys. Soc.* **85**, 455 (1965).
6. W. Gautchi, *SIAM Rev.* **9**, 24 (1967).
7. F. W. J. Olver and D. J. Sookne, *Math. Comput.* **26**, 941 (1972).
8. J. B. Campbell, *ACM Trans. Math. Software* **6**, 581 (1980).
9. M. Abramowitz and I. A. Stegun (Eds.), *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (National Bureau of Standards, Washington, DC, 1964), p. 452.
10. O. A. Sharafeddin, H. F. Bowen, and D. J. Kouri, *J. Comput. Phys.* **100**, 294 (1992).
11. L. H. Thomas, *J. Chem. Phys.* **22**, 1758 (1954).
12. A. Jablonski, *Physica A* **183**, 361 (1992).