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Exponentially - fitted multiderivative methods for the numerical solution of the Schrödinger equation

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In this paper exponentially fitted multiderivative methods are developed for the numerical solution of the one-dimensional Schrödinger equation. The methods are called multiderivative since uses derivatives of order two and four. An application to the the resonance problem of the radial Schrödinger equation indicates that the new method is more efficient than other similar well known methods of the literature.

KEY WORDS: multiderivative methods, multistep methods, numerical methods, schrödinger equation

AMS subject classification: 65L05

1. Introduction

The radial Schrödinger equation has the form

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]y(r). \tag{1}$$

Models of this type, which represent a boundary value problem, occur frequently in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry etc. (see for example [1–4]).

In the following we give some definitions for (1):

- the function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(r) \to 0$ as $r \to \infty$;
- k^2 is a real number denoting *the energy*;
- l is a given integer representing *angular momentum*;
- V is a given function which denotes the potential;

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- the boundary conditions are

$$y(0) = 0 \tag{2}$$

and a second boundary condition, for large values of r, determined by physical considerations.

From the literature is known that the last decades many numerical methods have been developed for the numerical solution of the Schrödinger equation (see [5–24]). The vision of the above activity was the development of fast and reliable methods.

The numerical methods for the approximate solution of the Schrödinger equation can be divided into two main categories:

- methods with constant coefficients;
- methods with coefficients dependent on the frequency of the problem.[1]

In this paper we will investigate methods of the second category.

In this paper we introduce an explicit exponentially fitted multiderivative method for the numerical solution of the Schrödinger equation. The method is called multiderivative since it includes second and fourth derivative of the function. We apply the new developed methods to the resonance problem of the Schrödinger equation. The comparison of the new methods with known methods of the literature shows the efficiency of the new developed methods. For comparison purposes we use the well known Numerov method and the exponentially fitted Numerov-type method of Raptis and Allison [25].

2. A new family of multiderivative methods

We introduce the following family of methods to integrate $y'' = f(x)\, y(x)$:

$$\bar{y}_{n+1} = 2\, y_n - y_{n-1} + a_0\, h^2\, y''_n + a_1\, h^4\, y^{(4)}_n, \tag{3}$$

$$\begin{aligned} y_{n+1} &= 2\, y_n - y_{n-1} + h^2 \left[c_0\, y''_n + c_1 \left(\bar{y}''_{n+1} + y''_{n-1}\right)\right] \\ &\quad + h^4 \left[c_2\, y^{(4)}_n + c_3 \left(\bar{y}^{(4)}_{n+1} + y^{(4)}_{n-1}\right)\right], \end{aligned} \tag{4}$$

where $y''_{n\pm i} = f_{n\pm i}\, y_{n\pm i}$, $y^{(4)}_{n\pm i} = \left(f''_{n\pm i} + f^2_{n\pm i}\right) y_{n\pm i} + 2\, f'_{n\pm i}\, y'_{n\pm i}$ and $i = -1(1)1$. We note also that $\bar{y}''_{n+1} = f_{n+1}\, \bar{y}_{n+1}$ where $\bar{y}_{n+1}$ is calculated from the relation (3). It is easy to see that in order the above method, (3) and (4) to be applicable, then approximate schemes for the first derivatives of y are needed.

[1] In the case of the radial Schrödinger equation the frequency of the problem is equal to: $\sqrt{|l(l+1)/r^2 + V(r) - k^2|}$.

2.1. Construction of the exponentially fitted and trigonometrically fitted scheme for equation (3)

In order the stage (3) of the above method to integrate exactly any linear combination of the functions:

$$\{1,\ x,\ \cos(\pm v\,x), \sin(\pm v\,x)\} \tag{5}$$

the appropriate parameters of the new method are the solution of a system of equations, which is produced in the following way.

We calculate $y_{n\pm i},\ i=-1(1)1,$ and $y''_n = f_n\,y_n,\ y^{(4)}_n = \left(f''_n + f^2_n\right)\,y_n + 2\,f'_n\,y'_n$ for $y(x)=x^n,\ \ n=0,\ 1$ and for $y(x)=\cos(v\,x),\ y(x)=\sin(v\,x)$. So, the following system of equations is hold:

$$1 = a_0, \tag{6}$$

$$2\cos(w) - 2 = w^2\,(-a_0 + a_1\,w^2), \tag{7}$$

where $w = vh$.

The solution of equations. (6) and (7) gives us the parameters $a_i,\ i=0,\ 1$ of the first layer of the new method.

Solving the system in the previous section equations. (6) and (7), we obtain the parameters of the first layer of the new method, which are

$$\begin{aligned} a_0 &= 1,\\ a_1 &= \frac{2\cos(w) - 2 + w^2}{w^4}. \end{aligned} \tag{8}$$

The above parameter a_1 converted into its Taylor series expansion which is given below:

$$\begin{aligned} a_1 = \frac{1}{12} - \frac{1}{360}\,w^2 + \frac{1}{20160}\,w^4 - \frac{1}{1814400}\,w^6 + \frac{1}{239500800}\,w^8 \\ - \frac{1}{43589145600}\,w^{10} + \frac{1}{10461394944000}\,w^{12} + \cdots \end{aligned} \tag{9}$$

In figure 1 we present the behavior of the quantity a[1] = a_1, where a_1 is given by equation (8).

2.2. Construction of the exponentially fitted and trigonometrically fitted scheme for equation (4)

In order the stage (4) of the above method to integrate exactly any linear combination of the functions:

$$\{\ 1,\ x,\ x^2,\ x^3,\ x^4,\ x^5,\ x^6,\ x^7,\ \cos(\pm v\,x), \sin(\pm v\,x)\ \}, \tag{10}$$

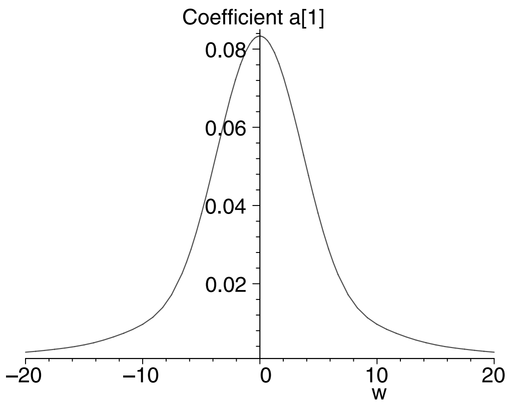

Figure 1. Behavior of the coefficient a_1 given by equation (8).

the appropriate parameters of the new method are the solution of a system of equations, which is produced in the following way.

We calculate $y_{n\pm i}$, and $y''_{n\pm i} = f_{n\pm i}\, y_{n\pm i}$, $y^{(4)}_{n\pm i} = \left(f''_{n\pm i} + f^2_{n\pm i}\right) y_{n\pm i} + 2 f'_{n\pm i}\, y'_{n\pm i}$, $i = -1(1)1$ for $y(x) = x^n$, $n = 0(1)7$ and for $y(x) = \cos(v\,x)$, $y(x) = \sin(v\,x)$. So, the following system of equations holds:

$$
\begin{aligned}
1 &= c_0 + 2\,c_1, && (11)\\
1 &= 12\,c_1 + 12\,c_2 + 24\,c_3, && (12)\\
1 &= 30\,c_1 + 360\,c_3, && (13)\\
2\cos(w) - 2 &= w^2\left(2\,w^2 c_3 \cos(w) - 2\cos(w)\,c_1 - c_0 + c_2\,w^2\right), && (14)
\end{aligned}
$$

where $w = vh$.

The solution of equations (11)–(13) gives us the parameters $c_i,\ i = 0(1)2$ as function of c_0:

$$
\begin{aligned}
c_1 &= \frac{1}{2} - \frac{1}{2}\,c_0,\\
c_2 &= -\frac{61}{180} + \frac{5}{12}\,c_0,\\
c_3 &= -\frac{7}{180} + \frac{1}{24}\,c_0.
\end{aligned}
\tag{15}
$$

Based on equations (15) and (14) we have the parameter c_0:

$$
c_0 = \frac{360\cos(w) - 360 + 14 w^4\cos(w) + 180\cos(w)\,w^2 + 61\,w^4}{15\,w^4\cos(w) + 180\cos(w)\,w^2 - 180\,w^2 + 75\,w^4}. \tag{16}
$$

The above parameter c_0 converted into its Taylor series expansion which is given below.

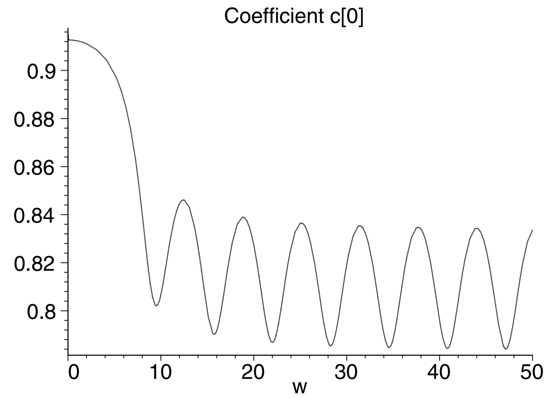

Figure 2. Behavior of the coefficient c_0 given by equation (16).

$$\begin{aligned} c_0 = {} & \frac{115}{126} - \frac{59}{158760}\,w^2 - \frac{233}{44008272}\,w^4 - \frac{451037}{7208554953600}\,w^6 \\ & - \frac{111679}{181655584830720}\,w^8 - \frac{1010455379}{2140084444890712320000}\,w^{10} \\ & - \frac{159482401}{78820956324128696832000}\,w^{12} + \cdots \end{aligned} \tag{17}$$

In figure 2 we present the behavior of the quantity $c[0] = c_0$, where c_0 is given by equation (16).

Based on the above coefficients we can find that the local truncation error of the above schemes (3) and (4) is given by

$$LTE(h) = -\frac{11}{90720}\,h^8\,\left(y_n^{(6)} + w^2\,y_n^{(4)}\right). \tag{18}$$

We note that if we substitute $w = -\mathrm{i}\,w$ in the above formulae, the exponentially fitted case is produced.

2.3. Stability analysis

In order to investigate the periodic stability properties of the numerical methods for problems of Schrödinger type, Lambert and Watson [29] have introduced the scalar test equation

$$y'' = -q^2\,y \tag{19}$$

and the *interval of periodicity*, where q is a constant.

Based on their theory when the symmetric two-step multiderivative method is applied to the scalar test equation (19), we obtain the difference equation

$$y_{n+1} - 2\,B(H)\,y_n + y_{n-1} = 0 \tag{20}$$

and the associate characteristic equation:

$$z^2 - 2\,B(H)\,z + 1 = 0, \tag{21}$$

where $H = qh$.

For our methods (3) and (4) we have

$$\begin{aligned} B(H) = 1 - H^2\left(\frac{1}{2}\,c_0 + c_1\right) + H^4\left(\frac{1}{2}\,c_1\,a_0 + \frac{1}{2}\,c_2 + c_3\right) \\ -H^6\left(\frac{1}{2}\,c_1\,a_1 + \frac{1}{2}\,c_3\,a_0\right) + \frac{1}{2}\,c_3\,a_1\,H^8. \end{aligned} \tag{22}$$

Definition 1. (see [29]). A symmetric two-step method with the characteristic equation given by equation (21) is said to have an interval of periodicity $\left(0, H_0^2\right)$ if, for all $H \in \left(0, H_0^2\right)$, the roots z_i, $i = 1, 2$, satisfy

$$z_1 = \mathrm{e}^{\mathrm{i}\,\theta(H)} \quad \text{and} \quad z_2 = \mathrm{e}^{-\mathrm{i}\,\theta(H)}, \tag{23}$$

where $\theta(H)$ is a real function of H.

Based on the above definition, it is easy for one to see that the following theorem holds.

Theorem 1. A method that has a characteristic equation given by equation (21) has a non-empty interval of periodicity $(0, H_0^2)$, if for all $H^2 \in (0, H_0^2)$, $|B(H)| < 1$.

So we have that in order the above methods (3) and (4) to have a non-empty interval of periodicity the following conditions must hold:

$$1 \pm B(H) > 0 \tag{24}$$

for all $H^2 \in \left(0, H_0^2\right)$.

Substituting in $B(H)$ the coefficients given by equations (8), (15) and (16), we obtain that in the case of $w = H$, equation (24) holds for every $H^2 \in \left(0, \pi^2\right)$, i.e. larger than the corresponding interval of periodicity of Numerov's method (which is equal to $(0, 6)$).

3. Computational implementation

As we have mentioned previously, in order the above methods (3) and (4) to be applicable we need approximate schemes for the first derivatives of y. This is due to the following formula:

$$y^{(4)}_{n\pm i} = \left(f''_{n\pm i} + f^2_{n\pm i}\right) y_{n\pm i} + 2\, f'_{n\pm i}\, y'_{n\pm i} \quad \text{and} \quad i = -1(1)1. \tag{25}$$

The general formulae of the first derivatives on the points x_i, $i = n-1(1)n+1$ are given by

$$\begin{aligned} h\, y'_{n+1} &= a_{2,n+1}\, y_{n+1} + a_{1,n+1}\, y_n + a_{0,n+1}\, y_{n-1} \\ &\quad + h^2 \left(b_{2,n+1}\, y''_{n+1} + b_{1,n+1}\, y''_n + b_{0,n+1}\, y''_{n-1}\right), \end{aligned} \tag{26}$$

$$\begin{aligned} h\, y'_n &= a_{2,n}\, y_{n+1} + a_{1,n}\, y_n + a_{0,n}\, y_{n-1} \\ &\quad + h^2 \left(b_{2,n}\, y''_{n+1} + b_{1,n}\, y''_n + b_{0,n}\, y''_{n-1}\right), \end{aligned} \tag{27}$$

$$\begin{aligned} h\, y'_{n-1} &= a_{2,n-1}\, y_{n+1} + a_{1,n-1}\, y_n + a_{0,n-1}\, y_{n-1} \\ &\quad + h^2 \left(b_{2,n-1}\, y''_{n+1} + b_{1,n-1}\, y''_n + b_{0,n-1}\, y''_{n-1}\right). \end{aligned} \tag{28}$$

In order the formulae (26) to integrate exactly any linear combination of the functions:

$$\{1,\ x,\ x^2,\ \cos(\pm v\, x), \sin(\pm v\, x)\}, \tag{29}$$

the appropriate parameters of the above formula are the solution of a system of equations, which is produced in the following way.

We calculate $y_{n\pm i}$, and $y''_{n\pm i} = f_{n\pm i} y_{n\pm i}$, $y'_{n\pm i}$ $i = -1(1)1$ for $y(x) = x^n$, $n = 0(1)2$ and for $y(x) = \cos(v\, x)$, $y(x) = \sin(v\, x)$. So, the following system of equations holds:

$$0 = a_{2,\,n+1} + a_{1,\,n+1} + a_{0,\,n+1}, \tag{30}$$

$$1 = a_{2,\,n+1} - a_{0,\,n+1}, \tag{31}$$

$$2 = a_{2,\,n+1} + a_{0,\,n+1} + 2\,b_{2,\,n+1} + 2\,b_{1,\,n+1} + 2\,b_{0,\,n+1}, \tag{32}$$

$$w\cos(w) = -\sin(w)\,(a_{0,\,n+1} - b_{0,\,n+1}\, w^2 + b_{2,\,n+1}\, w^2 - a_{2,\,n+1}), \tag{33}$$

$$\begin{aligned} -w\sin(w) &= a_{2,\,n+1}\cos(w) + a_{1,\,n+1} + a_{0,\,n+1}\cos(w) - b_{2,\,n+1}\, w^2\cos(w), \\ &\quad - b_{1,\,n+1}\, w^2 - b_{0,\,n+1}\, w^2\cos(w), \end{aligned} \tag{34}$$

$$0 = a_{2,\,n} + a_{1,\,n} + a_{0,\,n}, \tag{35}$$

$$1 = a_{2,\,n} - a_{0,\,n}, \tag{36}$$

$$0 = a_{2,\,n} + a_{0,\,n} + 2\,b_{2,\,n} + 2\,b_{1,\,n} + 2\,b_{0,\,n}, \tag{37}$$

$$w = -\sin(w)\,(a_{0,\,n} - b_{0,\,n}\, w^2 - a_{2,\,n} + b_{2,\,n}\, w^2), \tag{38}$$

$$\begin{aligned} 0 &= a_{2,\,n}\cos(w) + a_{1,\,n} + a_{0,\,n}\cos(w) - b_{2,\,n}\, w^2\cos(w) - b_{1,\,n}\, w^2 \\ &\quad - b_{0,\,n}\, w^2\cos(w), \end{aligned} \tag{39}$$

$$
\begin{aligned}
0 &= a_{2,n-1} + a_{1,n-1} + a_{0,n-1}, &(40)\\
1 &= a_{2,n-1} - a_{0,n-1}, &(41)\\
-2 &= a_{2,n-1} + a_{0,n-1} + 2\,b_{2,n-1} + 2\,b_{1,n-1} + 2\,b_{0,n-1}, &(42)\\
w\cos(w) &= -\sin(w)\,(a_{0,n-1} - b_{0,n-1}\,w^2 - a_{2,n-1} + b_{2,n-1}\,w^2), &(43)\\
w\sin(w) &= a_{2,n-1}\cos(w) + a_{1,n-1} + a_{0,n-1}\cos(w) - b_{2,n-1}\,w^2\cos(w)\\
&\quad - b_{1,n-1}\,w^2 - b_{0,n-1}\,w^2\cos(w), &(44)
\end{aligned}
$$

where $w = vh$.

Considering that

$$
b_{1,n+1} = b_{1,n} = b_{1,n-1} = 1, \tag{45}
$$

the solution of the above system of equations is given by:

$$
\begin{aligned}
a_{2,n+1} &= \frac{1}{2} - b_{2,n+1} - b_{0,n+1},\ a_{0,n+1} = -\frac{1}{2} - b_{2,n+1} - b_{0,n+1},\\
a_{1,n+1} &= 2\,b_{2,n+1} + 2\,b_{0,n+1},\\
b_{2,n+1} &= (2\,w + 2\,w\cos(2\,w) - 4\,w\cos(w) + 2\,w^3\cos(2\,w)\\
&\quad - 2\sin(2\,w) + 4\sin(w) - w^2\sin(2\,w)\\
&\quad + 2\,w^4\sin(w))/(-4\,w^2\sin(2\,w) + 8\,w^2\sin(w) - 2\,w^4\sin(2\,w)),\\
b_{0,n+1} &= (-2\,w - 2\,w\cos(2\,w) + 2\sin(2\,w)\\
&\quad + 4\,w\cos(w) - 4\sin(w) - 2\,w^3 + w^2\sin(2\,w)\\
&\quad + 2\,w^4\sin(w))/(-4\,w^2\sin(2\,w) + 8\,w^2\sin(w) - 2\,w^4\sin(2\,w)), &(46)\\
a_{0,n} &= -\frac{3}{2} - b_{2,n} - b_{0,n}, \quad a_{1,n} = 2 + 2\,b_{2,n} + 2\,b_{0,n},\\
a_{2,n} &= -\frac{1}{2} - b_{2,n} - b_{0,n},\\
b_{2,n} &= (-4\cos(w)\,w + 4\,w - 2\,w^3\cos(w) + 2\sin(2\,w)\\
&\quad - 4\sin(w) - w^2\sin(2\,w) + 4\,w^2\sin(w)\\
&\quad - 2\,w^4\sin(w))/(4\,w^2\sin(2\,w) - 8\,w^2\sin(w) + 2\,w^4\sin(2\,w)),\\
b_{0,n} &= (4\cos(w)\,w - 2\sin(2\,w) - 4\,w + 4\sin(w)\\
&\quad + 2\,w^3\cos(w) - 3\,w^2\sin(2\,w) + 4\,w^2\sin(w)\\
&\quad - 2\,w^4\sin(w))/(4\,w^2\sin(2\,w) - 8\,w^2\sin(w) + 2\,w^4\sin(2\,w)), &(47)\\
a_{0,n-1} &= -\frac{5}{2} - b_{2,n-1} - b_{0,n-1}, \quad a_{2,n-1} = -\frac{3}{2} - b_{2,n-1} - b_{0,n-1},\\
a_{1,n-1} &= 4 + 2\,b_{2,n-1} + 2\,b_{0,n-1},\\
b_{2,n-1} &= (2\,w + 2\,w\cos(2\,w) + 2\,w^3 - 4\,w\cos(w)\\
&\quad - 2\sin(2\,w) + 3\,w^2\sin(2\,w) + 4\sin(w) - 8\,w^2\sin(w)\\
&\quad + 2\,w^4\sin(w))/(-4\,w^2\sin(2\,w) - 2\,w^4\sin(2\,w) + 8\,w^2\sin(w)),
\end{aligned}
$$

$$
\begin{aligned}
b_{0,\,n-1} = {} & (-2\,w - 2\,w\cos(2\,w) + 2\sin(2\,w) \\
& -2\,w^3\cos(2\,w) + 5\,w^2\sin(2\,w) + 4\,w\cos(w) \\
& -4\sin(w) - 8\,w^2\sin(w) + 2\,w^4\sin(w))/ \\
& (-4\,w^2\sin(2\,w) - 2\,w^4\sin(2\,w) + 8\,w^2\sin(w)).
\end{aligned} \tag{48}
$$

The above parameters converted into its Taylor series expansion which are given below.

$$
\begin{aligned}
b_{2,\,n+1} = {} & \frac{11}{30} + \frac{89}{4500}\,w^2 + \frac{13819}{9450000}\,w^4 + \frac{8371}{67500000}\,w^6 \\
& + \frac{752613067}{65488500000000}\,w^8 + \frac{2912078681}{2606175000000000}\,w^{10} \\
& + \frac{301127030851}{2708842500000000000}\,w^{12} + \cdots\,, \\
b_{0,\,n+1} = {} & \frac{1}{30} - \frac{11}{4500}\,w^2 - \frac{883}{1350000}\,w^4 - \frac{13801}{157500000}\,w^6 \\
& - \frac{647386933}{65488500000000}\,w^8 - \frac{133708144631}{127702575000000000}\,w^{10} \\
& - \frac{9662807981917}{89391802500000000000}\,w^{12} + \cdots\,, \\
b_{2,\,n} = {} & \frac{1}{60} - \frac{67}{18000}\,w^2 - \frac{1963}{2700000}\,w^4 - \frac{49301}{540000000}\,w^6 \\
& - \frac{1317482263}{130977000000000}\,w^8 - \frac{76981425751}{72972900000000000}\,w^{10} \\
& - \frac{19388788306337}{178783605000000000000}\,w^{12} + \cdots\,, \\
b_{0,\,n} = {} & \frac{11}{60} + \frac{283}{18000}\,w^2 + \frac{25009}{18900000}\,w^4 + \frac{448643}{3780000000}\,w^6 \\
& + \frac{1477048987}{130977000000000}\,w^8 + \frac{43553090461}{39293100000000000}\,w^{10} \\
& + \frac{19806426537413}{178783605000000000000}\,w^{12} + \cdots\,, \\
b_{2,\,n-1} = {} & \frac{1}{6} + \frac{13}{900}\,w^2 + \frac{2363}{1890000}\,w^4 + \frac{3623}{31500000}\,w^6 \\
& + \frac{145434059}{13097700000000}\,w^8 + \frac{365034269}{331695000000000}\,w^{10} \\
& + \frac{1974325419491}{17878360500000000000}\,w^{12} + \cdots\,,
\end{aligned}
$$

$$
\begin{aligned}
b_{0,\,n-1} = {} & -\frac{1}{6} - \frac{7}{900}\, w^2 - \frac{1637}{1890000}\, w^4 - \frac{9131}{94500000}\, w^6 \\
& - \frac{134565941}{13097700000000}\, w^8 - \frac{27172361287}{25540515000000000}\, w^{10} \\
& - \frac{19653278591}{180589500000000000}\, w^{12} + \cdots\,.
\end{aligned} \tag{49}
$$

Based on the above coefficients we can find that the local truncation error of the formulae (26)–(28) are given by:

$$
\begin{aligned}
\mathrm{LTE}_{n+1} &= -\frac{1}{45}\, h^5\, \left(y_n^{(5)} + w^2\, y_n^{(3)}\right), \\
\mathrm{LTE}_{n} &= \frac{7}{360}\, h^5\, \left(y_n^{(5)} + w^2\, y_n^{(3)}\right), \\
\mathrm{LTE}_{n-1} &= -\frac{1}{45}\, h^5\, \left(y_n^{(5)} + w^2\, y_n^{(3)}\right).
\end{aligned} \tag{50}
$$

For the application of the first layer (3) of the methods (3) and (4) the following formula is also needed:

$$
h\, y_n' = aa_{1,n}\, y_n + aa_{0,n}\, y_{n-1} + h^2 \left(bb_{1,n}\, y_n'' + bb_{0,n}\, y_{n-1}''\right). \tag{51}
$$

In order the formula (51) to integrate exactly any linear combination of the functions:

$$
\{1,\ x,\ \cos(\pm v\, x), \sin(\pm v\, x)\}, \tag{52}
$$

the appropriate parameters of the above formula are the solution of a system of equations, which is produced in the following way.

We calculate $y_{n\pm i}$, and $y''_{n\pm i} = f_{n\pm i}\, y_{n\pm i}$, $y'_{n\pm i}$, $i = -1,\ 0$, for $y(x) = x^n$, $n = 0,\ 1$ and for $y(x) = \cos(v\, x)$, $y(x) = \sin(v\, x)$. So, the following system of equations holds:

$$0 = aa_{1,\,n} + aa_{0,\,n}, \tag{53}$$

$$1 = -aa_{0,\,n}, \tag{54}$$

$$w = \sin(w)\,(-aa_{0,\,n} + bb_{0,\,n}\, w^2), \tag{55}$$

$$0 = aa_{1,\,n} + aa_{0,\,n} \cos(w) - bb_{1,\,n}\, w^2 - bb_{0,\,n}\, w^2 \cos(w), \tag{56}$$

where $w = vh$.

Considering that

$$
bb_{1,\,n-1} = 1, \tag{57}
$$

the solution of the above system of equations is given by

$$\begin{aligned} aa_{0,\,n} &= -1, \quad aa_{1,\,n} = 1, \\ bb_{1,\,n} &= \frac{\sin(w) - \cos(w)\, w}{w^2 \sin(w)}, \\ bb_{0,\,n} &= \frac{w - \sin(w)}{w^2 \sin(w)}. \end{aligned} \tag{58}$$

The above parameters converted into its Taylor series expansion which are given below.

$$\begin{aligned} bb_{0,\,n} &= \frac{1}{6} + \frac{7}{360}\, w^2 + \frac{31}{15120}\, w^4 + \frac{127}{604800}\, w^6 + \frac{73}{3421440}\, w^8 \\ &\quad + \frac{1414477}{653837184000}\, w^{10} + \frac{8191}{37362124800}\, w^{12} + \cdots, \\ bb_{1,\,n} &= \frac{1}{3} + \frac{1}{45}\, w^2 + \frac{2}{945}\, w^4 + \frac{1}{4725}\, w^6 + \frac{2}{93555}\, w^8 \\ &\quad + \frac{1382}{638512875}\, w^{10} + \frac{4}{18243225}\, w^{12} + \cdots \end{aligned} \tag{59}$$

Based on the above coefficients we can find that the local truncation error of the formula (51) is given by

$$LTE_n = -\frac{1}{24}\, h^4 \left(y_n^{(4)} + w^2\, y_n^{(2)} \right). \tag{60}$$

We note here that the exponentially fitted versions of the above formulae can be constructed with similar procedures.

4. Numerical illustrations

In this section we present some numerical illustrations in order to investigate the performance of our new method. Consider the numerical integration of the radial Schrödinger equation (1) using the well-known Woods–Saxon potential (see [1,4–6,8]) which is given by

$$V(r) = V_w(r) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{61}$$

with $z = \exp[(r - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$. In figure 3, we give a graph of this potential. In the case of negative eigenenergies (i.e. when $E \in [-50, 0]$) we have the well-known *bound-states problem* while in the case of positive eigenenergies (i.e. when $E \in (0, 1000]$) we have the well-known *resonance problem* (see [5,6,28]).

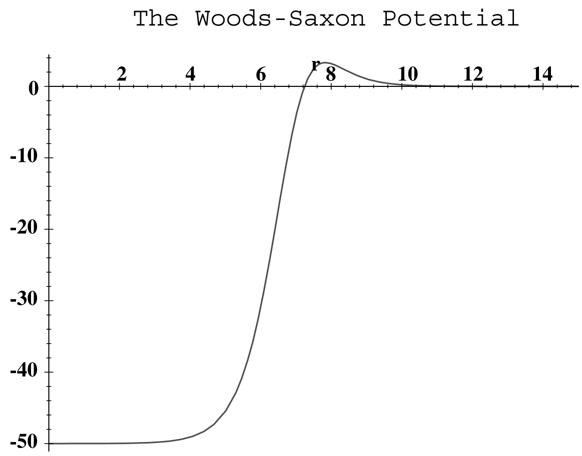

Figure 3. The Woods–Saxon potential.

4.1. *Resonance problem — The Woods–Saxon potential*

In the asymptotic region equation (1) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{62}$$

for x greater than some value X.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx), n_l(kx)$ are the *spherical Bessel and Neumann functions* respectively. Thus the solution of equation (1) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan \delta_l \cos(kx - \pi l/2)], \end{aligned} \tag{63}$$

where δ_l is the *phase shift* which may be calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{64}$$

for x_1 and x_2 distinct points on the asymptotic region (for which we have that x_1 is the right hand end point of the interval of integration and $x_2 = x_1 - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

Since the problem is treated as an initial-value problem, one needs y_0 and y_1 before starting a two-step method. From the initial condition, $y_0 = 0$. The value y_1 is computed using the Runge–Kutta–Nyström 12(10) method of Dormand et al. [36,37]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l from the above relation.

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (1) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods–Saxon one (61).

One can investigate the problem considered here, following two procedures. The first procedure consists of finding the *phase shift* $\delta(E) = \delta_l$ for $E \in [1, 1000]$. The second procedure consists of finding those E, for $E \in [1, 1000]$, at which δ equals $\pi/2$. In our case we follow the first procedure i.e. we try to find the phase shifts for given energies. The obtained phase shift is then compared to the analytic value of $\pi/2$.

The above problem is the so-called *resonance problem* when *the positive eigenenergies lie under the potential barrier*. We solve this problem, using the technique fully described in [5].

The boundary conditions for this problem are:

$$\begin{aligned} &y(0) = 0, \\ &y(x) \sim \cos[\sqrt{E}x] \quad \text{for large } x. \end{aligned}$$

The domain of numerical integration is [0, 15].

For comparison purposes in our numerical illustration we use the following methods:

- the well known Numerov's method (which is indicated as method [a]);
- the explicit version of Numerov's method which is developed by Chawla [32] (which is indicated as method [b]);
- the exponentially fitted method of Raptis and Allison [25] (which is indicated as method [c]);
- the exponentially fitted method of Ixaru and Rizea [28] (which is indicated as method [d]);
- the new multiderivative exponentially fitted method developed in this paper (which is indicated as method [e]).

The numerical results obtained for the five methods, with stepsizes equal to $h = 1/2^n$, were compared with the analytic solution of the Woods–Saxon potential resonance problem, rounded to six decimal places. Figure 4 shows the errors $Err = -\log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ of the highest eigenenergy $E_3 = 989.701916$ for several values of n.

5. Conclusions

In this paper a new approach for developing efficient methods for the numerical solution of the radial Schrödinger type equations is introduced. This approach is based on exponential fitting procedure and multiderivative methods.

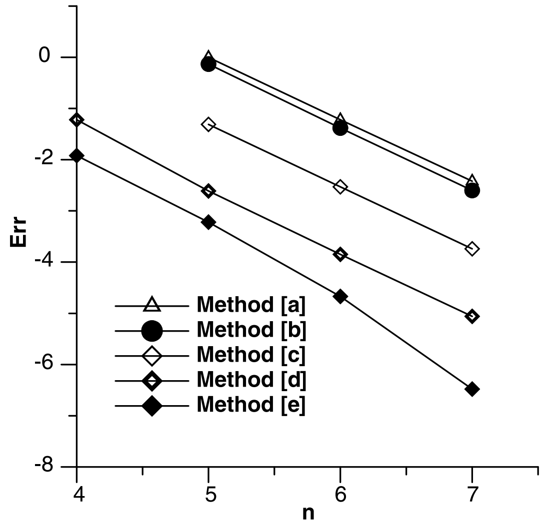

Figure 4. Error (Err) for several values of n for the eigenvalue $E_3 = 989.701916$. The non-existence of a value of Err indicates that for this value of n, Err is positive.

Using this new approach we have developed an exponentially fitted multiderivative method.

From the numerical results we have the following remarks:

- the Numerov's method and the explicit Numerov-type method of Chawla [32] have approximately the same behavior;
- the exponentially fitted Numerov-type method of Raptis and Allison [25] is more efficient than the Numerov's method and the explicit Numerov-type method of Chawla [32];
- the exponentially fitted Numerov-type method of Ixaru and Rizea [28] is more efficient than the exponentially fitted Numerov-type method of Raptis and Allison [25];
- the new developed exponentially fitted multiderivative method is the more efficient one compared with the other methods.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

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