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ORIGINAL PAPER

A family of four-step trigonometrically-fitted methods and its application to the schrödinger equation

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Abstract In this article we present a singularly almost P-stable exponentially-fitted four-step method for the approximate solution of the one-dimensional Schrödinger equation. More specifically we present a method that is singularly almost P-stable (a concept later introduced in this article) and also integrates exactly any linear combination of the functions $\{1,\ x,\ \exp(\pm I\ v\,x),\ x\ \exp(\pm I\ v\,x),\ x^2\ \exp(\pm I\ v\,x)\}$. The numerical experimentation showed that our method is considerably more efficient compared to well known methods used for the approximate solution of resonance problem of the radial Schrödinger equation.

Keywords Numerical solution · Schrödinger equation · Linear multistep methods · P-stability · Exponential fitting · Trigonometric fitting

Abbreviation

LTE Local truncation error

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1 Introduction

The radial Schrödinger equation can be written as:

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x). \quad (1)$$

The above boundary value problem occurs frequently in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. (see for example [1]–[4]).

We give some definitions for (1):

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

The boundary conditions are:

$$y(0) = 0 \quad (2)$$

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

The last decades a lot of research has been done on the development of numerical methods for the solution of the Schrödinger equation. The aim of this research is the development of fast and reliable methods for the solution of the Schrödinger equation and related problems (see for example [5]–[18], [19]–[61]).

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

1. Methods with constant coefficients
2. Methods with coefficients depending on the frequency of the problem.[1]

In this article we will investigate methods of the second category. We will investigate the exponentially-fitted methods. A book on the study of the exponential fitting technique has been published recently [19]. More specifically we will obtain an exponentially-fitted method of sixth algebraic order for the numerical solution of the radial Schrödinger equation. The developed method is also singularly almost P-stable i.e. it has an interval of periodicity equal to $(0, \infty) - S$[2] (in the case that the frequency of the exponential fitting is the same as the frequency of the scalar test equation). We apply the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The above application shows the efficiency of the new obtained method. The article is organized as follows. In Sect. 2 we present the development of the method. In the same section, the error analysis is

[1] When using the trigonometrically-fitted method for the solution of the radial Schrödinger equation, the fitted frequency is equal to: $\sqrt{|l(l+1)/x^2 + V(x) - k^2|}$

[2] where S is a set of distinct points

presented. The stability of the new method is also studied. In Sect. 3 the numerical results are presented. Finally, in Sect. 4 remarks and conclusions are discussed.

2 The new trigonometrically-fitted four-step method

2.1 Construction of the new method

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

$$\begin{aligned} & y_{n+2} + a\, y_{n+1} - (2 + 2\, a)\, y_n + a\, y_{n-1} + y_{n-2} \\ & \quad = h^2 \left[b_0 \left(y''_{n+2} + y''_{n-2} \right) + b_1 \left(y''_{n+1} + y''_{n-1} \right) + b_2 y''_n \right] \end{aligned} \tag{3}$$

In order the above method (3) to be exact for any linear combination of the functions

$$\{1,\ x,\ \exp(\pm I\ v\, x),\ x\ \exp(\pm I\ v\, x),\ x^2\ \exp(\pm I\ v\, x)\} \tag{4}$$

where $I = \sqrt{-1}$, the following system of equations must hold:

$$\begin{aligned} & 2\, a\ \cos(v\, h) - 2 + 2\ \cos(2\, v\, h) - 2\, a \\ & \quad = -2\, h^2\, v^2\ \cos(2\, v\, h)\, b_0 - 2\, h^2\, v^2\, b_1\ \cos(v\, h) - h^2\, v^2\, b_2 \end{aligned} \tag{5}$$

$$\begin{aligned} & -2\, x - 2\, x\, a + 2\, x\, a\ \cos(v\, h) + 2\, x\ \cos(2\, v\, h) \\ & \quad = -2\, h^2\, v^2\ \cos(2\, v\, h)\, b_0\, x - 2\, h^2\, v^2\, b_1\, x\ \cos(v\, h) - h^2\, v^2\, b_2\, x \end{aligned} \tag{6}$$

$$\begin{aligned} & 2\, a\, h\ \sin(v\, h) + 4\, h\ \sin(2\, v\, h) \\ & \quad = 4\, h^2\, v\ \cos(2\, v\, h)\, b_0 + 2\, h^2\, v\, b_2 - 4\, h^3\, v^2\, b_0\ \sin(2\, v\, h) \\ & \qquad -2\, h^3\, v^2\, b_1\ \sin(v\, h) + 4\, h^2\, v\, b_1\ \cos(v\, h) \end{aligned} \tag{7}$$

$$\begin{aligned} & -2\, x^2\, a - 2\, x^2 + 8\, h^2\ \cos(2\, v\, h) + 2\, x^2\ \cos(2\, v\, h) \\ & \qquad +2\, x^2\, a\ \cos(v\, h) + 2\, a\, h^2\ \cos(v\, h) \\ & \quad = -2\, h^4\, v^2\, b_1\ \cos(v\, h) + 4\, h^2\, b_1\ \cos(v\, h) \\ & \qquad -8\, h^4\ \cos(2\, v\, h)\, b_0\, v^2 - 8\, h^3\, b_1\, v\ \sin(v\, h) \\ & \qquad -2\, h^2\, b_1\, v^2\, x^2\ \cos(v\, h) - h^2\, b_2\, x^2\, v^2 \\ & \qquad -2\, h^2\ \cos(2\, v\, h)\, b_0\, v^2\, x^2 + 4\, h^2\ \cos(2\, v\, h)\, b_0 \\ & \qquad +2\, h^2\, b_2 - 16\, h^3\, b_0\, v\ \sin(2\, v\, h) \end{aligned} \tag{8}$$

$$\begin{aligned} & 8\, x\, h\ \sin(2\, v\, h) + 4\, a\, x\, h\ \sin(v\, h) \\ & \quad = -4\, h^3\, b_1\, v^2\, x\ \sin(v\, h) + 8\, h^2\ \cos(2\, v\, h)\, b_0\, v\, x \\ & \qquad -8\, h^3\, b_0\, v^2\, x\ \sin(2\, v\, h) + 4\, h^2\, b_2\, x\, v + 8\, h^2\, b_1\, v\, x\ \cos(v\, h) \end{aligned} \tag{9}$$

We apply the new method (3) to the scalar test equation:

$$y'' = -v^2 y. \tag{10}$$

We obtain the following difference equation:

$$A(v,h)\ (y_{n+2}+y_{n-2})+B(v,h)\ (y_{n+1}+y_{n-1})+C(v,h)\,y_n=0 \tag{11}$$

where

$$\begin{aligned}&A(v,h)=1+v^2\,h^2\,b_0,\ B(v,h)=a+v^2\,h^2\,b_1,\\&C(v,h)=-2-2\,a+v^2\,h^2\,b_2.\end{aligned} \tag{12}$$

The corresponding characteristic equation is given by:

$$A(v,h)\ \left(\lambda^4+1\right)+B(v,h)\ \left(\lambda^3+\lambda\right)+C(v,h)\,\lambda^2=0 \tag{13}$$

Definition 1 (*see* [62]) A symmetric four-step method with the characteristic equation given by (13) is said to have an *interval of periodicity* $\left(0,w_0^2\right)$ if, for all $w\in\left(0,w_0^2\right)$, the roots $z_i,\ i=1,2$ satisfy

$$z_{1,2}=e^{\pm i\,\theta(v\,h)},\ |z_i|\leq 1,\ i=3,4 \tag{14}$$

where $\theta(v\,h)$ is a real function of $v\,h$ and $w=v\,h$.

Definition 2 (*see* [62]) A method is called P-stable if its interval of periodicity is equal to $(0,\infty)$.

In order the new method to be P-stable[3] we require the characteristic Eq. (13) to have the following roots:

$$\exp(I\ v\,h), \exp(-I\ v\,h), -\exp(I\ v\,h), -\exp(-I\ v\,h) \tag{15}$$

In order (15) to be roots of the characteristic Eq. (13), the following system of equations must hold:

$$\begin{aligned}&4\,(1+v^2\,h^2\,b_0)\ \cos(v\,h)^2-2\,(a+v^2\,h^2\,b_1)\ \cos(v\,h)\\&\quad-4-2\,a+h^2\,v^2\,b_2-2\,v^2\,h^2\,b_0=0\end{aligned} \tag{16}$$

$$\begin{aligned}&4\,(1+v^2\,h^2\,b_0)\ \cos(v\,h)^2+2\,(a+v^2\,h^2\,b_1)\ \cos(v\,h)\\&\quad-4-2\,a+h^2\,v^2\,b_2-2\,v^2\,h^2\,b_0=0\end{aligned} \tag{17}$$

[3] in the case that the frequency of the exponential fitting is the same as the frequency of the scalar test equation (which in the case of (10) has been obtained)

Solving the system of Eqs. (5)–(8), (16), (17) we obtain the following values of the coefficients of the methods:

$$
\begin{aligned}
b_0 &= \frac{\sin(2\,w) - 4\,w\,\cos(w) + 4\,\sin(w) - 2\,w}{-3\,w^2\,\sin(2\,w) + 4\,w^3\,\cos(w) + 2\,w^3} \\
b_1 &= \frac{T_0}{-3\,w^2\,\sin(2\,w) + 4\,w^3\,\cos(w) + 2\,w^3} \\
b_2 &= \frac{T_1}{-3\,w^2\,\sin(2\,w) + 4\,w^3\,\cos(w) + 2\,w^3} \\
a &= \frac{T_2}{-3\,\sin(2\,w) + 4\,w\,\cos(w) + 2\,w}
\end{aligned}
\tag{18}
$$

where $w = v\,h$ and:

$$
\begin{aligned}
T_0 &= 2\,w\,\cos(3\,w) + 10\,w\,\cos(w) - 3\,\sin(3\,w) \\
&\quad -3\,\sin(w) + 4\,\cos(2\,w)\,w + 8\,w - 6\,\sin(2\,w) \\
T_1 &= -4\,w\,\cos(3\,w) - 12\,w\,\cos(w) + 2\,\sin(4\,w) \\
&\quad +6\,\sin(2\,w) + 2\,\sin(3\,w) + 10\,\sin(w) - 8\,\cos(2\,w)\,w - 12\,w \\
T_2 &= -2\,w\,\cos(3\,w) - 10\,w\,\cos(w) - 4\,\cos(2\,w)\,w \\
&\quad -8\,w + 3\,\sin(3\,w) + 3\,\sin(w) + 6\,\sin(2\,w)
\end{aligned}
$$

For small values of $|w|$ the formulae given by (18) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_0 &= \frac{1}{15} + \frac{17}{1575}\,w^2 + \frac{163}{94500}\,w^4 + \frac{60607}{218295000}\,w^6 \\
&\quad + \frac{1697747}{37837800000}\,w^8 + \frac{519335027}{71513442000000}\,w^{10} \\
&\quad + \frac{12254045443}{10420530120000000}\,w^{12} \\
&\quad + \frac{609739626367891}{3201499468767600000000}\,w^{14} + \ldots \\
b_1 &= \frac{16}{15} - \frac{208}{1575}\,w^2 + \frac{247}{23625}\,w^4 + \frac{4154}{27286875}\,w^6 \\
&\quad + \frac{1790779}{28378350000}\,w^8 + \frac{606383}{62511750000}\,w^{10} \\
&\quad + \frac{28752907369}{18235927710000000}\,w^{12} \\
&\quad + \frac{6387572067797}{25011714599746875000}\,w^{14} + \ldots
\end{aligned}
$$

$$b_2 = \frac{26}{15} - \frac{1298}{1575}\, w^2 + \frac{727}{6750}\, w^4 - \frac{1003979}{109147500}\, w^6 + \frac{13137323}{56756700000}\, w^8 - \frac{94972363}{2750517000000}\, w^{10} - \frac{127664236097}{36471855420000000}\, w^{12} - \frac{979315457827727}{1600749734383800000000}\, w^{14} + \ldots$$

$$a = -\frac{16}{15}\, w^2 + \frac{208}{1575}\, w^4 - \frac{247}{23625}\, w^6 - \frac{4154}{27286875}\, w^8 - \frac{1790779}{28378350000}\, w^{10} - \frac{606383}{62511750000}\, w^{12} - \frac{28752907369}{18235927710000000}\, w^{14} + \ldots \tag{19}$$

The local truncation error of this method is given by:

$$\text{LTE} = -\frac{2\,h^8}{945}\left(y_n^{(8)} + 3\,v^2\ y_n^{(6)} + 3\,v^4\ y_n^{(4)} + v^6\ y_n^{(2)}\right) \tag{20}$$

Studying the error of the new method we can observe the following:

The LTE of any method (3) which integrates exactly any linear combination of the functions (4) is given by:

$$\text{LTE} = h^8\left(-\frac{2}{945} + \frac{31\,a}{60480}\right)\left(y_n^{(8)} + 3\,v^2\ y_n^{(6)} + 3\,v^4\ y_n^{(4)} + v^6\ y_n^{(2)}\right) \tag{21}$$

From (21) it can be seen that in the interval $-4 \le a \le 0$ the absolute value of the error constant decreases for increasing a value. So, the error constant's smallest value can be obtained for $a = 0$.[4] Based on the above, we conclude that in this section we have developed a four-step exponentially-fitted method with the smallest possible error constant.

2.2 Error analysis

We will study the following methods:

Classical method[5]

$$\text{LTE}_{\text{CL}} = -\frac{2\,h^8}{945}\, y_n^{(8)} \tag{22}$$

[4] For this value the classical method i.e. the method produced from (18) and (19) for $w -> 0$ is completely unstable since the characteristic equation has no roots

[5] i.e. the method with constant coefficients

Trigonometrically-fitted method produced by Simos [66]

$$\mathrm{LTE}_{\mathrm{EXPOLD}} = -\frac{2\,h^8}{945}\left(y_n^{(8)} - v^2\,y_n^{(6)}\right) \tag{23}$$

Trigonometrically-fitted method produced in this article

$$\mathrm{LTE} = -\frac{2\,h^8}{945}\left(y_n^{(8)} + 3\,v^2\;y_n^{(6)} + 3\,v^4\;y_n^{(4)} + v^6\;y_n^{(2)}\right) \tag{24}$$

The steps for the error analysis are:

– The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)\,y(x) \tag{25}$$

– Based on the article of Ixaru and Rizea [20], the function f(x) can be written in the form:

$$f(x) = g(x) + G \tag{26}$$

where $g(x) = V(x) - V_c = g$, where V_c is the constant approximation of the potential and $G = v^2 = V_c - E$.
– We express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \ldots,$ which are terms of the local truncation error formulae, in terms of the Eq. (25). The expressions are presented as polynomials of G
– Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae

Based on the procedure mentioned above and on the formulae:

$$\begin{aligned}
y_n^{(2)} &= (\mathrm{V}(x) - V_c + G)\,\mathrm{y}(x) \\
y_n^{(4)} &= \left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x) + 2\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right) \\
&\quad + (\mathrm{V}(x) - V_c + G)\left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right)
\end{aligned}$$

$$
\begin{aligned}
y_n^{(6)} = & \left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x) + 4\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\\
& + 3\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right)\\
& + 4\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)\\
& + 6\,(\mathrm{V}(x) - V_c + G)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\\
& + 4\,(\,\mathrm{U}(x) - V_c + G)\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\\
& + (\mathrm{V}(x) - V_c + G)^2\left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right)\ldots
\end{aligned}
$$

we obtain the following expressions:

Classical method

$$
\begin{aligned}
\mathrm{LTE_{CL}} = & -\frac{2}{945}\,\mathrm{y}(x)\,G^4\\
& + \left(-\frac{8}{945}\,\mathrm{y}(x)\,\mathrm{V}(x) + \frac{8}{945}\,\mathrm{y}(x)\,V_c\right)G^3\\
& + \left(\frac{8}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)\,V_c - \frac{4}{315}\,\mathrm{y}(x)\,{V_c}^2\right.\\
& - \frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\\
& \left.-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\;\mathrm{y}(x)\right) - \frac{4}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\right)G^2\\
& + \left(-\frac{16}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{V}(x) + \frac{88}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,V_c\right.\\
& + \frac{16}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)V_c - \frac{8}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)\,{V_c}^2\\
& + \frac{8}{945}\,\mathrm{y}(x)\,{V_c}^3 - \frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)\\
& - \frac{88}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{V}(x) - \frac{8}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)^3
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)+\frac{8}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\,V_c\\
&-\frac{32}{945}\left(\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\right)G\\
&+\frac{8}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)\,{V_c}^3-\frac{2}{945}\left(\frac{d^6}{dx^6}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\\
&-\frac{4}{315}\left(\frac{d^5}{dx^5}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\\
&-\frac{52}{945}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\\
&-\frac{32}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)-\frac{2}{63}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)^2\,\mathrm{y}(x)\\
&+\frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)V_c-\frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\,\mathrm{V}(x)^2\\
&-\frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\,{V_c}^2\\
&+\frac{16}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\,\mathrm{V}(x)\,V_c\\
&+\frac{8}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)^3\,V_c+\frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\,\mathrm{y}(x)\,V_c\\
&-\frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\,\mathrm{y}(x)\,\mathrm{V}(x)-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\,\mathrm{V}(x)^2\\
&-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right){V_c}^2\\
&-\frac{4}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\,{V_c}^2\\
&-\frac{2}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)^4-\frac{2}{945}\,\mathrm{y}(x)\,{V_c}^4\\
&+\frac{88}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\,\mathrm{V}(x)\,V_c\\
&-\frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\,\mathrm{V}(x)\\
&-\frac{32}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\,\mathrm{V}(x)+\frac{32}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\,\mathrm{y}(x)\,V_c
\end{aligned}
\tag{27}
$$

Trigonometrically-fitted method produced by Simos [66]

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{EXPOLD}} = {} & \left(\frac{2}{945}\,\mathrm{y}(x)\,V_c - \frac{2}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)\right) G^3 \\
& + \left(\frac{4}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)\,V_c - \frac{4}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\right. \\
& - \frac{2}{63}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x) - \frac{2}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)^2 \\
& \left. - \frac{2}{315}\,\mathrm{y}(x)\,{V_c}^2\right) G^2 \\
& + \left(\frac{74}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,V_c\right. \\
& + \frac{4}{105}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right) V_c \\
& - \frac{74}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{V}(x) - \frac{2}{105}\,\mathrm{y}(x)\,\mathrm{V}(x)\,{V_c}^2 \\
& + \frac{2}{315}\,\mathrm{y}(x)\,{V_c}^3 - \frac{16}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x) \\
& + \frac{2}{105}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\,V_c - \frac{2}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)^3 \\
& - \frac{4}{105}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{V}(x) \\
& - \frac{2}{63}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x) \\
& \left. - \frac{8}{189}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\right) G \\
& + \frac{8}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)\,{V_c}^3 - \frac{2}{945}\left(\frac{d^6}{dx^6}\,\mathrm{V}(x)\right)\mathrm{y}(x) \\
& - \frac{4}{315}\left(\frac{d^5}{dx^5}\mathrm{V}(x)\right)\left(\frac{d}{dx}\mathrm{y}(x)\right) - \frac{52}{945}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\mathrm{y}(x)\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right) \\
& - \frac{32}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right) - \frac{2}{63}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)^2\mathrm{y}(x) \\
& + \frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right) V_c - \frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{V}(x)^2 \\
& - \frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,{V_c}^2 \\
& + \frac{16}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{V}(x)\,V_c
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{8}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)^3\,V_c+\frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)\,V_c\\
&-\frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)\,\mathrm{V}(x)-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{V}(x)^2\\
&-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)V_c{}^2-\frac{4}{315}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\,V_c{}^2\\
&-\frac{2}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)^4-\frac{2}{945}\,\mathrm{y}(x)\,V_c{}^4\\
&+\frac{88}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{V}(x)\,V_c-\frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{V}(x)\\
&-\frac{32}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{V}(x)+\frac{32}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,V_c \qquad (28)
\end{aligned}
$$

Trigonometrically-fitted Method produced in this article

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{NEW}}=&-\frac{8}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,G^2\\
&+\Bigg(-\frac{8}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)-\frac{32}{945}\left(\frac{d}{dx}\,\mathrm{U}(x)\right)^2\mathrm{y}(x)\\
&-\frac{26}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x)-\frac{2}{945}\,\mathrm{y}(x)\,\mathrm{U}(x)^3\\
&+\frac{46}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,V_c-\frac{2}{315}\,\mathrm{y}(x)\,\mathrm{U}(x)\,V_c{}^2\\
&+\frac{2}{945}\,\mathrm{y}(x)\,V_c{}^3-\frac{46}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{U}(x)\\
&+\frac{2}{315}\,\mathrm{y}(x)\,\mathrm{U}(x)^2\,V_c-\frac{4}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{U}(x)\\
&+\frac{4}{315}\left(\frac{d}{dx}\,\mathrm{U}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)V_c\Bigg)\,G\\
&-\frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,V_c{}^2-\frac{52}{945}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\mathrm{y}(x)\left(\frac{d^3}{dx^3}\,\mathrm{U}(x)\right)\\
&+\frac{88}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{U}(x)\,V_c-\frac{2}{945}\left(\frac{d^6}{dx^6}\,\mathrm{V}(x)\right)\mathrm{y}(x)\\
&-\frac{4}{315}\left(\frac{d^5}{dx^5}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)-\frac{2}{63}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{32}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)+\frac{32}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,V_c\\
&-\frac{32}{945}\left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{U}(x)-\frac{4}{315}\,\mathrm{y}(x)\,\mathrm{U}(x)^2\,{V_c}^2\\
&-\frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{U}(x)+\frac{16}{315}\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)V_c\\
&-\frac{44}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,\mathrm{U}(x)^2-\frac{2}{945}\,\mathrm{y}(x)\,{V_c}^4\\
&+\frac{16}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{U}(x)\,V_c-\frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)\,\mathrm{U}(x)\\
&+\frac{8}{135}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x)\,V_c-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\mathrm{U}(x)^2\\
&-\frac{8}{315}\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right){V_c}^2+\frac{8}{945}\,\mathrm{y}(x)\,\mathrm{U}(x)^3\,V_c\\
&+\frac{8}{945}\,\mathrm{y}(x)\,\mathrm{U}(x)\,{V_c}^3-\frac{2}{945}\,\mathrm{y}(x)\,\mathrm{U}(x)^4
\end{aligned}
\tag{29}
$$

We consider two situations in terms of the value of E:

- The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. Thus for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G, are the same for the three cases.
- $G \gg 0$ or $G \ll 0$. Then $\mid G \mid$ is a large number. So, we have the following asymptotic expansions of the Eqs. (27), (28) and (29).

Classical method

$$
\mathrm{LTE_{CL}} = -\frac{2}{945}\,\mathrm{y}(x)\,G^4 + \ldots \tag{30}
$$

Trigonometrically-fitted Method Produced by Simos [66]

$$
\mathrm{LTE_{EXPOLD}} = \left(-\frac{2}{945}\,V_c\,\mathrm{y}(x) + \frac{2}{945}\,\mathrm{y}(x)\,\mathrm{V}(x)\right) G^3 + \ldots \tag{31}
$$

Trigonometrically-fitted Method produced in this article

$$
\mathrm{LTE} = -\frac{8}{945}\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x)\,G^2 + \ldots \tag{32}
$$

From the above equations we have the following theorem:

Theorem 1 *For the Classical Four-Step Method the error increases as the fourth power of G. For the Trigonometrically-fitted Method produced by Simos* [66] *the error increases as the third power of G. Finally, for the Trigonometrically-fitted Four-Step Method developed in this article the error increases as the second power of G. So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Trigonometrically-fitted four-step Method is the most accurate one, especially for large values of* $\mid G \mid = \mid V_c - E \mid$.

2.3 Stability analysis

We apply the new method to the scalar test equation:

$$y'' = -q^2 y, \tag{33}$$

where $q \neq v$. We obtain the following difference equation:

$$A(q,h)\ (y_{n+2} + y_{n-2}) + B(q,h)\ (y_{n+1} + y_{n-1}) + C(q,h)\, y_n = 0 \tag{34}$$

where

$$\begin{aligned} &A(q,h) = 1 + q^2 h^2 b_0,\ B(q,h) = a + q^2 h^2 b_1, \\ &C(q,h) = -2\,(1+a) + q^2 h^2 b_2. \end{aligned} \tag{35}$$

The corresponding characteristic equation is given by:

$$A(q,h)\ \left(\lambda^4 + 1\right) + B(q,h)\ \left(\lambda^3 + \lambda\right) + C(q,h)\,\lambda^2 = 0 \tag{36}$$

Theorem 2 (see [63]) *A symmetric four-step method with the characteristic equation given by* (36) *is said to have a nonzero interval of periodicity* $\left(0, H_0^2\right)$ *if, for all* $H \in \left(0, H_0^2\right)$ *the following relations are hold*

$$\begin{aligned} P_1(H,w) \geq 0,\ P_2(H,w) \geq 0,\ P_3(H,w) \geq 0 \\ P_2(H,w)^2 - 4\,P_1(H,w)\,P_3(H,w) \geq 0 \end{aligned} \tag{37}$$

where $H = q\,h$, $w = v\,h$ *and:*

$$\begin{aligned} &P_1(H,w) = 2\,A(H,w) - 2\,B(H,w) + C(H,w) \geq 0, \\ &P_2(H,w) = 12\,A(H,w) - 2\,C(H,w) \geq 0, \\ &P_3(H,w) = 2\,A(H,w) + 2\,B(H,w) + C(H,w) \geq 0, \\ &N(H,w) = P_2(H,w)^2 - 4\,P_1(H,w)\,P_3(H,w) \geq 0 \end{aligned} \tag{38}$$

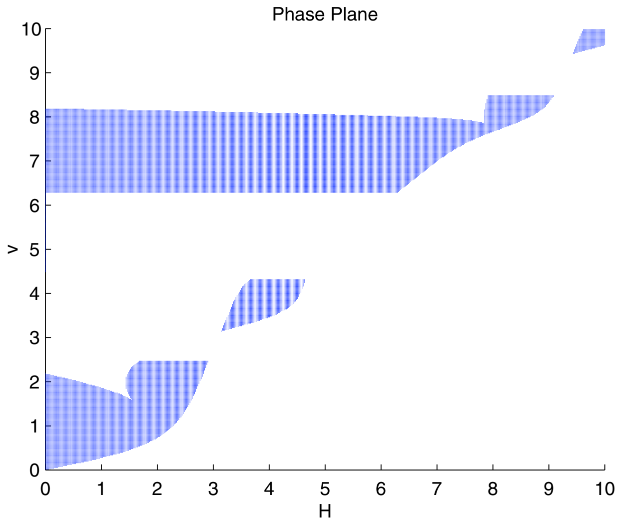

Fig. 1 The stability region in the $w - H$ plane for the new method

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$[6] only when the frequency of the exponential fitting is the same as the frequency of the scalar test equation, i.e. $H = w$.

Based on (35) the stability polynomials (38) take the form:

$$P_1(H, w) = -4\,a + H^2\,(2\,b_0 - 2\,b_1 + b_2)\,,$$
$$P_2(H, w) = 4\,(4 + a) + 2\,H^2\,(6\,b_0 - b_2)\,,$$
$$P_3(H, w) = H^2\,(2\,b_0 + 2\,b_1 + b_2) \tag{39}$$

In the Fig. 1, we present the $w - H$ plane. A method is P-stable if the $w - H$ plane is completely shadowed. It can be seen the following:

- If the frequency of the exponential fitting is equal to the frequency of the scalar test equation (first diagonal of the $w - H$ plane) the method is almost P-Stable (the empty area in the diagonal of the figure exists since we have cancelations in the denominators of the coefficients of the new proposed method. This can been seen by Fig. 2 in which we have computed the $w - H$ plane using the Taylor series expansions of the coefficients).
- If the frequency of the exponential fitting is different from the frequency of the scalar test equation the method is not P-stable (i.e. there are areas in the Fig. 1 that are white and in which the conditions of P-stability are not satisfied).

Remark 1 For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to

[6] where S is a set of distinct points

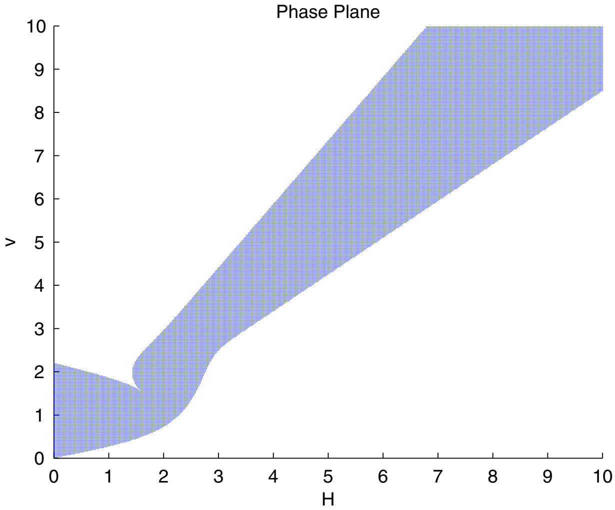

Fig. 2 The stability region in the $w - H$ plane for the new method using Taylor series expansions of the coefficients

observe the surroundings of the first diagonal of the $w - H$ plane. The new proposed method will never have stability problems for the following reason: It is obvious that the magnitude of the error is equal to $\frac{2w^8}{945}$ and we can have a reasonable accuracy when $|w| < 1.5$. It can be seen that large parts of the surroundings of the line between the points (0, 0) and (1.5, 1.5) are belonged in the stability region.

Remark 2 From the study of the stability regions, it can be seen that the family of the methods (3) has a non-empty region of stability when $-4 \leq a < 0$ and a being a fixed value. A serious problem occur since the smallest possible error constant (in the absolute value of the LTE), when $a \in [0, 4]$, is obtained at the point $a = 0$. Then, the produced method is completely unstable (see the footnote at the end of Sect. 2.1). We note that the produced method in this article has a non-empty region of stability and is almost P-stable in the case that the frequency of the exponential fitting is the same as the frequency of the scalar test equation.

3 Numerical results—conclusion

In order to illustrate the efficiency of the new obtained method given by coefficients (18) and (19) we apply it to the radial time independent Schrödinger equation.

In order to apply the new method to the radial Schrödinger equation the value of parameter v is needed. For every problem of the one-dimensional Schrödinger equation given by (1) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{40}$$

where $V(x)$ is the potential and E is the energy.

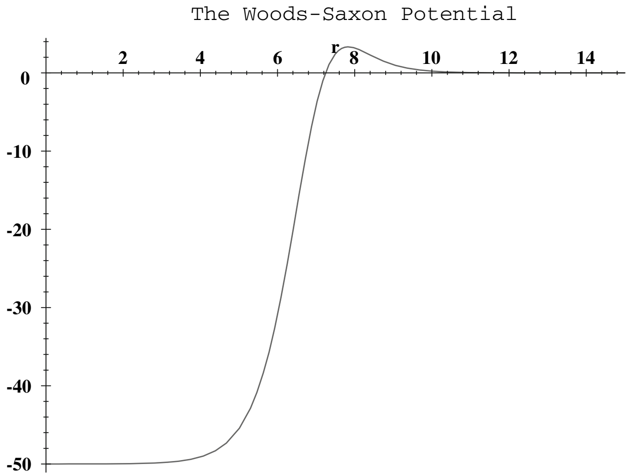

Fig. 3 The Woods–Saxon potential

3.1 Woods-Saxon potential

We use as potential the well known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{41}$$

with $z = exp\left[(x - X_0)/a\right],\ u_0 = -50,\ a = 0.6$, and $X_0 = 7.0$.

The behavior of Woods-Saxon potential is shown in the Fig. 3.

For some well known potentials, such as the Woods-Saxon potential, the definition of parameter v is not given as a function of x but based on some critical points which have been defined from the study of the appropriate potential (see for details [13]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [13]):

$$v = \begin{cases} \sqrt{-50+E}, & \text{for x} \in [0, 6.5 - 2\text{h}], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5 - h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5 + h \\ \sqrt{E}, & \text{for } x \in [6.5 + 2h, 15] \end{cases} \tag{42}$$

3.2 Radial Schrödinger equation—The resonance problem

Consider the numerical solution of the radial time independent Schrödinger Eq. (1) in the well-known case of the Woods-Saxon potential (41). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$. We consider Eq. (1) in a rather large domain of energies, i.e. $E \in [1, 1000]$.

In the case of positive energies, $E = k^2$, the potential dies away faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{43}$$

for x greater than some value X.

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[sin\left(kx - \frac{l\pi}{2}\right) + tan\delta_l cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{44}$$

where δ_l is the phase shift that may be calculated from the formula

$$tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{45}$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need y_0 before starting a one-step method. From the initial condition we obtain y_0. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l.

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$. We actually solve the latter problem, known as **the resonance problem** when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0, \;\; y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{46}$$

We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using:

- the Numerov's method which is indicated as **Method I**
- the Exponentially-fitted method of Numerov type developed by Raptis and Allison [10] which is indicated as **Method II**
- the Exponentially-fitted four-step method developed by Raptis [16] which is indicated as **Method III**
- the Two-Step P-stable exponentially-fitted method developed by Kalogiratou and Simos [18] which is indicated as **Method IV**
- the Four-Step method mentioned in Henrici [64] which is indicated as **Method V**

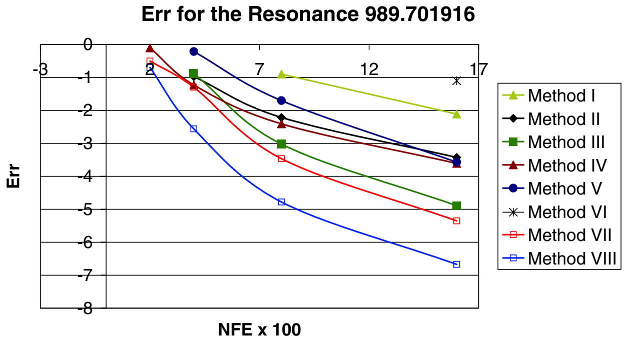

Fig. 4 Comparison of the maximum errors Err in the computation of the resonance $E_3 = 989.701916$ using the Methods I–VIII. The values of Err have been obtained based on the $NFEx100$. The absence of values of Err for some methods indicates that for these values of NFEx100 = Number of Function Evaluations, the Err is positive

- the Two-Step P-stable method obtained by Chawla [65] which is indicated as **Method VI**
- the P-stable trigonometrically-fitted four-step method obtained by Simos [66] which is indicated as **Method VII**
- the new P-stable trigonometrically-fitted four-step method produced in this article which is indicated as **Method VII**

The computed eigenenergies are compared with exact ones. In Fig. 4 we present the maximum absolute error $log_{10}(Err)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{47}$$

of the eigenenergy E_3, for several values of NFEx100 = Number of Function Evaluations.

4 Conclusions

In the present article we have obtained a new exponentially-fitted four-step method for the numerical solution of the radial Schrödinger equation. For this method we have examined the stability properties. The new method is almost P-stable only in the case that the frequency of the exponential fitting is the same as the frequency of the scalar test equation. The new method integrates also exactly every linear combination of the functions

$$\{1,\ x,\ \exp\left(\pm I\ v\, x\right),\ x\ \exp\left(\pm I\ v\right),\ x^2\ \exp\left(\pm I\ v\, x\right)\}. \tag{48}$$

We have applied the new method to the resonance problem of the radial Schrödinger equation.

Based on the results presented above we have the following conclusions:

- The P-stable exponentially-fitted Numerov's type method of Kalogiratou and Simos (see [18]) is more efficient than the Numerov's method and the method of Raptis and Allison [10].
- The exponentially-fitted four-step method developed by Raptis [16] is more efficient than Numerov's method. For number of function evaluations equal to 400 the behavior is worse than the methods of Raptis and Allison [10] and Kalogiratou and Simos [18].
- The exponentially-fitted method Raptis and Allison [10] is more efficient than the Numerov's method.
- The P-stable trigonometrically-fitted four-step method obtained by Simos [66] is more efficient than all the other methods (except the new one).
- Finally, the new obtained method is much more efficient than all the other methods.

The reason of the better behavior of the new method is the combination of the P-stability, smallest LTE constant and the exponential fitting property.

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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