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A four-step exponentially fitted method for the numerical solution of the Schrödinger equation

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In this paper, we present an exponentially fitted four-step method for the numerical solution of the radial Schrödinger equation. More specifically we present a method that integrates exactly the functions $\{\exp(\pm wx), x\{\exp(\pm wx)\}$. We illustrated the efficiency of our newly produced scheme against well known methods, with excellent results. The numerical results showed that our method is considerably more efficient compared to well known methods used for the numerical solution of resonance problem of the radial Schrödinger equation.

KEY WORDS: numerical solution, Schrödinger equation, linear multistep methods, stability, exponential fitting, trigonometric fitting

1. Introduction

The radial Schrödinger equation can be written as:

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

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

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 $r \to \infty$.
- The quantity k^2 is a real number denoting *the energy*.
- The quantity l is a given integer representing *angular momentum*.
- The quantity 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.

The last decades a lot of research has been done on the development of numerical methods for the numerical 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 (see, e.g. [5–62]).

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 dependent on the frequency of the problem.[1]

In this paper, we will investigate methods of the second category. We will investigate the exponentially-fitted methods. We note that recently Ixaru and Vanden Berghe [45] have published a very interesting book on exponential fitting. More specifically we will obtain an exponentially fitted method of sixth algebraic order for the numerical solution of the radial Schrödinger equation. We apply the new obtained method to the resonance problem of the radial Schrödinger equation. The above application shows the efficiency of the new obtained method.

2. The new trigonometrically fitted four-step method

2.1. Construction of the new method

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

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

In order the above method (3) to be exact for the functions

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

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

$$\begin{aligned} 2\cos(2\, v\, h) - 4\cos(v\, h) + 2\, a = &- 2\, h^2\, v^2 \cos(2\, v\, h)\, b_0 \\ &- 2\, h^2\, v^2\, b_1 \cos(v\, h) - h^2\, v^2\, b_2. \end{aligned} \tag{5}$$

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

In order the above method (3) to be exact for the functions

$$\{x \exp(\pm I\, v\, x)\}, \tag{6}$$

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

$$\begin{aligned} & h^2 v^2 b_2 x + 2 h^2 v^2 b_0 x \cosh(2 v h) \\ & +4 x \cosh(v h) - 4 \cos(v h) x + 2 x \cos(2 v h) \\ & - 2 x \cosh(2 v h) + 2 h^2 v^2 b_1 \cosh(v h) x \\ = & -h^2 v^2 b_2 x - 2 h^2 v^2 b_0 x \cos(2 v h) - 2 h^2 v^2 b_1 \cos(v h) x \qquad (7) \\ & -4 h \sin(v h) + 4 h \sin(2 v h) = -4 h^3 v^2 b_0 \sin(2 v h) \\ & +4 h^2 v \cos(2 v h) b_0 - 2 h^3 v^2 b_1 \sin(v h) \\ & + 4 h^2 v b_1 \cos(v h) + 2 h^2 v b_2. \qquad (8) \end{aligned}$$

We apply the coefficients founded from the solution of the system of equations (5)–(8) to the method (3) and we define the local truncation error expanding (LTE) the appropriate terms in Taylor series expansions. We find the following expression of the LTE:

$$\begin{aligned} LTE = & h^6 \left(\frac{13}{60} v^4 q_n^{(2)} - \frac{13}{60} v^2 q_n^{(4)} + \frac{13}{60} v^6 q_n + \frac{1}{4} v^2 q_n^{(4)} b_1 \right. \\ & \left. -\frac{1}{4} v^6 q_n b_1 - \frac{13}{60} q_n^{(6)} + \frac{1}{4} b_1 q_n^{(6)} - \frac{1}{4} b_1 q_n^{(2)} v^4 \right) \\ & + h^8 \left(\frac{1}{24} b_1 q_n^{(8)} - \frac{13}{180} v^2 q_n^{(6)} + \frac{1}{12} v^2 q_n^{(6)} b_1 - \frac{1}{12} v^6 q_n^{(2)} b_1 + \frac{19}{3024} v^4 q_n^{(4)} \right. \\ & \left. + \frac{13}{180} v^6 q_n^{(2)} + \frac{997}{30240} v^8 q_n - \frac{1}{24} v^8 q_n b_1 - \frac{1187}{30240} q_n^{(8)} \right) + \cdots \end{aligned} \tag{9}$$

In order the method to be of sixth order algebraic the following equation must hold:

$$\frac{13}{60} - \frac{1}{4} b_1. \tag{10}$$

Solving the system of equations (5), (7), (8) and (10) we obtain:

$$
\begin{aligned}
a = {} & -\cos(2\,v\,h) + 2\cos(v\,h) - h^2\,v^2\cos(2\,v\,h)\,b_0 \\
& -h^2\,v^2\,b_1\cos(v\,h) - \frac{1}{2}\,h^2\,v^2\,b_2 \\
b_0 = {} & (-60\,e^{(3\,v\,h)}\,h\,v\sin(2\,v\,h) - 30\cos(2\,v\,h)\,e^{(3\,v\,h)} \\
& -30\,e^{(4\,v\,h)} - 30\,e^{(2\,v\,h)} + 60\cos(v\,h)\,e^{(3\,v\,h)} \\
& -13\,h^2\,v^2\,e^{(2\,v\,h)} + 15\,e^{(5\,v\,h)} + 15\,e^{(v\,h)} - 13\,h^2\,v^2\,e^{(4\,v\,h)} \\
& +26\,h^2\,v^2\cos(v\,h)\,e^{(3\,v\,h)} + 60\,e^{(3\,v\,h)}\,h\,v\sin(v\,h) - 26\,e^{(3\,v\,h)}\,h^3\,v^3\sin(v\,h))/ \\
& (15\,v^2\,h^2\,e^{(5\,v\,h)} + 15\,v^2\,h^2\,e^{(v\,h)} - 30\,v^2\,h^2\cos(2\,v\,h)\,e^{(3\,v\,h)} \\
& +60\,v^3\,h^3\,e^{(3\,v\,h)}\sin(2\,v\,h)) \\
b_1 = {} & \frac{13}{15} \\
b_2 = {} & (-60\,e^{(3\,v\,h)}\cos(3\,v\,h) + 30\,e^{(3\,v\,h)}\cos(4\,v\,h) - 26\,h^3\,v^3\sin(2\,v\,h)\,e^{(2\,v\,h)} \\
& +90\,e^{(3\,v\,h)}\,h\,v\sin(v\,h) + 30\,h\,v\,e^{(3\,v\,h)}\sin(3\,v\,h) \\
& +30\,e^{(3\,v\,h)} - 26\,h^2\,v^2\cos(v\,h)\,e^{(v\,h)} \\
& -13\,h^3\,v^3\,e^{(3\,v\,h)}\sin(3\,v\,h) + 60\cos(2\,v\,h)\,e^{(2\,v\,h)} + 60\,e^{(4\,v\,h)}\cos(2\,v\,h) \\
& -60\cos(v\,h)\,e^{(3\,v\,h)} + 60\,h\,v\sin(2\,v\,h)\,e^{(5\,v\,h)} - 30\sin(v\,h)\,v\,h\,e^{(5\,v\,h)} \\
& -26\,h^2\,v^2\cos(v\,h)\,e^{(5\,v\,h)} - 60\,h\,v\sin(2\,v\,h)\,e^{(4\,v\,h)} - 30\cos(2\,v\,h)\,e^{(5\,v\,h)} \\
& -39\,e^{(3\,v\,h)}\,h^3\,v^3\sin(v\,h) - 60\,h\,v\sin(2\,v\,h)\,e^{(2\,v\,h)} + 60\,h\,v\sin(2\,v\,h)\,e^{(v\,h)} \\
& -30\sin(v\,h)\,v\,h\,e^{(v\,h)} - 30\cos(2\,v\,h)\,e^{(v\,h)} - 26\,h^3\,v^3\sin(2\,v\,h)\,e^{(4\,v\,h)} \\
& +26\cos(2\,v\,h)\,h^2\,v^2\,e^{(2\,v\,h)} + 26\cos(2\,v\,h)\,h^2\,v^2\,e^{(4\,v\,h)} \\
& +13\,h^3\,v^3\sin(v\,h)\,e^{(5\,v\,h)} + 13\,h^3\,v^3\sin(v\,h)\,e^{(v\,h)})/(15\,v^2\,h^2\,e^{(5\,v\,h)} \\
& +15\,v^2\,h^2\,e^{(v\,h)} - 30\,v^2\,h^2\cos(2\,v\,h)\,e^{(3\,v\,h)} + 60\,v^3\,h^3\,e^{(3\,v\,h)}\sin(2\,v\,h)).
\end{aligned}
\tag{11}
$$

For small values of v the formulae given by (11) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_0 = {} & \frac{3}{40} - \frac{19}{12096}\,h^4\,v^4 - \frac{31}{100800}\,h^6\,v^6 + \frac{8539}{479001600}\,h^8\,v^8 \\
& + \frac{1568477}{65383718400}\,h^{10}\,v^{10} + \frac{80060597}{15692092416000}\,h^{12}\,v^{12} + \cdots \\
b_2 = {} & \frac{7}{60} + \frac{19}{6048}\,h^4\,v^4 + \frac{31}{50400}\,h^6\,v^6 + \frac{389573}{239500800}\,h^8\,v^8 \\
& + \frac{2367383}{6538371840}\,h^{10}\,v^{10} - \frac{117196661}{7846046208000}\,h^{12}\,v^{12} + \cdots \\
a = {} & 1 - \frac{19}{12096}\,h^8\,v^8 - \frac{31}{50400}\,h^{10}\,v^{10} - \frac{3637}{39916800}\,h^{12}\,v^{12} + \cdots
\end{aligned}
\tag{12}
$$

The LTE of the new method is given by:

$$\text{LTE} = \frac{19\,h^8}{6048}\left(-q_n^{(8)} + 2\,v^4\,q_n^{(4)} - v^8\,q_n\right). \tag{13}$$

3. Stability of the method

We apply the new method to the scalar test equation:

$$y'' = -q^2 y, \tag{14}$$

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

$$A(q,h)\,\left(y_{n+2} + y_{n-2}\right) + B(q,h)\,\left(y_{n+1} + y_{n-1}\right) + C(q,h)\,y_n = 0, \tag{15}$$

where

$$A(q,h) = 1 + q^2\,h^2\,b_0,\ B(q,h) = -2 + q^2\,h^2\,b_1,\ \text{and}\ C(q,h) = 2\,a + q^2\,h^2\,b_2. \tag{16}$$

The corresponding characteristic equation is given by:

$$A(q,h)\,\left(\lambda^4 + 1\right) + B(q,h)\,\left(\lambda^3 + \lambda\right) + C(q,h)\,\lambda^2 = 0. \tag{17}$$

Definition 1 (see [56]). A symmetric four-step method with the characteristic equation given by (17) 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

$$z_{1,2} = e^{\pm i\,\theta(q\,h)}, \quad |z_i| \leq 1, \quad i = 3, 4, \tag{18}$$

where $\theta(q\,h)$ is a real functions of $q\,h$ and $H = q\,h$.

Definition 2 (see [56]). A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

We have the following Theorem:

Theorem 1 (see [39]). A symmetric four-step method with the characteristic equation given by (17) 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 following relations are hold

$$\begin{gathered} P_1(H,w) \geqslant 0,\ P_2(H,w) \geqslant 0,\ P_3(H,w) \geqslant 0, \\ N(H,w) = P_2(H,w)^2 - 4\,P_1(H,w)\,P_3(H,w) \geqslant 0 \end{gathered} \tag{19}$$

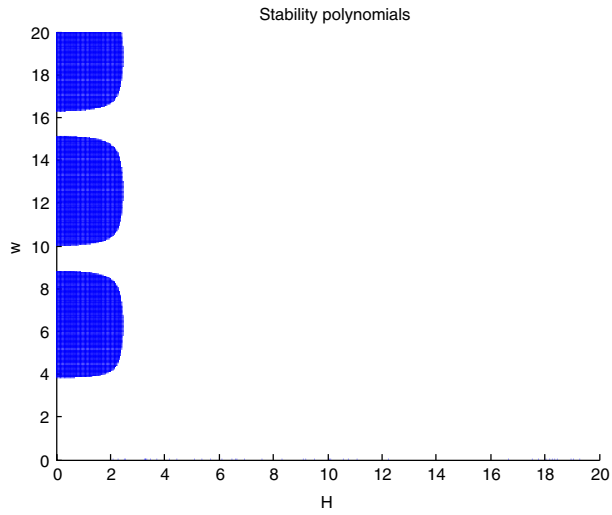

Figure 1. The $w - H$ plane for the new method.

and

$$\begin{aligned} P_1(H,w) &= 2\,A(H,w) - 2\,B(H,w) + C(H,w) \geqslant 0,\\ P_2(H,w) &= 12\,A(H,w) - 2\,C(H,w) \geqslant 0,\\ P_3(H,w) &= 2\,A(H,w) + 2\,B(H,w) + C(H,w) \geqslant 0,\\ N(H,w) &= P_2(H,w)^2 - 4\,P_1(H,w)\,P_3(H,w) \geqslant 0, \end{aligned} \tag{20}$$

where $w = v\,h$ and $H = q\,h$.

In figure 1, we present the $w - H$ plane. In figure 2 we present the stability polynomials $P_j(H,w)$, $j = 1(1)3$ in the case $H = w$. We note here that in the case $H = w$ the stability polynomial $N(H,w) \geqslant 0$ for $H^2 \in (0,\infty)$. It can be seen from figure 2 that the interval of periodicity of the new method is $(0, 9.02)$.

4. Numerical results – conclusion

In order to test the efficiency of the new method given by coefficients (11) and (12) we apply them to the radial Schrödinger equation.

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

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|}, \tag{21}$$

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

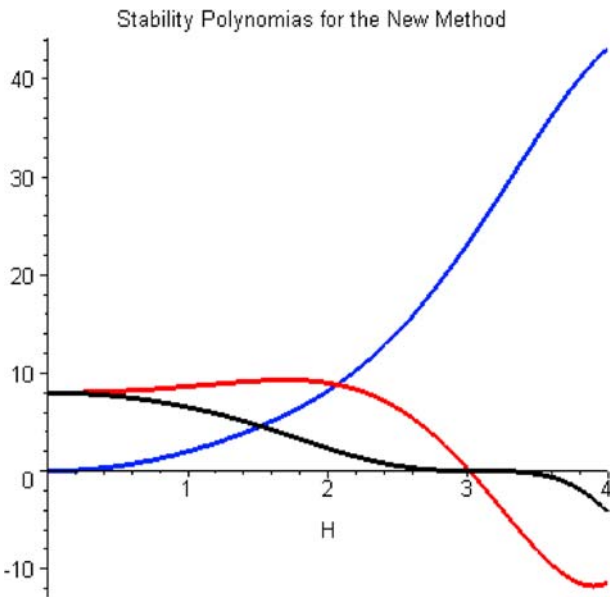

Figure 2. The stability polynomials $P_j(H)$; $j = 1(1)3$ for the new method in the case $H = w$.

For some well known potentials, such as Woods–Saxon potential, the definition of parameter v is given not 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 [28]).

4.1. *Woods–Saxon potential*

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

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\left(1+z^2\right)} \tag{22}$$

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 figure 2.

For the purpose of obtaining our results it is appropriate to choose v as follows (see for details [28])(figure 3):

$$v = \begin{cases} \sqrt{-50+E} & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E} & \text{for } x = 6.5-h, \\ \sqrt{-25+E} & \text{for } x = 6.5, \\ \sqrt{-12.5+E} & \text{for } x = 6.5+h, \\ \sqrt{E} & \text{for } x \in [6.5+2h, 15]. \end{cases} \tag{23}$$

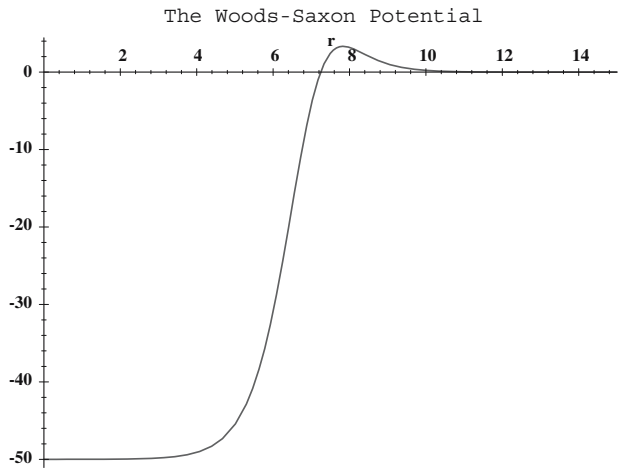

Figure 3. The Woods–Saxon potential.

4.2. *Radial Schrödinger equation - the resonance problem*

Consider the numerical solution of the radial Schrödinger equation (1) in the well-known case where the potential is the Woods–Saxon potential (22). 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 equation (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 Shrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{24}$$

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 equation (1) has (when $x \to 0$) the asymptotic form

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\,\delta_l\,\cos\left(kx - \frac{l\pi}{2}\right)\right], \end{aligned} \tag{25}$$

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

$$\tan\,\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{26}$$

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:

$$y(0) = 0, \quad y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{27}$$

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 [25] which is indicated as **Method II**;
- the exponentially fitted four-step method developed by Raptis [40] which is indicated as **Method III**;
- the two-step P-stable exponentially fitted method developed by Kalogiratou and Simos [42] which is indicated as **Method IV**;
- the four-step method mentioned in Henrici [43] which is indicated as **Method V**;
- the two-step P-stable method obtained by Chawla [44] which is indicated as **Method VI**
- the new P-stable trigonometrically fitted four-step method which is indicated as **Method VII**.

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

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}|, \tag{28}$$

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

The choice of the parameter v is based on (23).

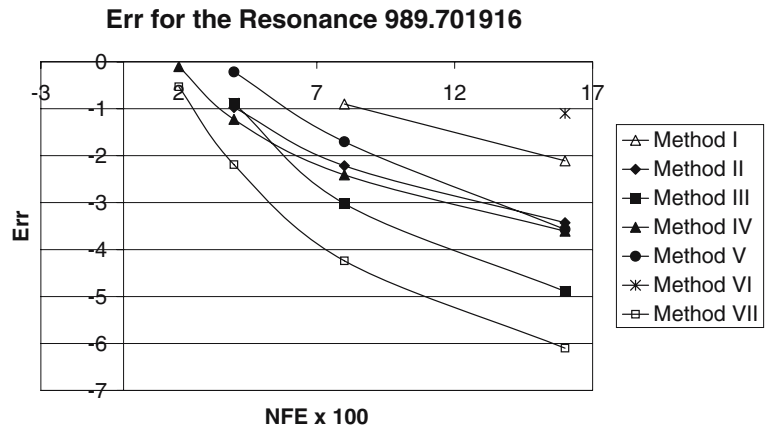

Figure 4. Comparison of the maximum errors Err in the computation of the resonance $E_3 = 989.701916$ using Methods I–VI. The values of Err have been obtained based on the $NFEx100$. The absence of values of Err for some methods indicates that for these values of NFEx100 = Number of Function Evaluations,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

5. Conclusions

In the present paper, we have developed an exponentially fitted four-step method for the numerical integration of the radial Schrödinger equation. The new method integrates exactly any linear combination of the functions

$$\{\exp(\pm w\,x)\,,\ x\,\exp(\pm w\,x)\}. \tag{29}$$

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 new exponentially fitted four-step method is much more efficient than all the other methods.
- The P-stable exponentially fitted Numerov's type method of Kalogiratou and Simos [42] has better behavior than the Numerov's method and the method of Raptis and Allison [25].
- The exponentially fitted four-step method developed by Raptis [40] is better then Numerov's method. For number of function evaluations equal to 200 and 400 is worse than the methods of Raptis and Allison [25] and Kalogiratou and Simos [42] but for number of function evaluations equal to 800 and 1600 is the second best method.
- Finally, the exponentially fitted method Raptis and Allison [25] has better behavior than the Numerov's method.

It is obvious that the combination of the minimization of the LTE and the exponential fitting property develops a new direction for the construction of efficient numerical methods for the solution of the Schrödinger equation and related problems.

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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Active Member of the European Academy of Sciences and Arts, Corresponding Member of the European Academy of Sciences and Corresponding Member of European Academy of Arts, Sciences and Humanities.

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