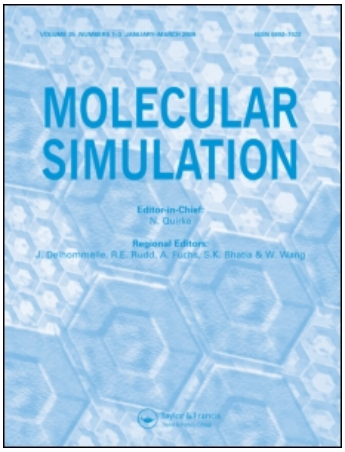

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A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation

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A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation

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In this paper we present a P-stable exponentially-fitted four-step method for the numerical integration of the radial Schrödinger equation. More specifically we present a method than satisfies the property of P-stability and also integrates exactly any linear combination of the functions $\{1, x, \exp(\pm wx), x\exp(\pm wx), x^2\exp(\pm wx)\}$. We tested the efficiency of our newly developed scheme against well known methods, with excellent results. The numerical illustration showed that our method is considerably more efficient compared to well-known methods used for the numerical integration of resonance problem of the radial Schrödinger equation.

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

PACS: 0.260; 95.10.E; *MSC*: 65L05; 65L06

1. Introduction

The radial Schrödinger equation can be written as:

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

The radial Schrödinger equation is a boundary value problem which occurs frequently in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics, etc. (see for example [1–4], [34–35], [39–52], [56–57]).

We give some definitions for equation (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.
- The boundary conditions are:

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

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

In recent decades a lot of research has been done on the construction of numerical methods for the solution of the Schrödinger equation. The aim of this research is the construction of fast and reliable methods for the numerical solution of the Schrödinger equation (see for example [5–17] and [18–32]).

The methods for the numerical 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. We will obtain an exponentially-fitted method of sixth algebraic order for the numerical solution of the one-dimensional Schrödinger equation. The developed method is also P-stable, i.e. it has an interval of periodicity equal to $(0, \infty)$. We apply the new developed method to

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the resonance problem of the one-dimensional Schrödinger equation. The above application shows the efficiency of the new constructed method.

2. The new P-stable trigonometrically-fitted four-step method

2.1 Construction of the new method

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

$$y_{n+2} + ay_{n+1} - (2+2a)y_n + ay_{n-1} + y_{n-2} = h^2[b_0(y''_{n+2} + y_{n-2}) + b_1(y''_{n+1} + y_{n-1}) + b_2 y''_n] \quad (3)$$

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

$$\{1, x, \exp(\pm wx), x\exp(\pm wx), x^2\exp(\pm wx)\} \quad (4)$$

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

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

$$\begin{aligned} 2h\sin(vh)(a + 4\cos(vh)) = &-2(2b_0 - b_2 - 2b_1\cos(vh) \\ &- 4b_0\cos(vh)^2 + hb_1v\sin(vh) \\ &+ 4hb_0v\cos(vh)\sin(vh))h^2v \end{aligned} \quad (6)$$

$$\begin{aligned} &-2x^2a - 8h^2 + 16h^2\cos(vh)^2 + 4x^2\cos(vh)^2 \\ &- 4x^2 + 2ah^2\cos(vh) + 2x^2a\cos(vh) \\ &= -h^2(4b_0 - 2b_2 + 8hb_1v\sin(vh) + 2b_1v^2x^2\cos(vh) \\ &+ 4b_0v^2x^2\cos(vh)^2 + 16h^2b_0v^2\cos(vh)^2 \\ &+ 2h^2b_1v^2\cos(vh) - 8b_0\cos(vh)^2 - 4b_1\cos(vh) \\ &+ 32hb_0v\cos(vh)\sin(vh) \\ &- 8h^2b_0v^2 - 2b_0v^2x^2 + b_2x^2v^2) \end{aligned} \quad (7)$$

We note here that in order to produce the corresponding system of equations for the exponentially-fitted method the substitute of $I\ v$ with v is sufficient.

2.2 Stability of the new method

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

$$y'' = -v^2y. \quad (8)$$

We obtain the following difference equation:

$$\begin{aligned} &A(v,h)(y_{n+2} + y_{n-2}) + B(v,h)(y_{n+1} + y_{n-1}) \\ &+ C(v,h)y_n = 0 \end{aligned} \quad (9)$$

where

$$\begin{aligned} &A(v,h) = 1 + v^2h^2b_0, B(v,h) = a + v^2h^2b_1, \\ &\text{and} \quad C(v,h) = -2 - 2a + v^2h^2b_2. \end{aligned} \quad (10)$$

The corresponding characteristic equation is given by:

$$A(v,h)(\lambda^4 + 1) + B(v,h)(\lambda^3 + \lambda) + C(v,h)\lambda^2 = 0 \quad (11)$$

Definition 1. (see [37]) A symmetric four-step method with the characteristic equation given by (11) 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

$$z_{1,2} = \mathrm{e}^{\pm i\theta(vh)}, \quad |z_i| \le 1, \quad i = 3, 4 \quad (12)$$

where $\theta(v\ h)$ is a real functions of $v\ h$.

Definition 2. (see [37]) 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 four-step method we require that the characteristic equation (11) have the following roots:

$$\exp(Ivh), \exp(-Ivh), -\exp(Ivh), -\exp(-Ivh) \quad (13)$$

In order (13) to be satisfied, the following system of equations must hold:

$$\begin{aligned} &4(1 + v^2h^2b_0)\cos(vh)^2 - 2(a + v^2h^2b_1)\cos(vh) \\ &- 4 - 2v^2h^2b_0 - 2a + v^2h^2b_2 = 0 \end{aligned} \quad (14)$$

$$\begin{aligned} &4(1 + v^2h^2b_0)\cos(vh)^2 + 2(a + v^2h^2b_1)\cos(vh) \\ &- 4 - 2v^2h^2b_0 - 2a + v^2h^2b_2 = 0 \end{aligned} \quad (15)$$

Solving the system of equations (5), (6), (7), (14), (15) we obtain the following values of the coefficients of the methods (we note hear that the equation (15) is an identity):

$$\begin{aligned} b_0 &= -\frac{2w\cos(w) + w - \sin(w)\cos(w) - 2\sin(w)}{(-3\sin(w)\cos(w) + 2w\cos(w) + w)w^2} \\ b_1 &= \frac{2(\cos(w)+1)(-3\sin(w)\cos(w) + 2w\cos(w)^2 + w)}{(-3\sin(w)\cos(w) + 2w\cos(w) + w)w^2} \\ b_2 &= -\frac{A(w)}{(-3\sin(w)\cos(w) + 2w\cos(w) + w)w^2} \\ a &= -\frac{B(w)}{-3\sin(w)\cos(w) + 2w\cos(w) + w} \end{aligned} \quad (16)$$

where

$$A(w)=2(4w\cos(w)^3+4w\cos(w)^2+w-4\sin(w)\cos(w)^3 -2\sin(w)\cos(w)^2-\sin(w)\cos(w)-2\sin(w))$$
$$B(w)=2(2w\cos(w)^3-3\sin(w)\cos(w)^2 +2w\cos(w)^2+w\cos(w)-3\sin(w)\cos(w)+w)$$

and $w = v\,h$.

For small values of w the formulae given by equation (16) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
b_0 &= \tfrac{1}{15}+\tfrac{17}{1575}w^2+\tfrac{163}{94500}w^4+\tfrac{60607}{218295000}w^6+\tfrac{1697747}{37837800000}w^8\\
&\quad+\tfrac{519335027}{71513442000000}w^{10}+\tfrac{12254045443}{10420530120000000}w^{12}\\
&\quad+\tfrac{609739626367891}{3201499468767600000000}w^{14}+\ldots\\
b_1 &= \tfrac{16}{15}-\tfrac{208}{1575}w^2+\tfrac{247}{23625}w^4+\tfrac{4154}{27286875}w^6+\tfrac{1790779}{28378350000}w^8\\
&\quad+\tfrac{606383}{62511750000}w^{10}+\tfrac{28752907369}{18235927710000000}w^{12}\\
&\quad+\tfrac{6387572067797}{25011714599746875000}w^{14}+\ldots\\
b_2 &= \tfrac{26}{15}-\tfrac{1298}{1575}w^2+\tfrac{727}{6750}w^4-\tfrac{1003979}{109147500}w^6+\tfrac{13137323}{56756700000}w^8\\
&\quad-\tfrac{94972363}{2750517000000}w^{10}-\tfrac{127664236097}{36471855420000000}w^{12}\\
&\quad-\tfrac{979315457827727}{160074973438380000000}w^{14}+\ldots\\
a &= -\tfrac{16}{15}w^2+\tfrac{208}{1575}w^4-\tfrac{247}{23625}w^6-\tfrac{4154}{27286875}w^8\\
&\quad-\tfrac{1790779}{28378350000}w^{10}-\tfrac{606383}{62511750000}w^{12}-\tfrac{28752907369}{18235927710000000}w^{14}+\ldots
\end{aligned} \tag{17}$$

The Local Truncation Error ($LTE(h)$) of the new method is given by:

$$\mathrm{LTE}(h) = -\frac{2h^8}{945}\left(y_n^{(8)}+3v^2y_n^{(6)}+3v^4y_n^{(4)}+v^6y_n^{(2)}\right) \tag{18}$$

Based on the theory developed in [5,6,53,54], a four-step method with a characteristic equation given by equation (11) is P-stable if the following theorem is hold:

Theorem 1. ([54]) A symmetric four-step method with the characteristic equation given by equation (11) 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

$$\begin{aligned}
P_1(w) &= 2A(w) - 2B(w) + C(w) \geq 0,\\
P_2(w) &= 12A(w) - 2C(w) \geq 0,\\
P_3(w) &= 2A(w) + 2B(w) + C(w) \geq 0
\end{aligned} \tag{19}$$

Based on the above theorem and substituting the polynomials $A(w)$, $B(w)$ and $C(w)$ given by equation (10) and the coefficients b_i, $i = 0(1)2$, a given by equation (16), it is easy for one to see that the conditions equation (19) are satisfied for all $H \in (0, \infty)$ except the values for which:

$$T(w) = -3\sin(2w) + 4w\cos(w) + 2w = 0 \tag{20}$$

i.e. the method is P-Stable. We note here that $T(w)$ is the denominator of the stability polynomials $P_i(w)$, $i = 1(1)3$.

3. Numerical results–conclusion

In order to illustrate the efficiency of the new method given by coefficients (16) and (17) we apply them to the one-dimensional 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 equation (1) the parameter v is defined by

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

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

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 and properties which have been defined from the study of the appropriate potential (see for details [36]).

3.1 Woods–Saxon potential

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

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

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

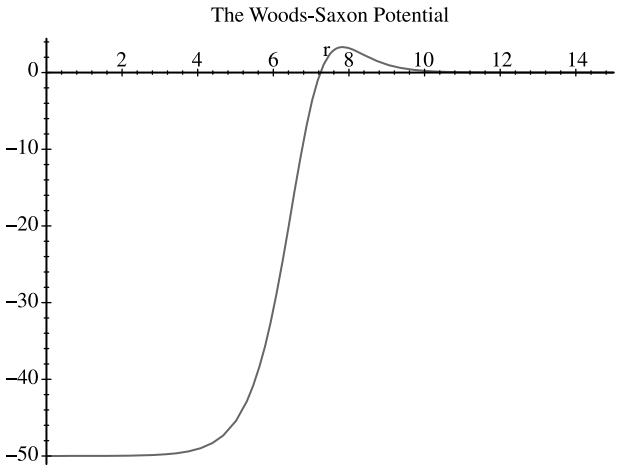

Figure 1. The Woods–Saxon potential.

The behavior of Woods–Saxon potential is shown in figure 1.

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [36]):

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

3.2 Radial Schrödinger equation—the resonance problem

Consider the numerical solution of the radial Shrödinger equation (1) in the well-known case where the potential is the Woods–Saxon potential equation (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 $l(l+1)/x^2$ 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

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

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 $\delta_l = \pi/2$. 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:

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

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 [33] which is indicated as Method II.
- the exponentially-fitted method of Numerov type developed by Ixaru and Rizea [36] which is indicated as Method III.
- the exponentially-fitted four-step method developed by Raptis [55] which is indicated as Method IV.
- the new P-stable trigonometrically-fitted four-step method which is indicated as Method V.

The computed eigenenergies are compared with exact ones. In figures 2, 3 and 4 we present the maximum absolute error $\log_{10}(\text{Err})$ where

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

of the eigenenergies E_1, E_2 and E_3 respectively, for several values of $NFEx100 = Number\ of\ Function\ Evaluations$.

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

4. Conclusions

In the present paper we have developed a P-stable exponentially-fitted four-step method for the numerical integration of the radial Schrödinger equation. The new

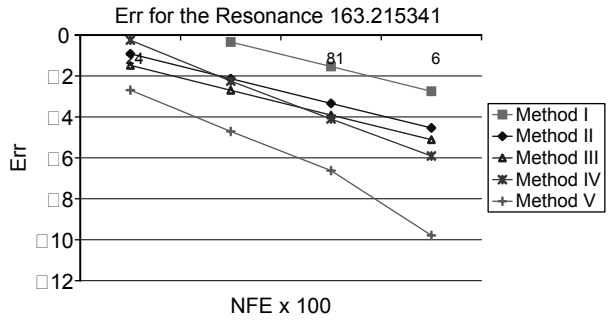

Figure 2. Comparison of the maximum errors Err in the computation of the resonance $E_1 = 163.215341$ using the Methods I–V. The values of Err have been obtained based on the *NFEx*100. The absence of values of Err for some methods indicates that for these values of NFEx100 = Number of Function Evaluations, the Err is positive.

method satisfies the property of P-stability and in the same time integrates exactly any linear combination of the functions

$$\{1, x, \exp(\pm wx), x\exp(\pm wx), x^2\exp(\pm wx)\}. \qquad (29)$$

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:

- For all the resonances the new P-stable exponentially-fitted four-step method is much more efficient than all the other methods.
- The exponentially fitted method developed by Ixaru and Rizea [36] has better behavior than the methods of Numerov, Raptis and Allison [33] and the exponentially-fitted four-step method developed by Raptis [55].
- The exponentially-fitted four-step method developed by Raptis [55] for the resonances 163.215341 341.495874 has better behavior for number of function evaluations equal to 1600 than the Numerov's method and the method developed by Raptis and Allison [33]. The method is better then Numerov's method for all the resonances. Finally for the resonance 989.701916 and

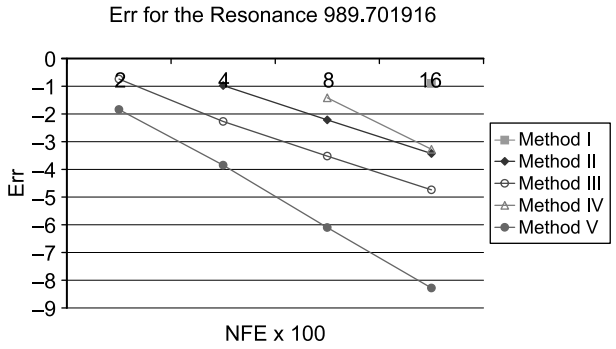

Figure 3. Comparison of the maximum errors Err in the computation of the resonance $E_2 = 341.495874$ using the Methods I–V. The values of Err have been obtained based on the *NFEx*100. The absence of values of Err for some methods indicates that for these values of NFEx100 = Number of Function Evaluations, the Err is positive.

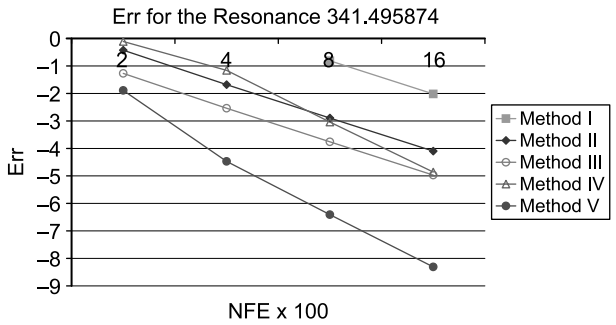

Figure 4. Comparison of the maximum errors Err in the computation of the resonance $E_3 = 989.701916$ using the Methods I–V. The values of Err have been obtained based on the *NFEx*100. The absence of values of Err for some methods indicates that for these values of NFEx100 = Number of Function Evaluations, the Err is positive.

for number of function evaluations equal to 200 and 400 for the other resonances is worse than the method of Raptis and Allison [33].

- Finally, the exponentially-fitted method Raptis and Allison [33] has better behavior than the Numerov's method.

It is obvious that the combination of the P-stability 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).

Note

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

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