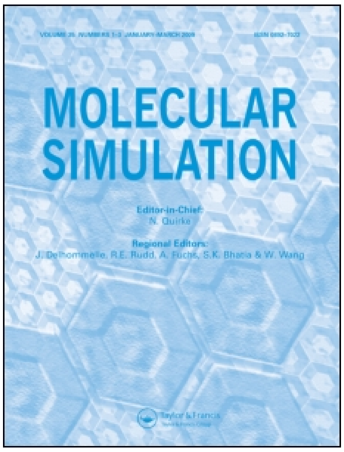

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An Accurate Exponentially-Fitted Four-Step Method for the Numerical Solution of the Radial Schrödinger Equation

T. E. Simos[a]
[a] Section of Mathematics, Department of Civil Engineering, School of Engineering, Democritus University of Thrace, Xanthi, Greece

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AN ACCURATE EXPONENTIALLY-FITTED FOUR-STEP METHOD FOR THE NUMERICAL SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION

T. E. SIMOS

Section of Mathematics, Department of Civil Engineering, School of Engineering, Democritus University of Thrace, GR-671 00 Xanthi, Greece

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We present here an accurate exponentially-fitted four-step method for the numerical integration of the one-dimensional Schrödinger equation. The formula considered contains free parameter which are defined in order to integrate exponential functions. Numerical results also indicate that the new method is much more accurate than other well known methods.

Keywords: Schrödinger equation; Numerov-type methods; exponentially-fitted methods; resonance problem

1. INTRODUCTION

There is a real need for the numerical solution of the Schrödinger equation for many scientific areas, such as the nuclear physics, the physical chemistry, the theoretical physics and chemistry (see [13, 27]).

There is much activity in the area of the solution of the one-dimensional Schrödinger equation. The result of this activity is the development of a great number of methods (see [1–4], [5–30], [36]).

The one dimensional Schrödinger equation has the form:

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

where k^2 is a real number denoting *the energy*, l is a given integer and V is a given function which denotes *the potential*. The function $W(x) = l(l+1)/x^2$

$+ V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$. The boundary conditions are:

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

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

Boundary value methods based on either collocation or finite differences are not very popular for the solution of (1) due to the fact that the problem is posed on an infinite interval. Initial value methods, such as shooting, also need to take into account the fact that $|y'(x)|$ may be very large near $x = 0$. The aim of this paper is to derive more efficient integrators to solve equation (1) in a shooting approach.

One of the most popular methods for the solution of (1) is **Numerov's method**. This method is only of order four, but in practice it has been found to have a superior performance to certain higher order four-step methods. The reason for this, as proved in [21], is that the Numerov method has the same phase-lag order as the four-step methods but it has a larger interval of periodicity. For this reason the improvement of the behavior of the four-step methods is an interesting area. This is the subject of the present paper.

An alternative approach to deriving higher order methods for (1) was given by Cash and Raptis [2]. In [2], a sixth order Runge-Kutta type method with a large interval of periodicity was derived. This method has a phase-lag of order six (while Numerov's method has phase-lag of order four) and a much larger interval of periodicity than the method of Numerov. More recently Simos [28] has derived a sixth order method with phase-lag of order eight and with a large interval of periodicity. Simos, also, in [36] has derived Numerov-type methods with phase-lag of order infinity for the numerical solution of the radial Schrödinger equation. Recently Simos [37] have derived an eighth order hybrid method, with constant coefficients, for accurate computation of elastic scattering phase shifts.

Another approach for developing efficient methods for the solution of (1) is to use exponential fitting. Raptis and Allison [19] have derived a Numerov type exponentially fitted method. Numerical results presented in [19] indicate that these fitted methods are much more efficient than Numerov's method for the solution of (1). Many authors have investigated the idea of exponential fitting, since Raptis and Allison. An interesting work in this general area is that of Ixaru and Rizea [7]. They showed that for the resonance problem defined by (1) it is generally more efficient to derive methods which exactly integrate functions of the form

$$\{1, x, x^2, \ldots, x^p, \exp(\pm vx), x\exp(\pm vx), \ldots, x^m\exp(\pm vx)\}, \tag{3}$$

where v is the frequency of the problem, than to use classical exponential fitting methods. The crucial concern when solving the Schrödinger equation is that the numerical method should integrate exactly the functions (3) with m as large as possible, as shown by [7] and [21]. For the method obtained by Ixaru and Rizea [7] we have $m=1$ and $p=1$. Another low order method of this type (with $m=2$ and $p=0$) was developed by Raptis [16]. Simos [22] has derived a four-step method of this type which integrates more exponential functions and gives much more accurate results than the four-step methods of Raptis [15,17]. For this mehtod we have $m=3$ and $p=0$. Simos [23] has derived a family of four-step methods which give more efficient results than other four-step methods. In particular, he has derived methods with $m=0$ and $p=5$, $m=1$ and $p=3$, $m=2$ and $p=1$ and finally $m=3$ and $p=0$. Also Raptis and Cash [20] have derived a two-step method fitted to (3) with $m=0$ and $p=5$ based on the well known Runge-Kutta-type sixth order formula of Cash and Raptis [2]. The method of Cash, Raptis and Simos [3] is also based on the formula proposed in [2] and is fitted to (3) with $m=1$ and $p=3$.

The purpose of this paper is to develop a simple and accurate exponentially fitted numerical method for the solution of the radial Schrödinger equation and in particular to derive a method with $m=4$ and $p=0$ i.e. to derive a method which integrates many more functions of the form (3) than the methods proposed previously. We note also that the above mentioned values of m is the largest value which we can obtain for this method. The new method is much more accurate than the exponentially-fitted methods obtained from Numerov's method and from the sixth order Runge-Kutta-type methods because it exactly integrates more exponential functions. We note also, that the new method is a very simple compared with the hybrid exponentially fitted methods [3,20,24]. We have applied the new method to *the resonance problem* (which arises from the one-dimensional Schrödinger equation) with two different types of potential. Note that *the resonance problem* is one of the most difficult to solve of all the problems based on the one-dimensional Schrödinger equation because it has highly oscillatory solutions, especially for large resonances.

2. BASIC THEORY OF THE EXPONENTIAL MULTISTEP METHODS

In this section we explain the derivation of the exponentially fitted methods.

For the numerical solution of the initial value problem

$$y^{(r)} = f(x, y), \quad y^{(j)}(A) = 0, \quad j = 0, 1, \dots, r-1 \tag{4}$$

the multistep methods of the form

$$\sum_{i=0}^{k} a_i y_{n+i} = h^r \sum_{i=0}^{k} b_i f(x_{n+i}, y_{n+i}) \tag{5}$$

over the equally spaced intervals $\{x_i\}_{i=0}^{k}$ in $[A, B]$ can be used.

The method (5) is associated with the operator

$$L(x) = \sum_{i=0}^{k} [a_i z(x+ih) - h^r b_i z^{(r)}(x+ih)] \tag{6}$$

where z is a continuously differentiable function.

DEFINITION 1 The multistep method (5) called algebraic (or exponential) of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \dots, x^{p+r-1}$(or $\exp(v_0 x)$, $\exp(v_1 x), \dots, \exp(v_{p+r-1} x)$ where v_i, $i = 0, 1, \dots, p+r-1$ are real or complex numbers).

Remark 1 (see [34]) If $v_i = v$ for $i = 0, 1, \dots, n, n \leqslant p+r-1$ then the operator L vanishes for any linear combination of $\exp(vx)$, $x\exp(vx)$, $x^2\exp(vx)$, $\dots, x^n\exp(vx)$, $\exp(v_{n+1}x), \dots, \exp(v_{p+r-1}x)$.

Remark 2 (see [34]) Every exponential multistep method corresponds in a unique way, to an algebraic multistep method (by setting $v_i = 0$ for all i).

LEMMA 1 *(For proof see* [34] *and* [35]*) Consider an operator L of the form (6). With $v \in \mathscr{C}$, $h \in \mathscr{R}$, $n \geqslant r$ if $v = 0$, and $n \geqslant 1$ otherwise, then we have*

$$L[x^m \exp(vx)] = 0, \quad m = 0, 1, \dots, n-1, \quad L[x^n \exp(vx)] \neq 0 \tag{7}$$

if and only if the function φ has a zero of exact multiplicity s at $\exp(vh)$, where $s = n$ if $v \neq 0$, and $s = n - r$ if $v = 0$, $\varphi(w) = \rho(w)/\log^r w - \sigma(w)$, $\rho(w) = \Sigma_{i=0}^{k} a_i w^i$ and $\sigma(w) = \Sigma_{i=0}^{k} b_i w^i$.

PROPOSITION 1 *(For proof see [18] and [21]) Consider an operator L with*

$$L[\exp(\pm v_j x)] = 0, \quad j = 0, 1, \ldots, k \leqslant \frac{p+r-1}{2} \tag{8}$$

then for given a_i and p with $a_i = (-1)^r a_{k-i}$ there is a unique set of b_i such that $b_i = b_{k-i}$.

In the present paper we investigate the case $r = 2$.

3. THE NEW METHOD

Consider the method:

$$\bar{y}_n = y_n - ah^2(y''_{n+2} - 4y''_{n+1} + 6y''_n - 4y''_{n-1} + y''_{n-2}) \tag{9}$$

$$y_{n+1} + a_1 y_n + y_{n-1} = h^2[b_0(y''_{n+2} + y''_{n-2}) + b_1(y''_{n+1} + y''_{n-1}) + b_2 \bar{y}''_n] \tag{10}$$

where, for example, $y''_{n+1} = f(x_{n+1})y_{n+1}$ with $x_{n+1} = x_n + h, f(x_{n+1}) = l(l+1)/x^2_{n+1} + V(x_{n+1}) - k^2$.

We have chosen to consider this family of methods because it has five free parameters. This is sufficient to allow the construction of methods which integrate more exponential functions than the analogue Runge-Kutta-type methods, with algebraic order six, proposed by Raptis and Cash [20], Cash, Raptis and Simos [3] and Simos [24].

We require that the family of methods (9)–(10) should integrate exactly any linear combination of the functions:

$$\{\exp(\pm vx), x\exp(\pm vx), x^2\exp(\pm vx), x^3\exp(\pm vx), x^4\exp(\pm vx)\} \tag{11}$$

To construct a method of the form (9)–(10) which integrates exactly the functions (11), we require that the method (9)–(10) integrates exactly (see section 2):

$$\{\exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x), \exp(\pm v_3 x), \exp(\pm v_4 x)\} \tag{12}$$

and then put:

$$v_0 = v_1 = v_2 = v_3 = v_4 = v \tag{13}$$

Demanding that (9)–(10) integrates (12) exactly, we obtain the following system of equations for b_0, b_1, b_2, a and a_1

$$-a_1+2w_j^2\cosh(2w_j)b_0+2w_j^2\cosh(w_j)b_1+b_2w_j^2-2w_j^4b_2a(\cosh(2w_j)-4\cosh(w_j)+3)=2\cos(w_j) \quad (14)$$

where $w_j=v_jh$, $j=0$, 1, 2, 3, and 4.

Solving for b_i, $i=0$, 1, 2, for a and a_1 we obtain:

$$\begin{aligned}
a_1={}&(-412w^3\sinh(4w)+2272w^3\sinh(w)+791\sinh(2w)w^3-15w^2\cosh(6w)\\
&-882w^2\cosh(4w)-1728w^2\cosh(3w)+6543w^2\cosh(2w)+4032w^2\cosh(w)\\
&-784w^3\sinh(3w)+11w^3\sinh(6w)-180w\sinh(6w)+16w^3\sinh(5w)\\
&+4896w\sinh(3w)-7950w^2+520w^4-1800+2w^4\cosh(6w)\\
&-72w^4\cosh(4w)-450w^4\cosh(2w)-432w\sinh(4w)-288w\sinh(5w)\\
&-4032w\sinh(w)-3204w\sinh(2w)+1800\cosh(4w)+180\cosh(2w)\\
&+2880\cosh(w)-2880\cosh(3w)\ -180\cosh(6w))/(68w^3\sinh(4w)\\
&-1472w^3\sinh(w)+152\sinh(2w)w^3\ +228w^2\cosh(4w)-270w^2\cosh(3w)\\
&-1920w^2\cosh(2w)+1212w^2\cosh(w)+8w^4\cosh(5w)-368w^4\cosh(w)\\
&+72w^4\cosh(3w)+192w^3\sinh(3w)+180\cosh(5w)+64w^3\sinh(5w)\\
&-1620w\sinh(3w)+210w^2\cosh(5w)+540w^2+72w^4-2880\\
&+8w^4\cosh(4w)+208w^4\cosh(2w)+288w\sinh(4w)+324w\sinh(5w)\\
&+7848w\sinh(w)-2880w\sinh(2w)+2880\cosh(2w)\\
&+1800\cosh(w)-1980\cosh(3w)),
\end{aligned}$$

$$\begin{aligned}
b_0={}&(36w^3\sinh(4w)+816w^3\sinh(w)-552\sinh(2w)w^3+228w^2\cosh(4w)\\
&-48w^2\cosh(3w)-672w^2\cosh(2w)-528w^2\cosh(w)+944w^4\cosh(w)
\end{aligned}$$

$$+ 16w^4\cosh(3w) + 48w^3\sinh(3w) - 288w\sinh(3w) + 1020w^2 + 65w^4$$

$$- 180 - 18w^6 - 49w^4\cosh(4w) - 976w^4\cosh(2w) + 216w\sinh(4w)$$

$$+ 2016w\sinh(w) - 1008w\sinh(w) + 36\cosh(4w) + 144\cosh(2w)$$

$$+ 144\cosh(w) - 144\cosh(3w) - 52w^6\cosh(2w) - 21w^5\sinh(4w)$$

$$- 462w^5\sinh(2w) - 2w^6\cosh(4w))/(180w^4\cosh(5w) + 1800w^4\cosh(w)$$

$$- 1980w^4\cosh(3w) - 1472w^7\sinh(w) + 68w^7\sinh(4w) - 368w^8\cosh(w)$$

$$+ 8w^8\cosh(5w) - 2880w^4 + 540w^6 + 72w^8 - 1620w^5\sinh(3w)$$

$$+ 208w^8\cosh(2w) + 324w^5\sinh(5w) + 2880w^4\cosh(2w) - 1920w^6\cosh(2w)$$

$$+ 152\sinh(2w)w^7 + 288w^5\sinh(4w) + 8w^8\cosh(4w) + 7848w^5\sinh(w)$$

$$- 2880w^5\sinh(2w) + 192w^7\sinh(3w) - 270w^6\cosh(3w) + 64w^7\sinh(5w)$$

$$+ 210w^6\cosh(5w) + 72w^8\cosh(3w) + 228w^6\cosh(4w) + 1212w^6\cosh(w)),$$

$$b_1 = (216w^3\sinh(4w) + 2556w^3\sinh(w) - 1200\sinh(2w)w^3 + 168w^2\cosh(4w)$$

$$- 1110w^2\cosh(3w) + 2052w^2\cosh(w) - 73w^4\cosh(5w) - 606w^4\cosh(w)$$

$$- 665w^4\cosh(3w) - 390w^3\sinh(3w) + 36\cosh(5w) + 30w^3\sinh(5w)$$

$$- 900w\sinh(3w) + 144 + 210w^2\cosh(5w) - 1320w^2 + 908w^4 - 72w^6$$

$$- 288w^5\sinh(3w) - 32w^5\sinh(5w) - 44w^4\cosh(4w) + 480w^4\cosh(2w)$$

$$- 144w\sinh(4w) + 180w\sinh(5w) - 504w\sinh(w) + 1440w\sinh(2w)$$

$$- 144\cosh(4w) - 216\cosh(w) + 180\cosh(3w) - 208w^6\cosh(2w)$$

$$- 52w^5\sinh(4w) + 160w^5\sinh(w) - 472w^5\sinh(2w) - 36w^6\cosh(3w)$$

$$- 4w^6\cosh(5w) - 8w^6\cosh(4w) + 184w^6\cosh(w))/(- 90w^4\cosh(5w)$$

$$- 900w^4\cosh(w) + 990w^4\cosh(3w) + 736w^7\sinh(w) - 34w^7\sinh(4w)$$

$$+ 184w^8\cosh(w) - 4w^8\cosh(5w) + 1440w^4 - 270w^6 - 36w^8$$

$$+ 810w^5\sinh(3w) - 104w^8\cosh(2w) - 162w^5\sinh(5w) - 1440w^4\cosh(2w)$$

$$+ 960w^6\cosh(2w) - 76\sinh(2w)w^7 - 144w^5\sinh(4w) - 4w^8\cosh(4w)$$

$$- 3924w^5\sinh(w) + 1440w^5\sinh(2w) - 96w^7\sinh(3w) + 135w^6\cosh(3w)$$

$$- 32w^7\sinh(5w) - 105w^6\cosh(5w) - 36w^8\cosh(3w) - 114w^6\cosh(4w)$$

$$- 606w^6\cosh(w)), \tag{15}$$

$$b_2 = (- 1752w^3\sinh(4w) - 8256w^3\sinh(w) + 6924\sinh(2w)w^3$$

$$+ 228w^2\cosh(6w) - 1056w^2\cosh(4w) + 1296w^2\cosh(3w) - 996w^2\cosh(2w)$$

$$- 4992w^2\cosh(w) + 112w^4\cosh(5w) + 6656w^4\cosh(w) - 3312w^4\cosh(3w)$$

$$- 336w^3 \sinh(3w) - 144\cosh(5w) + 204w^3\sinh(6w) + 144w\sinh(6w)$$

$$+ 240w^3\sinh(5w) + 576w\sinh(3w) + 240w^2\cosh(5w) + 2w^6\cosh(6w)$$

$$+ 5280w^2 - 6752w^4 + 412w^6 - 784w^5\sinh(3w) + 16w^5\sinh(5w)$$

$$+ 101w^4\cosh(6w) - 1472w^4 \cosh(4w) + 4667w^4\cosh(2w) - 432w\sinh(4w)$$

$$+ 5184w\sinh(w) - 3024w\sinh(2w) + 288\cosh(4w) + 252\cosh(2w)$$

$$+ 576\cosh(w) - 432\cosh(3w) + 36\cosh(6w) - 762w^6\cosh(2w)$$

$$- 586w^5\sinh(4w) + 2272w^5\sinh(w) - 576 - 1921 w^5\sinh(2w)$$

$$+ 23w^5\sinh(6w) - 84w^6 \cosh(4w))/(180w^4\cosh(5w) + 1800w^4\cosh(w)$$

$$- 1980w^4\cosh(3w) - 1472w^7\sinh(w) + 68w^7\sinh(4w) - 368w^8\cosh(w)$$

$$+ 8w^8\cosh(5w) - 2880w^4 + 540w^6 + 72w^8 - 1620w^5\sinh(3w)$$

$$+ 208w^8\cosh(2w) + 324w^5\sinh(5w) + 2880w^4\cosh(2w)$$

$$- 1920w^6\cosh(2w) + 152\sinh(2w)\,w^7 + 288w^5\sinh(4w)$$

$$+ 8w^8\cosh(4w) + 7848w^5\sinh(w) - 2880w^5\sinh(2w)$$

$$+ 192w^7\sinh(3w) - 270w^6\cosh(3w) + 64w^7\sinh(5w) + 210w^6\cosh(5w)$$

$$+ 72w^8\cosh(3w) + 228w^6\cosh(4w) + 1212w^6\cosh(w)),$$

$$a = (-45w^2 - 36\cosh(4w) + 144\cosh(2w) + 2w^4\cosh(4w) + 52w^4\cosh(2w)$$

$$+ 18w^4 - 108 - 36w\sinh(4w) - 3w^2\cosh(4w) + 72w\sinh(2w) + 9w^3\sinh(4w)$$

$$+ 198\sinh(2w)w^3 + 48w^2\cosh(2w))/(1752w^3\sinh(4w) + 8256w^3\sinh(4w)$$

$$- 6924\sinh(2w)w^3 - 228w^2\cosh(6w) + 1056w^2\cosh(4w) - 1296w^2\cosh(3w)$$

$$+ 996w^2\cosh(2w) + 4992w^2\cosh(w) - 112w^4\cosh(5w) - 6656w^4\cosh(w)$$

$$+ 3312w^4\cosh(3w) + 336w^3\sinh(3w) + 144\cosh(5w) - 204w^3\sinh(6w)$$

$$- 144w\sinh(6w) - 240w^3\sinh(5w) - 576w\sinh(3w) - 240w^2\cosh(5w)$$

$$- 2w^6\cosh(6w) - 5280w^2 + 6752w^4 - 412w^6 + 784w^5\sinh(3w)$$

$$- 16w^5\sinh(5w) - 101w^4\cosh(6w) + 1472w^4\cosh(4w) - 4667w^4\cosh(2w)$$

$$+ 432w\sinh(4w) - 5184w\sinh(w) + 3024w\sinh(2w) - 288\cosh(4w)$$

$$- 252\cosh(2w) - 576\cosh(w) + 432\cosh(3w) - 36\cosh(6w)$$

$$+ 762w^6\cosh(2w) + 586w^5\sinh(4w) - 2272w^5\sinh(w)$$

$$+ 576 + 1921w^5\sinh(2w) - 23w^5\sinh(6w) + 84w^6\cosh(4w)).$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use the following series expansion for the coefficients $b_i, i = 0, 1, a, b$ and a_1 of the method:

$$a_1 = -2 + \frac{67}{1814400}w^{10} - \frac{109}{10644480}w^{12},$$

$$b_0 = -\frac{1}{240} + \frac{67}{181440}w^4 - \frac{2699}{23950080}w^6 + \frac{1316057}{74724249600}w^8$$

$$-\frac{2800351}{2241727488000}w^{10} - \frac{77176907}{914624815104000}w^{12},$$

$$b_1 = \frac{1}{10} - \frac{67}{45360}w^4 + \frac{61}{748440}w^6 + \frac{490229}{9340531200}w^8$$

$$-\frac{4450711}{280215936000}w^{10} + \frac{156102617}{72754246656000}w^{12},$$

$$b_2 = \frac{97}{120} - \frac{67}{30240}w^4 + \frac{83}{1330560}w^6 + \frac{553477}{12454041600}w^8$$

$$-\frac{7861747}{373621248000}w^{10} + \frac{4670097431}{1067062284288000}w^{12},$$

$$a = -\frac{31}{48888} + \frac{67}{293328}w^2 - \frac{1906909}{52580803968}w^4 + \frac{1307021}{759500501760}w^6$$

$$+\frac{93203489}{174049033734576}w^8 - \frac{42886910725223}{292924523775291408000}w^{10}$$

$$+\frac{98578337594141 95307}{58045736159616529222778880 0}w^{12}. \tag{16}$$

The local truncation error of the above scheme is given by

$$L.T.E.(h) = \frac{31}{60480}h^8(y^{(8)})(x) + y^{(6)}(x)F_n) \tag{17}$$

where $y^{(n)}(x)$ is the n-th derivative of the $y(x)$ and $F_n = \partial f/\partial y$.

If $v = i\phi$, then the family of methods (4) is exact for any linear combination of the functions:

$$\{\sin(\phi x), \cos(\phi x), x\sin(\phi x), x\cos(\phi x), x^2\sin(\phi x), x^2\cos(\phi x),$$

$$x^3\sin(\phi x), x^3\cos(\phi x), x^4\sin(\phi x), x^4\cos(\phi x)\} \tag{18}$$

4. STABILITY ANALYSIS

If we apply the method (9)–(10) to the scalar test equation $y'' = -\phi^2 y$, we obtain the difference equation.

$$A_2(H)y_{n+2} + A_1(H)y_{n+1} + A_0(H)y_n + A_1(H)y_{n-1} + A_2(H)y_{n-2} = 0 \quad (19)$$

where $H = wh$, h is the step length and $A_0(H)$, $A_1(H)$, $A_2(H)$ are polynomials of H, y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2, \ldots$ and

$$A_2(H) = h^2 b_0 + h^4 b_2 a$$

$$A_1(H) = 1 + h^2 b_1 - 4h^4 b_2 a$$

$$A_0(H) = a_1 + h^2 b_2 + 6h^4 b_2 a. \quad (20)$$

The characteristic equation associated with (19) is

$$A_2(H)s^2 + A_1(H)s + A_0(H) + A_1(H)s^{-1} + A_2(H)s^{-2} = 0 \quad (21)$$

Based on Lambert and Watson [19] we have the following definition

DEFINITION 2 A symmetric 4-step method with the characteristic equation given by (21) is said to have an **interval of periodicity** $[H_0, H_1]$ if, for all $H \in [H_0, H_1]$, all the roots s_i, $i = 1, \ldots, 4$ of (21) satisfy:

$$s_1 = e^{i\theta(H)}, \quad s_2 = e^{-i\theta(H)}, \text{ and } |s_i| \leqslant 1, \quad i = 3,4 \quad (22)$$

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

Based on the paper of Raptis and Simos [38] we have the following lemma.

LEMMA 2 *(for the proof see [38]). All four-step methods with stability polynomial given by (21) have interval of periodicity $(0, H_0^2)$ if:*

$$P_1(H), P_2(H), P_3(H) \geqslant 0$$

$$S(H) = P_2(H)^2 - 4P_1(H)\,P_3(H) \geqslant 0 \quad (23)$$

where $P_1(H) = 2A_2(H) - 2A_1(H) + A_0(H)$, $P_2(H) = 2(6A_2(H) - A_0(H))$ and $P_3(H) = 2A_2(H) + 2A_1(H) + A_0(H)$.

For the method derived in Section 2 we find that, for the values of coefficients given by (15) (with $w = vh$ and $v = i\phi$), $P_i(H) \geqslant 0$, $i = 1(1)3$ and $S(H) \geqslant 0$ for all $H^2 \in (0, \infty) - \{H^2 : H = q\pi, q = 1, 2, \dots\}$.

We find the same result for the cases $w = 1.1vh$ and $w = 1.2vh$ i.e. in the cases where there is a 10% and a 20% error in the estimation of the frequency of the problem, respectively.

5. NUMERICAL ILLUSTRATIONS

In this section we present some numerical results to illustrate the performance of our new methods. We consider the numerical integration of the Schrödinger equation:

$$y''(x) = (W(x) - E)\, y(x) \tag{24}$$

in the well-known case where the potential $V(x)$ is the Woods-Saxon potential

$$V(x) = V_w(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{25}$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$ and $X_0 = 7.0$. In order to solve this problem numerically we need to approximate the true (infinite) interval of integration $[0, \infty)$ by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $0 \leqslant x \leqslant 15$. We consider (24) in a rather large domain of energies, i.e. $E \in [1, 1000]$. The problem we consider is the so-called *resonance problem*.

5.1. The Resonance Problem Woods-Saxon Potential

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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{26}$$

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 (when $x \to 0$) the asymptotic form

$$y(x) \simeq Akj_l(kx) - Bkxn_l(kx)$$

$$\simeq AC[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)] \tag{27}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{28}$$

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_i, $i = 0(1)3$ before starting a four-step method. From the initial condition, $y_0 = 0$. It can be shown that, for values of x close to the origin, the solution behaves like $y(x) \sim cx^{l+1}$ as $x \to 0$, where c is an independent constant. In view of this we take $y_1 = h^{l+1}$ [2, 21]. The other values of y (i.e. y_2 and y_3) can be determined using the method of Raptis [16]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l and the normalization factor C from the above relations.

For positive energies one has the so-called resonance problem. This problem consists either of finding the **phase shift** $\delta(E) = \delta_l$ or finding those E, for $E \in [1, 1000]$, at which δ equals $\pi/2$. 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:

$$y(0) = 0,$$

$$y(x) \sim \cos[\sqrt{E}\,x] \text{ for large } x.$$

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

In our numerical illustration we find the positive *eigenenergies* or *resonances* by the following four methods:

Method MI: Numerov's method

Method MII: Derived by Ixaru and Rizea [7]

Method MIII: Derived by Raptis [16]

Method MIV: New exponentially-fitted method.

The numerical results obtained for the four methods, with stepsizes equal to $h = 1/2^n$, were compared with the analytic solution of the Wood-Saxon potential resonance problem, rounded to six decimal places. Table I shows the errors $Err = |E_{\text{calculated}} - E_{\text{analytical}}|$ of the eigenenergies for several values of n.

The performance of the present method is dependent on the choice of the fitting parameter v. For the purpose of obtaining our numerical results it is appropriate to choose v in the way suggested by Ixaru and Rizea [7]. That is, we choose:

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5] \\ (-E)^{1/2} & \text{for } x \in [6.5, 15] \end{cases} \tag{29}$$

For a discussion of the reasons for choosing the values 50 and 6.5 and the extent to which the results obtained depend on these values see [7, pp. 25].

5.2. Modified Woods-Saxon Potential

In Table II some results for $Err = |E_{\text{calculated}} - E_{\text{analytical}}|$ of the eigenenergies for several values of n, obtained with another potential in (24) are shown.

TABLE I Absolute errors (Real time of computation), in 10^{-7} units (in seconds), of the resonances calculated by the nine algorithms MI-MIV for the resonance problem with the Wood-Saxon potential

The resonance	*n*	*MI*	*MII*	*MIII*	*MIV*
53.5888719	1				9(0.010)
	2			675482(0.021)	0(0.020)
	3		456721(0.040)	87657(0.043)	0(0.035)
	4	2283232(0.080)	8109(0.080)	3135(0.085)	0(0.060)
341.4958743	1				13(0.010)
	2				0(0.020)
	3			665765(0.043)	0(0.035)
	4		284209(0.085)	12843(0.085)	0(0.065)
989.7019159	1				185(0.010)
	2				1(0.020)
	3			4325238(0.043)	0(0.035)
	4		2978039(0.080)	22283(0.090)	0(0.065)

TABLE II Absolute errors (Real time of computation), in 10^{-6} units (in seconds), of the positive eigenvalues calculated by the nine algorithms MI-MIV for the resonance problem with the modified Wood-Saxon potential

The resonance	*n*	*MI*	*MII*	*MIII*	*MIV*
61.482588	1				60(0.010)
	2				0(0.020)
	3			211345(0.050)	0(0.040)
	4	253692(0.090)	3244(0.090)	1265(0.102)	0(0.080)
352.682070	1				41(0.010)
	2				0(0.020)
	3			123357(0.050)	0(0.040)
	4		203007(0.090)	9171(0.100)	0(0.040)
1002.768393	1				512(0.010)
	2				8(0.020)
	3				0(0.040)
	4			545667(0.105)	0(0.080)

This potential is

$$V(x) = V_W(x) + \frac{D}{x} \tag{30}$$

where V_W is the Woods-Saxon potential (25). For the purpose of our numerical experiments we use the same parameters as in [7], i.e. $D = 20$, $l = 2$.

Since $V(x)$ is singular at the origin, we use the special strategy of [7]. We start the integration from a point $\varepsilon > 0$ and the initial values $y(\varepsilon)$ and $y(\varepsilon + h)$ for the integration scheme are obtained using a perturbative method (see [6]). As in [7] we use the value $\varepsilon = 1/4$ for our numerical experiments.

For the purpose of obtaining our numerical results it is appropriate to choose v in the way suggested by Ixaru and Rizea [7]. That is, we choose:

$$v = \begin{cases} \dfrac{[V(a_1) + V(\varepsilon)]}{2} & \text{for } x \in [\varepsilon, a_1] \\ \dfrac{V(a_1)}{2} & \text{for } x \in (a_1, a_2) \\ V(a_3) & \text{for } x \in (a_2, a_3) \\ V(15) & \text{for } x \in (a_3, 15). \end{cases}$$

where a_i, $i = 1, \ldots, 3$ are fully defined in [7].

All computations were carried out on an IBM *PC*-AT compatible 80486 using double precision arithmetic (16 significant digits precision).

6. CONCLUSION

We investigate here the exponentially fitted methods. The crucial concern when solving the Schrödinger equation is that the numerical method should integrate exactly the functions (11) with m as large as possible, as shown by [7] and [21]. The new method integrates exactly more functions of the form (3) than the known Numerov-type exponentially-fitted methods.

As predicted by the analysis, method MIV is the most accurate of all the methods for the problems tested.

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