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A New Numerov-Type Exponentially Fitted Method For The Numerical Integration Of The Schrödinger Equation

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Abstract. A new predictor-corrector exponentially fitted Numerov-type method is developed for the numerical integration of the radial Schrödinger equation and of coupled differential equations arising from the Schrödinger equation. The Numerov-type method considered contains free parameters which allow it to be fitted to exponential functions. The new fourth algebraic order method is very simple and integrate more exponential functions than both the well known fourth order Numerov type exponentially fitted methods and the sixth algebraic order Runge-Kutta type methods. Numerical results also indicate that the new method is much more accurate than the other exponentially fitted methods. Based on the method developed in the present paper and on the method of Simos [24] a new variable-step procedure is developed for the numerical solution of the coupled differential equations arising from the Schrödinger equation. Numerical illustrations indicate that the new variable-step method is more efficient than other well known variable-step methods.

Keywords: Schrödinger equation, predictor-corrector methods, Numerov-type methods, exponentially-fitted methods, resonance problem, bound-states problem.

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1 Introduction

The one-dimensional Schrödinger equation has the form:

$$y''(x) + f(x)y(x) = 0 \tag{1.1}$$

where $0 \leq x < \infty$ and $f(x) = E - l(l+1)/x^2 - V(x)$. We call the term $l(l+1)/x^2$ *the centrifugal potential*, and the function $V(x)$ *the potential*, where $V(x) \to 0$ as $x \to \infty$. According of the sign of the energy E there are two main categories of problems for the (1.1) (see for details [28]). In (1.1), E 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:

$$y(0) = 0 \tag{1.2}$$

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

There is a real need for the numerical solution of the one-dimensional Schrödinger equation in many scientific areas. Some of these areas are the nuclear physics, the physical chemistry, the theoretical physics and chemistry (see [1, 5, 27]).

There is much activity in the area of the solution of the radial Schrödinger equation (1.1). The result of this activity is the development of a great number of methods (see [1-3], [5-12], [15-26]). The most important characteristics of an efficient method for the solution of the problem (1.1) are the accuracy and the computational efficiency. The development of methods with the above mentioned characterisitcs is an open problem.

The **Numerov's method** is one of the most popular methods for the solution of (1.1). The reason of this popularity is explained in [35].

An alternative approach to deriving higher order methods for (1.1) was given by Cash and Raptis [2] (see for details in [35]). The characteristic of these type of methods is that are very complicated compared with the Numerov-type methods.

Another approach for developing efficient methods for the solution of (1.1) 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 (1.1). Many authors have investigated

the idea of exponential fitting, since Raptis and Allison. An intersting work in this general area was that of Ixaru and Rizea [7]. They showed that for the resonance problem defined by (1.1) it is generally more efficient to derive methods which exactly integrate functions of the form

$$\{1, x, x^2, \ldots, x^p, \exp(\pm vx), x\exp(\pm vx), \ldots, x^m \exp(\pm vx)\}, \tag{1.3}$$

where v is the frequency of the problem, than to use classical exponential fitting methods. The reason for this is explained in [25]. 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 method 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 (1.3) 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 (1.3) with $m = 1$ and $p = 3$. We note that the method of Cash, Raptis and Simos [3] is a Runge-Kutta type method and it is very complicated. In [35] Simos has derived a simple explicit exponentially-fitted method with $m = 3$ and $p = 0$.

The purpose of this paper is to derive a simple Numerov-type predictor-corrector method fitted to (1.3) and in particular to derive a method with $m = 4$ and $p = 1$ i.e. to derive a method which integrate much more functions of the form (1.3) than the methods proposed previously. We note also that the above mentioned values of m and p are the largest values 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 they integrate exactly more exponential functions. We note also, that the new method is 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. We note, as in [35], that *the resonance problem* is one of the most difficult to solve of all the problems based on the radial Schrödinger equation because it has highly oscillatory solutions, especially for large resonances (see section 5). We have also applied the new method to *the bound-states problem.* Based on the method developed in the present paper and on the method of Simos [24] a new variable-step procedure is developed for the numerical solution of the coupled differential equations arising from the Schrödinger equation.

The basic theory of the expomentially-fitted methods has been described in [35].

2 The New Method

Consider the family of methods:

$$\begin{aligned}
\overline{y}_{n+1} &= y_{n+1} - ah^2(y''_n - y''_{n+1}) \\
\overline{y}_{n-1} &= y_{n-1} - ah^2(y''_n - y''_{n-1}) \\
\overline{y}_n &= y_n - bh^2(\overline{y}''_{n+1} - 2y''_n + \overline{y}''_{n-1}) \\
\overline{\overline{y}}_n &= y_n - ch^2(y''_{n+1} - 2\overline{y}''_n + y''_{n-1}) \\
y_{n+1} - 2y_n + y_{n-1} &= h^2(b_0 y''_{n+1} + b_1 \overline{\overline{y}}''_n + b_0 y''_{n-1})
\end{aligned} \tag{2.1}$$

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

We have chosen to consider this family of methods because it has five free parameters. So, we will construct a method which integrate more exponential functions than the Numerov-type exponentially fitted methods [7, 16-19] and the Runge-Kutta-type methods proposed by Cash, Raptis and Simos [2,3,24]. When one solves the Schrödinger's equation numerically, it follows from [6,7,19,21] that the exact integration of the exponential functions (1.3) with m as large as possible is an important property for a numerical method. The new family of methods (2.1) has only five free parameters while the Runge-Kutta-type methods of Cash, Raptis and Simos [3, 20, 24] have at least eleven free parameters, making the derivation of suitable methods very difficult.

We require that the family of methods (2.1) should integrate exactly any linear combination of the functions:

$$\{1, x, \exp(\pm vx), x\exp(\pm vx), x^2\exp(\pm vx), x^3\exp(\pm vx), x^4\exp(\pm vx)\}. \tag{2.2}$$

To construct a method of the form (2.1) which integrates exactly the functions (2.2), we require that the method (2.1) integrates exactly (see previous section):

$$\{1, x, \exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x), \exp(\pm v_3 x), \exp(\pm v_4 x)\} \tag{2.3}$$

and then put:

$$v_0 = v_1 = v_2 = v_3 = v_4 = v, \tag{2.4}$$

Demanding that (2.1) integrates (2.3) exactly, we obtain the following system of equations for b_0, b_1, a, b and c

$$\begin{aligned}
2\cosh(w) - 2 = {} & 2\,w^2\cosh(w)\,b_0 + w^2\,b_1 + 2\,w^4\,[1-\cosh(w)]\,b_1\,c \\
& +4\,w^6\,[1-\cosh(w)]\,b_1\,c\,b + 4\,w^8\,[1-\cosh(w)]\,b_1\,c\,b\,a
\end{aligned} \tag{2.5}$$

Based on (2.5) and on a computer algebra program (an analogous program for explicit four-step methods has been developed in [38]) we can determine the coefficients b_0, b_1, b_2, a, b and c via the following algorithm:

(1) We introduce the environment *linalg* of the computer-algebra manipulation package Maple.

(2) We calculate the determinants of matrices of denoninators and numerators for each of the quantities b_0, b_1, $b_1\ c$, $b_1\ c\ b$ and $b_1\ c\ b\ a$

(3) We define the derivatives of the above determinants in order to avoid formulae of the form $\frac{0}{0}$, i.e. we apply the *L' Hôspital's rule.*

(4) We apply the relation (2.4).

(5) We define the coefficients of the method.

(6) We define the Taylor series expansions of the coefficients of the method.

The explicit expressions of the coefficients of the new method are given in the Appendix.

If $w = i\phi$, then the method (2.1) is exact for any linear combination of the functions:

$$\{1, x, sin(\phi x), cos(\phi x), xsin(\phi x), xcos(\phi x), x^2 sin(\phi x), x^2 cos(\phi x), x^3 sin(\phi x), x^3 cos(\phi x)\}, x^4 sin(\phi x), x^4 cos(\phi x)\}. \tag{2.6}$$

The local truncation error of the new method is given by:

$$\begin{aligned} L.T.E.(h) = h^6[&-\frac{1}{240}(D^{(6)})(y)(x) - \frac{1}{240}(D^{(4)})(y)(x) + \frac{45821}{37661021798400}(D^{(6)})(y)(x)\,w^{12} \\ &-\frac{36671}{426824913715200}(D^{(6)})(y)(x)\,w^{14} - \frac{81643}{96663289282560000}(D^{(4)})(y)(x)\,w^{16} \\ &+\frac{280627931279}{6426712449222760763228160000000}(D^{(4)})(y)(x)\,w^{28} \\ &+\frac{132424307}{1583344678448332800000}(D^{(4)})(y)(x)\,w^{18} \\ &-\frac{240113207617}{504691116255406080000000000}(D^{(4)})(y)(x)\,w^{20} \\ &+\frac{1810042244123}{10126122556548467589120000000}(D^{(4)})(y)(x)\,w^{22} \\ &+\frac{7467774706373}{212648573687517819371520000000}(D^{(4)})(y)(x)\,w^{24} + \frac{1}{12773376}(D^{(6)})(y)(x)\,w^{8} \\ &-\frac{67633}{5230697472000}(D^{(6)})(y)(x)\,w^{10} + \frac{1}{47308800}(D^{(4)})(y)(x)\,w^{10} + \frac{1}{532224}(D^{(4)})(y)(x)\,w^{6} \\ &-\frac{180932053319}{2142237483074253587742720000000}(D^{(4)})(y)(x)\,w^{26} - \frac{691}{2641766400}(D^{(4)})(y)(x)\,w^{8} \\ &-\frac{1389923}{1067062284288000}(D^{(4)})(y)(x)\,w^{12} + \frac{75631}{1113092422041600}(D^{(4)})(y)(x)\,w^{14}]. \end{aligned} \tag{2.7}$$

3 Stability Analysis

If we apply the method (2.1) to the scalar test equation $y'' = -s^2 y$, we obtain the difference equation

$$A(H^2)y_{n+1} - 2B(H^2)y_n + A(H^2) = 0 \tag{3.1}$$

where

$$\begin{aligned} A(H^2) &= 1 + H^2\, b_0 + H^4\, b_1\, c - 2H^6\, b_1\, c\, b + 2H^8\, b_1\, a\, b\, c \\ B(H^2) &= 1 - \frac{1}{2} H^2\, b_1 + H^4\, b_1\, c - 2H^6\, b_1\, c\, b + 2H^8\, b_1\, a\, b\, c \end{aligned} \tag{3.2}$$

and $H = sh$.

The stability polynomial of the difference equation (3.1) is given by

$$C(t; H^2) = A(H^2)t^2 - 2B(H^2)t + A(H^2). \tag{3.3}$$

We have the following definitions:

Definition 1 *[13] A symmetric two-step method with stability polynomial given by (3.3) is said to have a non-zero interval of periodicity $(0, H_0^2)$ if, for all $H^2 \in (0, H_0^2)$, the roots of the stability polynomial satisfy*

$$t_1 = e^{i\theta(H)}, \;\; t_2 = e^{-i\theta(H)} \tag{3.4}$$

where θ is a real function of $H = sh$.

Definition 2 *[13] A method is said to be P-stable if its interval of periodicity is $(0, \infty)$.*

Definition 3 *A method is said to be almost P-stable if its interval of periodicity is $(0, \infty) - S$, where S is a set of distinct points.*

Remark 1 *A symmetric two-step method with stability polynomial given by (3.3) has an interval of periodicity $(0, H_0^2)$ if, for all $H^2 \in (0, H_0^2)$, $A(H^2) \pm B(H^2) > 0$.*

In our stability analysis $s = v$. For the method derived in section 2 we find that: $A(H^2) - B(H^2) > 0$ for all $H^2 \in (0, \infty)$ and $A(H^2) + B(H^2) > 0$ for all $H^2 \in (0, \infty) - \{H^2 : H = sq\pi,\; q = 1, 2, \ldots\}$. Thus, the method is almost P-stable.

For comparison purposes in the Table 1 we list the properties of the two-step exponentially fitted method introduced in this paper, together with the corresponding properties of some two-step exponentially fitted methods presented previously in the literature. We note that all the methods are implicit.

Method	A. O.	Int. Per.	Integr. Expon. Func.
Numerov's method	4	$(0,6)$	$1, x, x^2, x^3, x^4, x^5$
Derived by Raptis and Allison [19]	4	$(0,\infty) - S$	m=0, p=3
Derived by Ixaru and Rizea [7]	4	$(0,\infty) - S$	m=1, p=1
Derived by Raptis [16]	4	$(0,\infty) - S$	m=2, p=0
Derived by Raptis and Cash [20]*	6	$(0,\infty) - S$	m=0, p=5
Derived by Cash, Raptis and Simos [3]*	6	$(0,\infty) - S$	m=1, p=3
Derived by Simos [24]*	6	$(0,\infty) - S$	m=2, p=0
Derived by Simos [35]	4	$(0,\infty) - S$	m=3, p=0
New Method	4	$(0,\infty) - S$	m=4, p=1

Table 1: Properties of some two-step exponentially-fitted methods. $S = \{H^2 : H = sq\pi, q = 1, 2, \ldots\}$. The quantities m and p are defined by (3). A.O. is the algebraic order of the method. Int. Per. is the interval of periodicity of the method. $*=$ hybrid two-step method

The new method is of algebraic order four and have the same interval of periodicity as the other well known exponentially-fitted methods listed in Table 1. However, the new method integrate exactly more functions of the form (1.3) than all the other methods developed in the literature. The crucial concern when solving the Schrödinger equation is that the numerical method should integrate exactly the functions (1.3) with m as large as possible, as shown by [7] and [21].

4 Numerical Illustrations

In this section some numerical results to illustrate the efficiency of our new method are presented. We consider the numerical integration of the Schrödinger equation:

$$y''(x) = (W(x) - E)y(x) \tag{4.1}$$

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

$$V(x) = V_w(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{4.2}$$

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 $0 \leq x \leq 15$. We consider (4.1) in a rather large domain of energies, i.e., $E \in [1, 1000]$. The problems we consider are (i) the so-called *resonance problem* and (ii) the so-called *bound-states problem.*

4.1 The Resonance Problem

4.1.1 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 (1.1) effectively reduces to

$$y''(x) + (k^2 - \frac{l(l+1)}{x^2})y(x) = 0, \tag{4.3}$$

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)] \end{aligned} \tag{4.4}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{4.5}$$

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

Since the problem is treated as an initial-value problem, one needs y_0 and y_1 before starting a two-step method. From the initial condition, $y_0 = 0$. 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]. 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:

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

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

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

Method MI: Numerov's method

Method MII: Derived by Ixaru and Rizea [7]

Method MIII: Derived by Raptis and Cash [20]

Method MIV: Derived by Cash, Raptis and Simos [3]

Method MV: Derived by Simos [24]

Method MVI: Derived by Simos [35]

Method MVII: New exponential - fitted method

The numerical results obtained for the seven methods were compared with the analytic solution of the Woods-Saxon potential resonance problem, rounded to six decimal places. Table 2 shows the absolute errors of the eigenenergies in 10^{-7} units and the CPU time required for the calculation for different choices of constant stepsize, which are shown in column 2. The empty areas indicate that the corresponding absolute errors are larger than 1.

The resonance	h	MI	MII	MIII
53.5888719	1/2			
	1/4			328432(0.022)
	1/8		456721(0.040)	9875(0.045)
	1/16	2283232(0.080)	8109(0.080)	109(0.090)
341.4958743	1/2			
	1/4			
	1/8			375432(0.045)
	1/16		284209(0.085)	25418(0.090)
989.7019159	1/2			
	1/4			
	1/8			
	1/16		2978039(0.080)	661239(0.095)

Table 2: Absolute errors (Real time of computation), in 10^{-7} units (in seconds), of the resonances calculated by the six algorithms MI-MVI for the resonance problem with the Woods-Saxon potential. The empty areas indicate that the error is greater than 1.

The performance of the different methods is dependent on the choice of the fitting parameter v. For the purpose of obtaining our numerical results it is appropriate to choose v

The resonance	h	MIV	MV	MVI	MVII
53.5888719	1/2		112345(0.023)	256432(0.005)	345(0.005)
	1/4	40326(0.030)	8923(0.046)	12324(0.010)	23(0.010)
	1/8	987(0.060)	93(0.095)	632(0.022)	1(0.020)
	1/16	12(0.110)	3(0.190)	9(0.041)	0(0.040)
341.4958743	1/2				812(0.005)
	1/4	543941(0.028)	23568(0.046)	148769(0.010)	78(0.010)
	1/8	9318(0.055)	871(0.095)	5011(0.023)	4(0.020)
	1/16	372(0.110)	13(0.190)	159(0.042)	0(0.040)
989.7019159	1/2				2456(0.005)
	1/4		765901(0.046)	995647(0.010)	236(0.010)
	1/8	45678(0.060)	3561(0.095)	15848(0.022)	7(0.020)
	1/16	6813(0.115)	53(0.190)	64(0.041)	1(0.040)

Table 2: continued

in the way suggested by Ixaru and Rizea [7]. That is, we choose:

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5] \\ (-E)^{1/2} & \text{for } x \in (6.5, 15] \end{cases} \tag{4.6}$$

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].

4.1.2 Modified Woods-Saxon Potential

In Table 3 some results obtained with another potential in (4.1) are shown. This potential is

$$V(x) = V_W(x) + \frac{D}{x} \tag{4.7}$$

where V_W is the Woods-Saxon potential (4.2). 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 $\epsilon > 0$ and the initial values $y(\epsilon)$ and $y(\epsilon + h)$ for the integration scheme are obtained using a perturbative method (see [6]). As in [7] we use the value $\epsilon = \frac{1}{4}$ for our numerical experiments.

For the purpose of obtaining our numerical results it is appropriate to choose ϵ in the

The resonance	h	MI	MII	MIII
61.482588	1/2			
	1/4			
	1/8			82345(0.050)
	1/16	253692(0.090)	3244(0.090)	275(0.102)
173.075711	1/2			
	1/4			
	1/8		234768(0.045)	93426(0.050)
	1/16		41986(0.090)	2925(0.100)
352.682070	1/2			
	1/4			
	1/8			456578(0.050)
	1/16		203007(0.090)	63550(0.105)
1002.768393	1/2			
	1/4			
	1/8			
	1/16			

Table 3: Absolute errors (Real time of computation), in 10^{-6} units (in seconds), of the positive eigenvalues calculated by the six algorithms MI-MVI for the resonance problem with the modified Woods-Saxon potential. The empty areas indicate that the error is greater than 1.

way suggested by Ixaru and Rizea [7]. That is, we choose:

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

For the choice of the values $a_i, i = 1(1)3$ see for details [7].

4.2 The Bound-States Problem

For negative energies we solve the so-called bound-states problem, i.e., with the boundary conditions

$$\begin{aligned} y(0) &= 0, \\ y(x) &\sim exp(-\sqrt{-E}x) \text{ for large } x. \end{aligned}$$

In order to solve this problem numerically we use a strategy which has been proposed by Cooley [5] and has been improved by Blatt [1]. This strategy involves integrating forward from the point $x = 0$, backward from the point $x_b = 15$ and matching up the solution at some

The resonance	h	MIV	MV	MVI	MVII
61.482588	1/2		867892(0.025)	1123439(0.006)	19(0.005)
	1/4	97459(0.025)	4561(0.050)	13452(0.011)	0(0.011)
	1/8	945(0.050)	35(0.100)	794(0.026)	0(0.025)
	1/16	11(0.120)	1(0.200)	0(0.052)	0(0.050)
173.075711	1/2				105(0.005)
	1/4	435671(0.030)	11234(0.050)	173217(0.012)	8(0.011)
	1/8	3451(0.060)	96(0.100)	631(0.027)	0(0.025)
	1/16	115(0.115)	8(0.200)	32(0.051)	0(0.050)
352.682070	1/2				1134(0.005)
	1/4	989763(0.030)	90785(0.050)	565482(0.013)	95(0.011)
	1/8	5464(0.060)	428(0.100)	7944(0.026)	2(0.025)
	1/16	856(0.120)	11(0.200)	501(0.051)	0(0.050)
1002.768393	1/2				4326(0.006)
	1/4		456327(0.050)	789437(0.012)	114(0.011)
	1/8		1238(0.100)	31623(0.027)	7(0.025)
	1/16	80927(0.120)	25(0.200)	159(0.052)	0(0.050)

Table 3: continued

internal point in the range of integration. As initial conditions for the backward integration we take (see [3]):

$$y(x_b) = exp(-\sqrt{-E}x_b) \text{ and } y(x_b - h) = exp[-\sqrt{-E}(x_b - h)] \ , \tag{4.8}$$

where h is the steplength of integration of the numerical method.

The true solutions to the Woods-Saxon bound-states problem were obtained correct to nine decimal places using the analytic solution and the numerical results obtained for the six methods mentioned above were compared to this true solution. In Table 4 we present the absolute errors of the eigenenergies in 10^{-9} units and the CPU time required for the calculation for different choices of constant stepsize, which are shown in column 2. The empty areas indicate that the corresponding absolute errors are larger than 1.

5 Error Estimation

It is known from the literature (see for example [20] and references therein) that there are many methods for the estimation of the local truncation error (LTE) in the integration of systems of initial-value problems. We note that the LTE is based on the algebraic order of the method.

Our local error estimation technique is based on an embedded pair of integration methods and on the fact that when the local truncation error is of higher algebraic order then the

The resonance	h	MI	MII	MIII
-49.457788728	1/2	43544(0.013)	323(0.013)	45(0.020)
	1/4	3423(0.025)	68(0.025)	8(0.040)
-41.232607772	1/2	65667443(0.015)	445331(0.017)	54663(0.023)
	1/4	4876771(0.030)	66789(0.033)	8767(0.043)
-26.873448915	1/2		544551(0.015)	76758(0.020)
	1/4		23439(0.030)	9421(0.040)
-8.676081670	1/2		5456779(0.014)	656447(0.022)
	1/4		323451(0.028)	43545(0.043)

Table 4: Absolute errors (Real time of computation), in 10^{-9} units (in seconds), of the eigenvalues calculated by the six algorithms MI-MVI for the bound-states problem with the Woods-Saxon potential. The empty areas indicate that the error is greater than 1.

The resonance	h	MIV	MV	MVI	MVII
-49.457788728	1/2	11(0.015)	1(0.024)	7(0.008)	0(0.007)
	1/4	0(0.030)	0(0.048)	0(0.016)	0(0.015)
-41.232607772	1/2	6548(0.015)	767(0.024)	2347(0.008)	1(0.007)
	1/4	785(0.030)	86(0.048)	213(0.017)	0(0.015)
-26.873448915	1/2	8789(0.015)	989(0.024)	3326(0.009)	2(0.007)
	1/4	946(0.030)	66(0.048)	451(0.018)	0(0.015)
-8.676081670	1/2	82338(0.015)	5663(0.024)	32659(0.009)	8(0.007)
	1/4	5456(0.030)	438(0.048)	1487(0.018)	0(0.015)

Table 4: continued

approximation of the solution for the problems which have a periodic or oscillating solution is better. The new error control procedure is, also, based on the fact that when a method exactly integrates functions of the form (1.3) with m and p as large as possible then the approximation of the solution for the problems which have a periodic or oscillating solution is more efficient and accurate.

Denoting the solution obtained with higher algebraic order method as y_{n+1}^H and the solution obtained with lower algebraic order method as y_{n+1}^L, we have the following definition

Definition 4 *We define the* **local truncation error** *estimate in the lower order solution* y_{n+1}^L *by the quantity*

$$L.T.E = \mid y_{n+1}^H - y_{n+1}^L \mid . \tag{5.1}$$

Under the assumption that when h is sufficiently small, the **local truncation error** *in* y_{n+1}^H *can be neglected compared with that in* y_{n+1}^L.

We assume that the solution y_{n+1}^H is obtained using and the solution y_{n+1}^L is obtained

using the present method.

In our variable-step procedure the solution y_{n+1}^{H}, i.e. the solution with high algebraic order, is obtained using the method of Simos [24], and the solution y_{n+1}^{L}, i.e. the solution with low algebraic order, is obtained using the present method.

If the local truncation error is bounded by acc and the step size of the integration used for the nth step length is h_n, the estimated step size for the $(n+1)st$ step, which will give a local truncation error bounded by acc, must be

$$h_{n+1} = h_n \left(\frac{acc}{L.T.E} \right)^{1/q}, \tag{5.2}$$

where q is the algebraic order.

Following [20], we have considered all step changes to halving and doubling. Thus, based on the procedure developed in [20], the step control procedure which we introduce for the Local Truncation Error is

$$If\ L.T.E\ <\ acc,\ h_{n+1} = 2h_n$$

$$If\ 100\ acc\ >\ L.T.E\ \geq\ acc,\ h_{n+1} = h_n \tag{5.3}$$

$$If\ L.T.E\ \geq\ 100\ acc,\ h_{n+1} = \frac{h_n}{2}\ and\ repeat\ the\ step. \tag{5.4}$$

It is known that the local error estimate is obtained to the lower order solution. This is applied, also, in our case.

In the third case of the above procedure (i.e. $h_{n+1} = \frac{h_n}{2}$), the required values of y are determined using high order interpolation formulae (see for details [31] pp. 397-400).

6 Coupled Differential Equations

In this section we present some numerical results to illustrate the performance of the new variable-step method. We consider the numerical integration of the coupled differential equations arising from the Schrödinger equation.

There are many problems in theoretical physics, atomic physics, physical chemistry, quantum chemistry and chemical physics which can be transformed to the solution of coupled differential equations of the Schrödinger type. On of the most important problems of the above category is the collision of an atom with a homonuclear diatomic molecule. In our example the collison is taken place such that vibration excitation and chemical reaction can be ignored (see for details and relevant theory in [32-33] and references therein).

The close-coupling differential equations of the Schrödinger type may be written in the form

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{6.1}$$

for $1 \leq i \leq N$ and $m \neq i$.

We have investigated the case in which all channels are open. So we have the following boundary conditions (see for details [32]):

$$y_{ij} = 0 \ at \ x = 0 \tag{6.2}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{li}(k_i x) \tag{6.3}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. We note here that since the methods presented in this paper have much larger intervals of periodicity (the property which must have a method to avoid instabilities) than the Numerov's method, the method of Hajj et. al. [36], the method of Cash and Raptis [2] and other finite difference methods, we can use the present methods to problems involving closed channels.

Based on the detailed analysis developed in [32] and defining a matrix K' and diagonal matrices M, N by:

$$K'_{ij} = \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}$$
$$M_{ij} = k_i x j_{l_i}(k_i x)\delta_{ij}$$
$$N_{ij} = k_i x n_{l_i}(k_i x)\delta_{ij}$$

we find that the asymptotic condition (6.3) may be written as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}' \tag{6.4}$$

One of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation is the Iterative Numerov method of Allison [32].

A real problem in theoretical physics, atomic physics, quantum chemistry and molecular physics which can be transformed to close-coupling differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [32], the entrance channel by the quantum numbers (j,l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we find that

$$[\frac{d^2}{dx^2} + k^2_{j'j} - \frac{l'(l'+1)}{x^2}]y^{Jjl}_{j'l'}(x) = \frac{2\mu}{\hbar^2}\sum_{j''}\sum_{l''} < j'l'; J \mid V \mid j''l''; J > y^{Jjl}_{j''l''}(x) \tag{6.5}$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}] \tag{6.6}$$

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

Following the analysis of [32], the potential V may be written as

$$V(x, \hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \tag{6.7}$$

and the coupling matrix element is given by

$$< j'l'; J \mid V \mid j''l''; J >= \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x) \tag{6.8}$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [33] and $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and $P_i,\ i = 0, 2$ are Legendre polynomials (see for details [33]). The boundary conditions may then be written as (see [32])

$$y^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \tag{6.9}$$

$$y^{Jjl}_{j'l'}(x) \sim \delta_{jj'}\delta_{ll'}\exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l')\exp[i(k_{j'j}x - 1/2l'\pi)] \tag{6.10}$$

where the scattering S matrix is related to the K matrix of (6.3) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \tag{6.11}$$

The calculation of the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles requires the existance of the numerical method for step-by-step integration from the initial value to matching points.

In our numerical test we choose the S matrix which is calculated using the following parameters

$$\frac{2\mu}{\hbar^2} = 1000.0,\ \frac{\mu}{I} = 2.351,\ E = 1.1,$$
$$V_0(x) = \frac{1}{x^{12}} - 2\frac{1}{x^6},\ V_2(x) = 0.2283V_0(x).$$

As is described in [32], we take J=6 and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of **four, nine and sixteen coupled differential equations**, respectively. Following Bernstein [34] and Allison [32] a reduction of the interval $[0, \infty)$ to $[0, x_0]$ is obtained. The wavefunctions are then vanished in this region and consequently the boundary condition (6.9) may be written as

$$y^{Jjl}_{j'l'}(x_0) = 0 \tag{6.12}$$

For the numerical solution of this problem we have used (i) the well known Iterative Numerov method of Allison [32], (ii) the variable-step method of Raptis and Cash [17], (iii) the variable step method of Simos [37] and (iv) the new embedded variable-step method. In Table 5 we present the real time of computation required by the methods mentioned above to calculate the square of the modulus of the S matrix for sets of 4, 9 and 16 coupled

Method	N	hmax	RTC
Iterative Numerov [32]	4	0.014	3.25
	9	0.014	23.51
	16	0.014	99.15
Variable-step Method of Raptis and Cash [20]	4	0.056	1.65
	9	0.056	8.68
	16	0.056	45.21
Variable-step Method of Simos [37]	4	0.112	1.43
	9	0.112	8.22
	16	0.112	40.13
New Variable-step method	4	0.448	0.26
	9	0.448	1.00
	16	0.448	5.28

Table 5: RTC (Real time of computation (in seconds)) to calculate $\mid S \mid^2$ for the variable-step methods (i)-(iv). $acc = 10^{-6}$. hmax is the maximum stepsize

differential equations. In Table 3 N indicates the number of equations of the set of coupled differential equations.

The variable step method developed in this paper is more efficient than other well known finite difference ones.

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

7 Conclusion

The method proposed in this paper is much more accurate than the Numerov-type methods of Raptis and Allison [19], Ixaru and Rizea [7] and Raptis [16]. We note also that the new method require the same amount of work as the Numerov-type methods of Raptis and Allison [19], Ixaru and Rizea [7] and Raptis [16] and less work than the Runge-Kutta-type hybrid methods of Raptis and Cash [20].

The crucial concern when solving the Schrödinger equation is that the numerical method should integrate exactly the functions (1.3) with m as large as possible, as shown by [7] and [21].

The new method integrate exactly more functions of the form (1.3) than the hybrid methods of Raptis and Cash [20] and Cash, Raptis and Simos [3], Simos [24].

As predicted by the analysis, method MVII is the most accurate of all the methods for the problems tested. We note here that this method is much more simpler compared with the Runge-Kutta type exponentially fitted methods of Raptis and Cash [20], Cash, Raptis and Simos [3], and Simos [24]

Based on the exponentially-fitted methods obtained above and the exponentially-fitted method of Simos [24], a variable-step exponentially-fitted method is introduced. Numerical results indicate that the new variable-step method is much more efficient than other well known methods in the literature for the numerical solution of the coupled equations arising from the Schrödinger equation.

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Appendix

The explicit expressions of the coefficients of the new method are given below.

$$b_0 = (12\,w^2\cosh(4\,w) + 544\,w^3\sinh(2\,w) - 24\,w^2\cosh(3\,w) - 16\,w^3\sinh(4\,w)$$

$$+128\,w^4\cosh(2\,w) - 300\,w^2 + 2856\,w\sinh(2\,w) - 2856\sinh(w)\,w + 204\,w\sinh(4\,w)$$
$$-3072\cosh(3\,w) - 96\,w^3\sinh(3\,w) - 4\,w^4\cosh(4\,w) + 10752\cosh(2\,w) + 13440$$
$$-736\sinh(w)\,w^3 - 21504\cosh(w) - 88\,w^4\cosh(3\,w) - 1224\,w\sinh(3\,w)$$
$$+384\cosh(4\,w) - 96\,w^2\cosh(2\,w) + 408\,w^2\cosh(w) - 380\,w^4 + 344\,w^4\cosh(w))/$$

$$(86\,w^6\cosh(w) - 276\,w^5\sinh(w) - 36\,w^5\sinh(3\,w) - 210\,w^3\sinh(2\,w) - 22\,w^6\cosh(3\,w)$$
$$-15\,w^3\sinh(4\,w) + 120\,w^4\cosh(2\,w) - w^6\cosh(4\,w) + 32\,w^6\cosh(2\,w)$$
$$+90\,w^3\sinh(3\,w) - 15\,w^4\cosh(4\,w) + 210\sinh(w)\,w^3 - 6\,w^5\sinh(4\,w)$$
$$+204\,w^5\sinh(2\,w) + 30\,w^4\cosh(3\,w) - 95\,w^6 + 375\,w^4 - 510\,w^4\cosh(w))$$
$$b_1 = -(24\,w^2\cosh(4\,w) + 1088\,w^3\sinh(2\,w) + 384\cosh(5\,w) - 48\,w^2\cosh(3\,w)$$

$$-32\,w^3\sinh(4\,w) + 256\,w^4\cosh(2\,w) - 600\,w^2 + 5712\,w\sinh(2\,w) - 5712\sinh(w)\,w$$
$$+408\,w\sinh(4\,w) + 11136\cosh(3\,w) - 192\,w^3\sinh(3\,w) - 8\,w^4\cosh(4\,w)$$
$$-24576\cosh(2\,w) - 21504 - 1472\sinh(w)\,w^3 + 37632\cosh(w) - 176\,w^4\cosh(3\,w)$$
$$-2448\,w\sinh(3\,w) - 3072\cosh(4\,w) - 192\,w^2\cosh(2\,w) + 816\,w^2\cosh(w) - 760\,w^4$$
$$+688\,w^4\cosh(w))/(86\,w^6\cosh(w) - 276\,w^5\sinh(w) - 36\,w^5\sinh(3\,w) - 210\,w^3\sinh(2\,w)$$
$$-22\,w^6\cosh(3\,w) - 15\,w^3\sinh(4\,w) + 120\,w^4\cosh(2\,w) - w^6\cosh(4\,w)$$
$$+32\,w^6\cosh(2\,w) + 90\,w^3\sinh(3\,w) - 15\,w^4\cosh(4\,w) + 210\sinh(w)\,w^3$$
$$-6\,w^5\sinh(4\,w) + 204\,w^5\sinh(2\,w) + 30\,w^4\cosh(3\,w) - 95\,w^6 + 375\,w^4$$
$$-510\,w^4\cosh(w))$$
$$c = (3\,w^3\cosh(4\,w) - 135\sinh(4\,w) - 1890\sinh(2\,w) + 66\,w^3\cosh(3\,w)$$

$$+1890\sinh(w) + 285\,w^3 - 204\,w^2\sinh(2\,w) + 276\,w^2\sinh(w) + 6\,w^2\sinh(4\,w)$$
$$+78\,w\cosh(3\,w) + 312\,w\cosh(2\,w) + 975\,w - 1326\,w\cosh(w) + 36\,w^2\sinh(3\,w)$$
$$-39\,w\cosh(4\,w) - 96\,w^3\cosh(2\,w) - 258\,w^3\cosh(w) + 810\sinh(3\,w))/(12\,w^3\cosh(4\,w)$$
$$+544\,w^4\sinh(2\,w) + 192\,w\cosh(5\,w) - 24\,w^3\cosh(3\,w) - 16\,w^4\sinh(4\,w)$$
$$+128\,w^5\cosh(2\,w) - 300\,w^3 + 2856\,w^2\sinh(2\,w) - 2856\,w^2\sinh(w) + 204\,w^2\sinh(4\,w)$$
$$+5568\,w\cosh(3\,w) - 96\,w^4\sinh(3\,w) - 4\,w^5\cosh(4\,w) - 12288\,w\cosh(2\,w) - 10752\,w$$
$$-736\sinh(w)\,w^4 + 18816\,w\cosh(w) - 88\,w^5\cosh(3\,w) - 1224\,w^2\sinh(3\,w)$$
$$-1536\,w\cosh(4\,w) - 96\,w^3\cosh(2\,w) + 408\,w^3\cosh(w) - 380\,w^5 + 344\,w^5\cosh(w))$$
$$b = (95\,w^3 + 120\,w\cosh(2\,w) - 15\,w\cosh(4\,w) + 375\,w + w^3\cosh(4\,w)$$

$$-86\,w^3\cosh(w) - 32\,w^3\cosh(2\,w) + 22\,w^3\cosh(3\,w) + 210\sinh(w) - 15\sinh(4\,w)$$
$$+90\sinh(3\,w) + 30\,w\cosh(3\,w) - 210\sinh(2\,w) - 510\,w\cosh(w))/(-3\,w^5\cosh(4\,w)$$
$$+135\,w^2\sinh(4\,w) + 1890\,w^2\sinh(2\,w) - 66\,w^5\cosh(3\,w) - 1890\,w^2\sinh(w) - 285\,w^5$$
$$+204\,w^4\sinh(2\,w) - 276\sinh(w)\,w^4 - 6\,w^4\sinh(4\,w) - 78\,w^3\cosh(3\,w)$$
$$-312\,w^3\cosh(2\,w) - 975\,w^3 + 1326\,w^3\cosh(w) - 36\,w^4\sinh(3\,w) + 39\,w^3\cosh(4\,w)$$
$$+96\,w^5\cosh(2\,w) + 258\,w^5\cosh(w) - 810\,w^2\sinh(3\,w))$$
$$a = (-32\,w^3\cosh(2\,w) + w^3\cosh(4\,w) + 95\,w^3 - 92\,w^2\sinh(w) - 2\,w^2\sinh(4\,w)$$

$$-12\,w^2\sinh(3\,w) + 22\,w^3\cosh(3\,w) - 306\,w\cosh(w) + 126\sinh(w) + 54\sinh(3\,w)$$
$$+18\,w\cosh(3\,w) - 9\,w\cosh(4\,w) + 72\,w\cosh(2\,w) - 9\sinh(4\,w) - 126\sinh(2\,w)$$
$$+68\,w^2\sinh(2\,w) - 86\,w^3\cosh(w) + 225\,w)/(-380\,w^5 - 480\,w^3\cosh(2\,w)$$
$$+60\,w^3\cosh(4\,w) - 1500\,w^3 - 4\,w^5\cosh(4\,w) + 344\,w^5\cosh(w) + 128\,w^5\cosh(2\,w)$$
$$-88\,w^5\cosh(3\,w) - 840\,w^2\sinh(w) + 60\,w^2\sinh(4\,w) - 360\,w^2\sinh(3\,w)$$

$$-120\,w^3\cosh(3\,w) + 840\,w^2\sinh(2\,w) + 2040\,w^3\cosh(w)).$$

As before, the formulae for a, b, c, b_0, b_1 are subject to heavy cancellations for small values of $w = vh$ and so instead we use the following series expansions for the coefficients of the method:

$$b_0 = \frac{1}{12} - \frac{1}{1064448}\,w^8 + \frac{67633}{435891456000}\,w^{10} - \frac{45821}{3138418483200}\,w^{12} + \cdots\ ,$$

$$b_1 = \frac{5}{6} + \frac{1}{532224}\,w^8 - \frac{26683}{217945728000}\,w^{10} + \frac{43}{313841848320}\,w^{12} + \cdots\ ,$$

$$c = \frac{1}{200} - \frac{1}{443520}\,w^6 + \frac{229}{756756000}\,w^8 - \frac{223673}{9081072000000}\,w^{10} + \frac{8269}{5292967680000}\,w^{12} + \cdots\ ,$$

$$b = -\frac{5}{252} + \frac{5}{22176}\,w^4 - \frac{20077}{544864320}\,w^6 + \frac{10489}{3051240192}\,w^8 - \frac{47339}{339632092800}\,w^{10} - \frac{64919671}{3902780304783360}\,w^{12} + \cdots\ ,$$

$$a = -\frac{7}{200} + \frac{1}{176}\,w^2 - \frac{6667}{7207200}\,w^4 + \frac{28429}{188760000}\,w^6 - \frac{94423}{3850704000}\,w^8 + \frac{2763014635489}{692085297103200000}\,w^{10} - \frac{214214956667}{329564427192000000}\,w^{12} + \cdots$$