

# Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation

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Received 8 February 2002

In the present paper we present a family of twelve steps symmetric multistep methods. The explicit part of new family of methods is applied to the scattering problems of the radial Schrödinger equation. This application shows the efficiency of the new family of methods.

**KEY WORDS:** symmetric multistep methods, exponential fitted methods, Schrödinger equation

**AMS subject classification:** 65L05

## 1. Introduction

Let us consider IVP of the form:

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \quad (1)$$

which solution has an oscillatory behavior. This type of equations are very important in many areas of quantum mechanics, physical chemistry, chemical physics, celestial mechanics or electronics.

For the solution of the above type of problems the most important properties are the following: (i) algebraic order of the method, (ii) interval of periodicity of the method, (iii) minimization of the phase-lag of the method, (iv) symmetry of the method, (v) exponential fitting and in special cases (vi) other adaptive properties such as Bessel and Neumann fitting. The development of methods with these properties is a continuing quest.

One of the most common proposed method that verifies all these properties (i)–(iv) are the symmetric multistep methods. Lambert and Watson [1] proved that a convergent

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multistep method with a non-zero interval of periodicity must be a symmetric method and must have even order. They gave examples of explicit methods with orders 2, 4, 6 and implicit methods with orders 4, 6, 8. Since the publication of that paper to nowadays several methods has been appear independently without a theory for its construction. In this paper we put some light in the construction of the existing and new symmetric methods, showing that they are part of the general family presented here.

In fact, we will extend this family to the case of exponential fitting methods with respect to one frequency (property (v)). That is to say when we take  $w = 0$  in our family we have a family that contains the classic symmetric methods. When we take  $w \neq 0$  then we have construct their exponential fitting extension. Finally the obtained methods have been applied to the resonance problem of the radial Schrödinger equation.

## 2. Family of twelve steps symmetric multistep methods

**Definition.** An ordinary polinomial of degree  $n$  in the variable  $\xi$  (real or complex)

$$\rho(\xi) = \sum_{i=0}^n a_i \xi^i, \quad a_i \in \mathbb{R}, \quad (2)$$

is said to be symmetric if  $a_i = a_{n-i}$ ,  $i = 0, 1, \dots, n$ , and  $a_0 \neq 0$ .

A classical multistep method represented by the polynomials  $(\rho, \sigma)$  is said symmetric if both polynomials are symmetric (see Lambert and Watson [1] for more details).

### 2.1. Explicit symmetric family

Given  $h > 0$ , for the integration of  $y''(x) = f(x, y)$  we consider the family of 12 step symmetric multistep methods:

$$\begin{aligned} & a_0 y_{n-6} + a_1 y_{n+5} + a_2 y_{-4+n} + a_3 y_{n-3} + a_4 y_{n-2} \\ & + a_5 y_{n-1} + a_5 y_{n+1} + a_4 y_{n+2} + a_3 y_{n+3} + a_2 y_{n+4} + a_1 y_{n+5} + a_0 y_{n+6} \\ & = \frac{h^2}{3628800} (50(18289152\alpha - 29786771a_0 - 1435008a_1 - 176979a_2 \\ & - 152192a_3 - 72339a_4) f_n + (36288000\alpha - 58366945a_0 \\ & - 6209664a_1 - 214305a_2 + 6272a_3 - 993a_4) f_{-4+n} \\ & + (-163296000\alpha + 238634060a_0 + 3516672a_1 - 4059060a_2 \\ & - 276736a_3 + 17484a_4) f_{n-3} \\ & + (435456000\alpha - 702113860a_0 \\ & - 38671872a_1 - 6211140a_2 - 3787264a_3 - 342084a_4) f_{n-2} \\ & + (-762048000\alpha + 1203012020a_0 + 33694464a_1 - 12307020a_2 \\ & - 6652672a_3 - 3309132a_4) f_{n-1} + (-762048000\alpha + 1203012020a_0 \end{aligned}$$

$$\begin{aligned}
 &+ 33694464a_1 - 12307020a_2 - 6652672a_3 - 3309132a_4) f_{n+1} \\
 &+ (435456000\alpha - 702113860a_0 - 38671872a_1 - 6211140a_2 \\
 &- 3787264a_3 - 342084a_4) f_{n+2} + (-163296000\alpha + 238634060a_0 \\
 &+ 3516672a_1 - 4059060a_2 - 276736a_3 + 17484a_4) f_{n+3} \\
 &+ (36288000\alpha - 58366945a_0 - 6209664a_1 - 214305a_2 + 6272a_3 - 993a_4) f_{n+4} \\
 &- 3628800\alpha f_{n-5} - 3628800\alpha f_{n+5}) \tag{3}
 \end{aligned}$$

where

$$a_5 = -a_0 - a_1 - a_2 - a_3 - a_4 \tag{4}$$

and

$$\begin{aligned}
 &\sin\left(\frac{wh}{2}\right)^{10} 1857945600 wh^2\alpha \\
 &= wh^2(708794075a_1 + 740244800a_2 + 740864475a_3 \\
 &+ 742860800a_4 + 744669275a_5) \\
 &+ (c_1a_5 - 4wh^2(292329389a_1 + 303829760a_2 + 302416173a_3 + 301580288a_4 \\
 &+ 300753005a_5)) \cos(wh) \\
 &+ (c_1a_4 + 4wh^2(165860497a_1 + 173975680a_2 + 174581649a_3 + 175442944a_4 \\
 &+ 175528465a_5)) \cos(2wh) \\
 &+ (c_1a_3 + wh^2(-235117388a_1 - 242693120a_2 - 238910796a_3 - 238616576a_4 \\
 &- 238634060a_5)) \cos(3wh) \\
 &+ (c_1a_2 + wh^2(52157281a_1 + 58152640a_2 + 58373217a_3 + 58365952a_4 \\
 &+ 58366945a_5)) \cos(4wh) \\
 &+ c_1a_1 \cos(5wh) + c_1a_0 \cos(6wh) \tag{5}
 \end{aligned}$$

where  $c_1 = -3628800$ .

The local truncation error is:

$$C_{14}h^{14}(w^2y^{(14)}(t) + y^{(16)}(t)) + O(h^{16}) \tag{6}$$

where

$$\begin{aligned}
 C_{14} = \frac{1}{2615348736000} &(139817479445a_0 - 3127899648a_1 + 299126805a_2 \\
 &- 44632576a_3 + 15936789a_4). \tag{7}
 \end{aligned}$$

## 2.2. Implicit symmetric family

$$\begin{aligned}
& a_0 y_{n-6} + a_1 y_{n-5} + a_2 y_{n-4} + a_3 y_{n-3} + a_4 y_{n-2} \\
& + a_5 y_{n-1} + a_5 y_{n+1} + a_4 y_{n+2} + a_3 y_{n+3} + a_2 y_{n+4} + a_1 y_{n+5} + a_0 y_{n+6} \\
= & h^2 \left( \frac{36883123200\alpha - 1970300185a_0 + 226371072a_1 + 111928935a_2 + 82237952a_3 + 40168167a_4}{39916800} f_n \right. \\
& - \alpha f_{n-6} + \left( 12\alpha - \frac{8323367a_0}{4561920} - \frac{34901a_1}{623700} + \frac{6617a_2}{4561920} - \frac{13a_3}{89100} + \frac{6059a_4}{159667200} \right) f_{n-5} \\
& + \left( -66\alpha + \frac{4929041a_0}{2280960} - \frac{179569a_1}{155925} - \frac{167791a_2}{2280960} + \frac{71a_3}{22275} - \frac{52141a_4}{79833600} \right) f_{n-4} \\
& + \left( 220\alpha - \frac{7455441a_0}{4561920} - \frac{322039a_1}{207900} - \frac{11211791a_2}{10644480} - \frac{51659a_3}{623700} + \frac{347317a_4}{53222400} \right) f_{n-3} \\
& + \left( -495\alpha + \frac{14518327a_0}{570240} - \frac{204884a_1}{51975} - \frac{2509013a_2}{1330560} - \frac{160004a_3}{155925} - \frac{657449a_4}{6652800} \right) f_{n-2} \\
& + \left( 792\alpha - \frac{11774551a_0}{2280960} - \frac{28481a_1}{11550} - \frac{1825459a_2}{591360} - \frac{581269a_3}{311850} - \frac{2672767a_4}{2956800} \right) f_{n-1} \\
& + \left( 792\alpha - \frac{11774551a_0}{2280960} - \frac{28481a_1}{11550} - \frac{1825459a_2}{591360} - \frac{581269a_3}{311850} - \frac{2672767a_4}{2956800} \right) f_{n+1} \\
& + \left( -495\alpha + \frac{14518327a_0}{570240} - \frac{204884a_1}{51975} - \frac{2509013a_2}{1330560} - \frac{160004a_3}{155925} - \frac{657449a_4}{6652800} \right) f_{n+2} \\
& + \left( 220\alpha - \frac{7455441a_0}{4561920} - \frac{322039a_1}{207900} - \frac{11211791a_2}{10644480} - \frac{51659a_3}{623700} + \frac{347317a_4}{53222400} \right) f_{n+3} \\
& + \left( -66\alpha + \frac{4929041a_0}{2280960} - \frac{179569a_1}{155925} - \frac{167791a_2}{2280960} + \frac{71a_3}{22275} - \frac{52141a_4}{79833600} \right) f_{n+4} \\
& \left. + \left( 12\alpha - \frac{8323367a_0}{4561920} - \frac{34901a_1}{623700} + \frac{6617a_2}{4561920} - \frac{13a_3}{89100} + \frac{6059a_4}{159667200} \right) f_{n+5} - \alpha f_{n+6} \right) \quad (8)
\end{aligned}$$

where

$$a_5 = -a_0 - a_1 - a_2 - a_3 - a_4 \quad (9)$$

and

$$\begin{aligned}
& 326998425600 \sin\left(\frac{wh}{2}\right)^{12} \alpha \\
= & wh^2(-3940600370a_0 + 452742144a_1 + 223857870a_2 + 164475904a_3 \\
& + 80336334a_4) + (c_2 a_5 + wh^2(8244218570a_0 + 393721344a_1 \\
& + 492873930a_2 + 297609728a_3 + 14432941a_4)) \cos(wh) \\
& + (c_2 a_4 - 8wh^2(508141445a_0 - 78675456a_1 - 37635195a_2 \\
& - 20480512a_3 - 1972347a_4)) \cos(2wh) \\
& + (c_2 a_3 + wh^2(2609404385a_0 + 247325952a_1 + 168176865a_2 \\
& + 13224704a_3 - 1041951a_4)) \cos(3wh) \\
& + (c_2 a_2 + wh^2(-345032870a_0 + 183878656a_1 + 11745370a_2 \\
& - 508928a_3 + 104282a_4)) \cos(4wh) \\
& + (c_2 a_1 + wh^2(291317845a_0 + 8934656a_1 - 231595a_2 \\
& + 23296a_3 - 6059a_4)) \cos(5wh) + c_2 a_0 \cos(6wh) \quad (10)
\end{aligned}$$

where  $c_2 = 159667200$ .

The local truncation error is:

$$C_{16}h^{16}(w^2y^{(14)}(t) + y^{(16)}(t)) + O(h^{18}) \tag{11}$$

where

$$C_{16} = -\frac{1}{31384184832000}(31861537855a_0 - 2660090880a_1 + 402680895a_2 - 74464256a_3 + 33586239a_4). \tag{12}$$

### 3. Properties

#### Corollary.

- (i) If  $a_0 \neq 0$  then the explicit multistep symmetric (3) integrates exactly the equation (1) when  $y(x)$  is any linear combination of the functions:

$$1, \quad x, \quad x^2, \quad \dots, \quad x^{11}, \quad \cos(wx), \quad \sin(wx). \tag{13}$$

- (ii) If  $a_0 \neq 0$  then the implicit multistep symmetric (8) integrates exactly the equation (1) when  $y(x)$  is any linear combination of the functions:

$$1, \quad x, \quad x^2, \quad \dots, \quad x^{13}, \quad \cos(wx), \quad \sin(wx). \tag{14}$$

#### Theorem.

- (i) The explicit multistep symmetric methods given by (3) when  $wh$  tends to zero are the maximum order methods with twelve steps.
- (ii) The implicit multistep symmetric given by (8) when  $wh$  tends to zero are the maximum order methods with twelve steps.

*Proof.* The conditions over the polynomial  $\rho$  comes from the consistency of the method. Ones that  $\rho$  has been choose  $\sigma$  is unique if we ask for maximum order methods. To prove that our choice of  $\sigma$  is right a simple Taylor expansion is enough.

When  $wh$  tends to zero the coefficient  $\alpha$  of the explicit method tends to

$$\frac{291317845a_0 + 8934656a_1 - 231595a_2 + 23296a_3 - 6059a_4}{159667200}. \tag{15}$$

When  $wh$  tends to zero the coefficient  $\alpha$  of the implicit method tends to

$$\frac{139817479445a_0 - 3127899648a_1 + 299126805a_2 - 44632576a_3 + 15936789a_4}{2615348736000}. \tag{16}$$

For example, all the twelve step methods that appear in the paper of Quinlan and Tremaine [2] are particular choices of  $a_i, i = 0, 1, 2, 3, 4$ , in our family. □

#### 4. Numerical illustrations – the radial Schrödinger equation

The radial Schrödinger equation can be written as

$$y''(x) = \left[ \frac{l(l+1)}{x^2} + V(x) - k^2 \right] y(x). \quad (17)$$

Equations of this type occur frequently in theoretical physics and chemistry (see for example [3–8]). In (17) the function  $W(x) = l(l+1)/x^2 + V(x)$  denotes *the effective potential*, which satisfies  $W(x) \rightarrow 0$  as  $x \rightarrow \infty$ ,  $k^2$  is a real number denoting *the energy*,  $l$  is a given integer representing *angular momentum* and  $V$  is a given function which denotes the potential. The boundary conditions are:

$$y(0) = 0 \quad (18)$$

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

There is much research activity in developing techniques for the numerical solution of the Schrödinger equation (for a review see [9,10]). A prime aim of this activity is the construction of a fast and reliable methods.

A fruitful way for developing efficient methods for the solution of (17) is to use exponential fitting. Up till the present the exponential fitting was applied to *symmetric multistep methods*. Raptis and Allison [11] have derived a Numerov type exponentially fitted method. The computational results obtained in [11] indicate that these fitted methods are much more efficient than Numerov's method for the solution of (17). Since then, exponential fitting has been the subject of great activity for the construction of symmetric exponentially-fitted multistep methods. An important contribution in this general area is that of Ixaru and Rizea [6]. They showed that for the resonance problem defined by (17) it is generally more efficient to derive methods which exactly integrate functions of the form

$$\{1, x, x^2, \dots, x^p, \exp(\pm vx), x \exp(\pm vx), \dots, x^m \exp(\pm vx)\}, \quad (19)$$

where  $v$  is the frequency of the problem, than to use classical exponential fitting methods. The reason for this is explained in [12]. We note that the resonance problem is a stiff oscillatory problem. For the method obtained by Ixaru and Rizea [6] we have  $m = 1$  and  $p = 1$ . Another low order method of this type (with  $m = 2$  and  $p = 0$ ) was developed by Raptis [13]. Raptis (see [14,15]) has derived four-step exponentially-fitted methods. For these methods we have  $m = 0$ ,  $p = 5$  and  $m = 2$  and  $p = 1$ . Simos [16] has also derived a four-step exponentially-fitted method. For this method we have  $m = 3$  and  $p = 0$ . Simos [17] 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  $p = 0$ . We note here that also hybrid exponentially-fitted methods have been derived during these years (for a full review see [10]).

In this section we present some numerical results to illustrate the performance of our new methods. Consider the numerical integration of the Schrödinger equation (17) using the well-known Woods–Saxon potential which is given by

$$V(x) = V_W(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{20}$$

with  $z = \exp[(x - R_0)/a]$ ,  $u_0 = -50$ ,  $a = 0.6$  and  $R_0 = 7.0$ . In the case of negative eigenenergies (i.e. when  $E \in [-50, 0]$ ) we have the well-known *bound-states problem* while in the case of positive eigenenergies (i.e. when  $E \in [1, 1000]$ ) we have the well-known *resonance problem*.

#### 4.1. Resonance problem

In the asymptotic region the equation (17) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right)y(x) = 0, \tag{21}$$

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 the asymptotic form (when  $x \rightarrow \infty$ )

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan \delta_l \cos(kx - \pi l/2)] \end{aligned} \tag{22}$$

where  $\delta_l$  is the *phase shift* which may be calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{23}$$

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 multistep method. From the initial condition,  $y_0 = 0$ . The values  $y_i$ ,  $i = 2, \dots, 8$ , are computed using the Runge–Kutta–Nyström 12(10) method of Dormand et al. [20,21]. With these starting values we evaluate at  $x_1$  of the asymptotic region the phase shift  $\delta_l$  from the above relation.

#### 4.2. The Woods–Saxon potential

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (17) with  $l = 0$  in the well-known case where the potential  $V(r)$  is the Woods–Saxon one (20).

One can investigate the problem considered here, following two procedures. The first procedure consists of finding the *phase shift*  $\delta(E) = \delta_l$  for  $E \in [1, 1000]$ . The

second procedure consists of finding those  $E$ , for  $E \in [1, 1000]$ , at which  $\delta$  equals  $\pi/2$ . In our case we follow the first procedure i.e. we try to find the phase shifts for given energies. The obtained phase shift is then compared to the analytic value of  $\pi/2$ .

The above problem is the so-called *resonance problem* when *the positive eigenenergies lie under the potential barrier*. We solve this problem, using the technique fully described in [1].

The boundary conditions for this problem are:

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

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

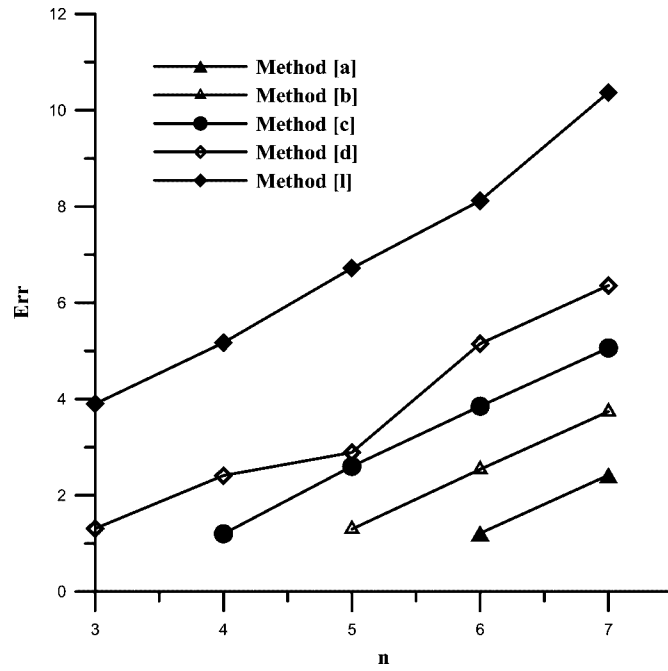
For comparison purposes in our numerical illustration we use the well-known Numerov's method (which is indicated as method [a]), the exponentially fitted method of Raptis and Allison [11] (which is indicated as method [b]), the exponentially-fitted method of Ixaru and Rizea [6] (which is indicated as method [c]), the exponentially-fitted method of Raptis [13] (which is indicated as method [d]), the classical Cowell method of order 8 mentioned in Henrici [18] (which is indicated as method [e]), the Cowell method of fourth algebraic order which integrates exactly functions of the form  $\{1, x, x^2, x^3, \cos(w, x), \sin(w, x)\}$ , which has been developed by Stiefel and Bettis [19] (which is indicated as method [f]), the exponentially-fitted Cowell method of fourth algebraic order which integrates exactly functions of the form

$$\{1, x, \cos(w, x), \sin(w, x), x \cos(w, x), x \sin(w, x)\},$$

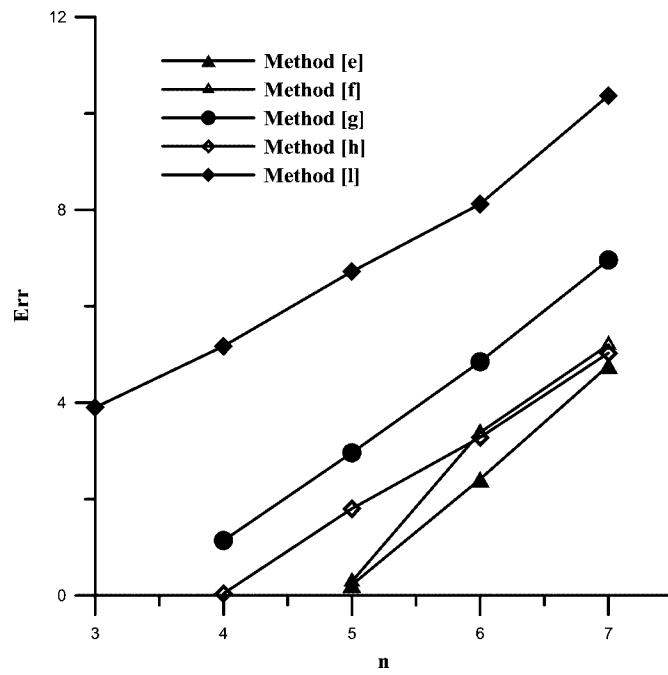
which has been developed by Stiefel and Bettis [19] (which is indicated as method [g]), the exponentially-fitted Cowell method of sixth algebraic order which integrates exactly functions of the form  $\{1, x, x^2, x^3, x^4, x^5, \cos(w, x), \sin(w, x)\}$ , which has been developed by Stiefel and Bettis [19] (which is indicated as method [h]), the exponentially-fitted Cowell method of sixth algebraic order which integrates exactly functions of the form  $\{1, x, x^2, x^3, \cos(w, x), \sin(w, x), x \cos(w, x), x \sin(w, x)\}$ , which has been developed by Stiefel and Bettis [19] (which is indicated as method [i]), the exponentially-fitted Cowell method of sixth algebraic order which integrates exactly functions of the form  $\{1, x, \cos(w, x), \sin(w, x), x \cos(w, x), x \sin(w, x), x^2 \cos(w, x), x^2 \sin(w, x)\}$ , which has been developed by Stiefel and Bettis [19] (which is indicated as method [k]) and the exponentially-fitted symmetric twelve step method of algebraic order twelve developed in this paper (which is indicated as method [l]).

The numerical results obtained for the methods mentioned above, with stepsizes equal to  $h = 1/2^n$ , were compared with the analytic solution of the Woods–Saxon potential resonance problem, rounded to six decimal places. Figure 1 show the errors  $\text{Err} = -\log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$  of the highest eigenenergy  $E_3 = 989.701916$  for several values of  $n$ .



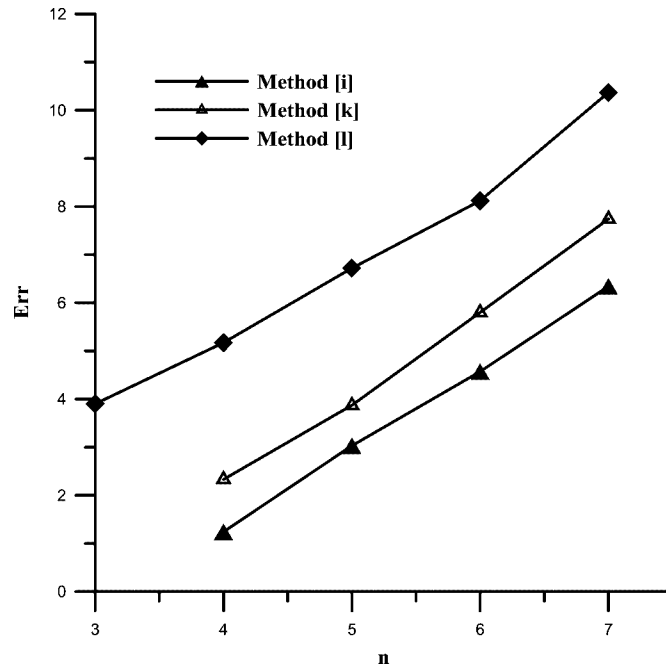


(a)



(b)

Figure 1. Values of Err for several values of  $n$  for the resonance  $E_3 = 989.7019159$ . The nonexistence of a value of Err indicates that the value of Err is negative.



(c)

Figure 1. (Continued).

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 [6]. That is, we choose:

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5], \\ (-E)^{1/2} & \text{for } x \in (6.5, 15]. \end{cases} \quad (24)$$

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 [6, p. 25].

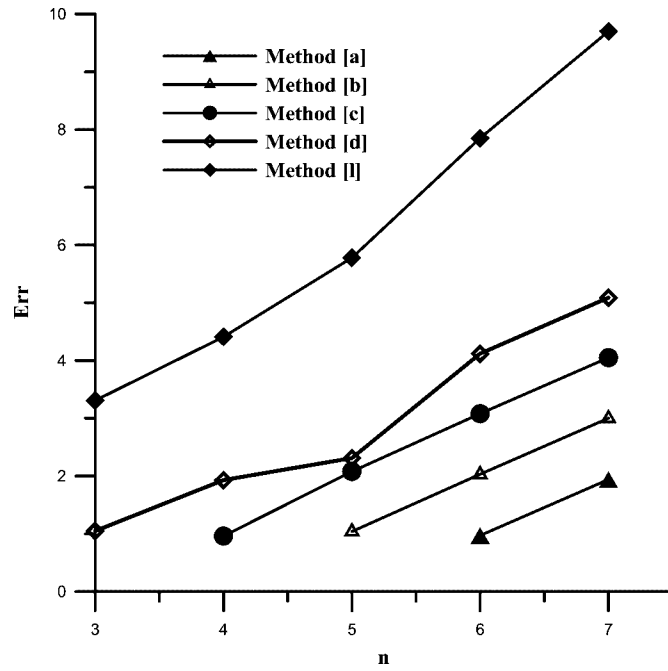
#### 4.3. Modified Woods–Saxon potential

In figure 2 some results for  $\text{Err} = -\log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$  of the highest eigenenergy  $E_3 = 1002.768393$ , for several values of  $n$ , obtained with another potential in (17) using the methods mentioned above are shown. This potential is

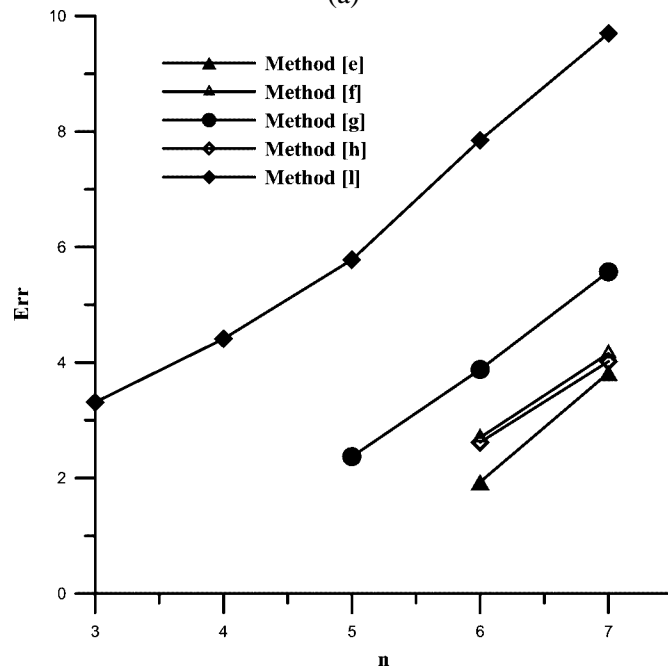
$$V(x) = V_W(x) + \frac{D}{x} \quad (25)$$

where  $V_W$  is the Woods–Saxon potential (20). For the purpose of our numerical experiments we use the same parameters as in [6], i.e.  $D = 20$ ,  $l = 2$ .

Since  $V(x)$  is singular at the origin, we use the special strategy of [6]. We start the integration from a point  $\varepsilon > 0$  and the initial values  $y(\varepsilon)$  and  $y(\varepsilon + h)$  for the integration



(a)



(b)

Figure 2. Values of Err for several values of  $n$  for the resonance  $E_3 = 1002.768393$ . The nonexistence of a value of Err indicates that the value of Err is negative.

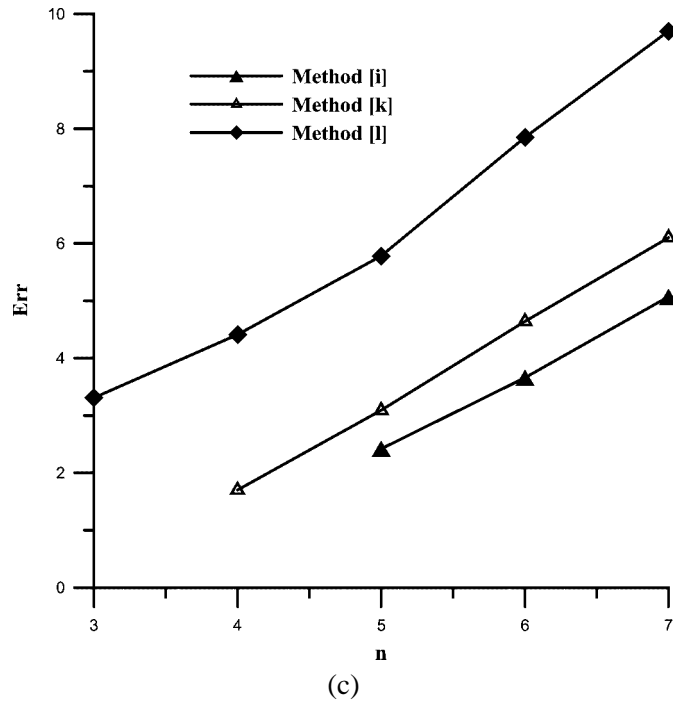


Figure 2. (Continued).

scheme are obtained using a perturbation method (see [6]). As in [6] 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 [6]. That is, we choose:

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

where  $a_i, i = 1, \dots, 3$ , are fully defined in [6].

We note here that each figure has three parts. In each part for comparison purposes we have included the method [n] which is the most accurate one.

### 5. Conclusions

A family of twelve steps symmetric multistep methods is presented in the present paper. The development of the new family of methods is done via a general family of methods, which is constructed in the paper. Part of this family of methods are existing

well known symmetric multistep methods. The explicit part of new family of methods is applied to the scattering problems of the radial Schrödinger equation. This application shows the efficiency of the new family of methods.

### Acknowledgements

The work was done during the visit of the second author to University of Salamanca. The authors wish to thank Spanish Ministry of Education grant SAB 1999/0153, JCYL under project SA 66/01 and CICYT under project BMF-2000-1115.

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