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P-stable Exponentially Fitted Methods for the Numerical Integration of the Schrödinger Equation

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A P-stable exponentially fitted method is developed in this paper for the numerical integration of the Schrödinger equation. An application to the bound-states problem (we solve the radial Schrödinger equation in order to find eigenvalues for which the wavefunction and its derivative are continuous and the boundary conditions are satisfied) and the resonance problem (the point of a resonance is that phase changes rapidly through π) of the radial Schrödinger equation indicates that the new method is generally more efficient than the previously developed exponentially fitted methods of the same kind. The method can be applied to any problem of physics and chemistry, which can be expressed as system of coupled second-order differential equations which have oscillatory or periodic solutions. This is because it has the property of the P-stability (i.e., the interval of periodic stability of the proposed method is equal to $(0, \infty)$) which allow is to integrate successful problems with high oscillatory or periodic solution.

Key Words: radial Schrödinger equation, exponentially fitted, multistep methods, finite difference methods, phase shift, bound-states problem, resonance problem.

1. INTRODUCTION

The numerical solution of the Schrödinger equation has been the subject of great activity, (see [1–3, 5–12, 15–26, 28, 31]) the aim being to achieve a fast and reliable method that generates a numerical solution. The radial form of the Schrödinger equation can be written as

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

Equations of this type occur very frequently in theoretical physics and chemistry, quantum

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physics and chemistry, physical chemistry (see, for example, [6–7, 14, 27]), and it is needed to be able to solve them both efficiently and reliably by numerical methods. In (1) the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, E is a real number denoting *the energy*, l is a given integer, and V is a given function which denotes the potential. The boundary conditions are

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

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

A fruitful way 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. The computational results obtained in [19] indicate that these fitted methods are much more efficient than Numerov's method for the solution of (1). Since then, exponential fitting has been the subject of great activity. An interesting paper 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 (if a problem can be written in the form $y''(x) = f(x)y(x)$, then the *frequency of the problem* is defined to be equal to $\sqrt{f(x)}$), rather than using classical exponential fitting methods. The reason for this is explained in [25]. We note here that the resonance problem is a stiff oscillatory problem. 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 (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 $p = 3$. All the above methods are not P-stable. Recently Coleman and Ixaru [34] have derived P-stable exponentially fitted methods. The main problem of their approach is the requirement for the knowledge of two frequencies for the same problem. For many real problems this is impossible.

In this paper we introduce a new approach for exponential fitting. The purpose of this paper is to derive a family of simple P-stable Numerov-type predictor–corrector methods fitted to (3) and, in particular, to derive methods with $m = 0$ and $p = 3$ and $m = 1$ and $p = 1$. The new methods are much more accurate than the corresponding exponentially fitted methods of Ixaru *et al.* [7] and Raptis [16]. We have applied the new methods 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 (see Section 4). We have also

applied the new methods to *the bound-states problem*. We note here that the method can be applied to any problem of physics and chemistry, which can be expressed as a system of coupled second-order differential equations which have oscillatory or periodic solutions. Problems of the above type are, for example, the Duffin's type equations, the Bessel's type equations, many problems of celestial mechanics, problems of molecular dynamics, and many others.

2. EXPONENTIAL MULTISTEP METHODS

For the numerical solution of the rth-order initial value problem

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

where A is low bound of the interval of integration, 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, where B is the upper bound of the interval of integration.

The method (5) is associated with the operator

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

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 $1, x, x^2, \ldots, x^{p+r-1}$ (or $\exp(v_0 x), \exp(v_1 x), \ldots, \exp(v_{p+r-1} x)$ where v_i, $i = 0, 1, \ldots, p + r - 1$ are real or complex numbers).

Remark 1 (See [30, 21]). If $v_i = v$ for $i = 0, 1, \ldots, n$, $n \le p + r - 1$, then the operator L vanishes for any linear combination of $\exp(vx), x\exp(vx), x^2\exp(vx), \ldots, x^n \exp(vx), \exp(v_{n+1}x), \ldots, \exp(v_{p+r-1}x)$.

Remark 2 (See [30, 21]). 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 [29, 30]). *Consider an operator L of the form* (6). *With $v \in \mathcal{C}$, $h \in \mathcal{R}$, $n \ge r$ if $v = 0$, and $n \ge 1$ otherwise, then we have*

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

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

PROPOSITION 1 (For proof see [31, 21]). *Consider an operator L with*

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

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 DERIVATION OF EXPONENTIALLY FITTED METHODS FOR GENERAL PROBLEMS

Consider the construction of an exponentially fitted multistep method (5) which exactly integrates the set of functions $\{\exp(\pm v_j x)\}_{j=0}^{k}$. We will use this for the numerical solution of the general problem (4).

From Lemma 1 we obtain the equations

$$\rho[\exp(\pm v_j h)] - (\pm v_j h)^r \sigma[\exp(\pm v_j h)] = 0, \tag{9}$$

or equivalently,

$$\sum_{i=0}^{k} [a_i \exp(\pm v_j h) - (\pm v_j h)^r b_i \exp(\pm v_j h)] = 0, \quad j = 0, 1, \ldots, n, \tag{10}$$

where $n \leq k$ and $a_i, b_i, i = 0(1)k$ are the coefficients of the multistep method (5).

We investigate here the case where k is a positive number. Then, from Proposition 1 we have a set of k equations:

$$a_i = (-1)^r a_{k-i}, \quad b_i = b_{k-i}, \quad i = 0, 1, \ldots, k. \tag{11}$$

We now let $a_k = 1$, which is the case adopted for all families of known multistep methods. Then (10) and (11) give the system of equations,

$$2 \sum_{i=1}^{k/2-1} a_i \sinh\left[\left(\frac{k}{2} - i\right) w_j\right] + a_{k/2} - w_j^r \left[2 \sum_{i=0}^{k/2-1} b_i \cosh\left[\left(\frac{k}{2} - i\right) w_j\right] + b_{k/2}\right]$$
$$= -2 \sinh\left(\frac{k w_j}{2}\right) \quad \text{for } r = 1, 3, 5, \ldots \tag{12}$$

$$2 \sum_{i=1}^{k/2-1} a_i \cosh\left[\left(\frac{k}{2} - i\right) w_j\right] + a_{k/2} - w_j^r \left[2 \sum_{i=0}^{k/2-1} b_i \cosh\left[\left(\frac{k}{2} - i\right) w_j\right] + b_{k/2}\right]$$
$$= -2 \cosh\left(\frac{k w_j}{2}\right) \quad \text{for } r = 2, 4, 6, \ldots, \tag{13}$$

where $w_j = v_j h$ and $j = 0, 1, \ldots, k$.

We now prove that the system of Eqs. (i) has a unique solution when $w_i \neq \pm w_j$ and (ii) lead to undetermined expressions of the form (0/0) when $w_i = \pm w_j$ for some i and j.

Let $X(w)$ and $Y(w)$ $(w = vh)$ be the matrices of the unknown coefficients in the systems of Eqs. (12) and (13), respectively. Consider case (i). In order to make the matrices $X(w)$

(or $Y(w)$) singular, then their columns would be linearly dependent. The elements in a row consist of terms like $\cosh Mw_j$, $\sinh Nw_j$, and powers of w_j. The multiple angle hyperbolic functions can be expressed in terms of powers of $\cosh w_j$, $\sinh x_j$, and their products. These with powers of w_j form a linearly independent set of functions. Therefore the columns cannot be linearly dependent. Hence, in this case $\det X(w) \neq 0$ (or $\det Y(w) \neq 0$). Thus the system of equations (12) and (13) has a unique solution.

Consider case (ii). Here we simply have two rows of the matrix of coefficients the same and, hence, $\det X(w) = 0$ (or $\det Y(w) = 0$). Similarly, we have the right-hand side of two of the equations in (10) or (11) the same so that the numerator determinant which is formed when a column of $X(w)$ (or $Y(w)$) is replaced by the right-hand column will also give two identical rows. Hence, the numerator determinant is 0. In these cases L'Hopital's rule must be used.

4. THE FAMILY OF EXPONENTIALLY FITTED METHOD

Consider the family of methods,

$$\begin{aligned} \bar{y}_{n+1} &= y_{n+1} - ah^2(f_n + f_{n+1}) \\ \bar{y}_{n-1} &= y_{n-1} - ah^2(f_n + f_{n-1}) \\ y_{n+1} - 2y_n + y_{n-1} &= h^2[b_0(\bar{f}_{n+1} + \bar{f}_{n-1}) + b_1 f_n], \end{aligned} \tag{14}$$

where $y_i = y(x_i), i = n-1, n, n+1$; $\bar{y}_{n\pm1} = \bar{y}(x_{n\pm1})$; $f_i = [l(l+1)/x_i^2 + V(x_i) - E]y(x_i)$, $i = n-1, n, n+1$; $\bar{f}_{n\pm1} = [l(l+1)/x_{n\pm1}^2 + V(x_{n\pm1}) - E]\bar{y}(x_{n\pm1})$.

This method for appropriate values of b_i, $i = 0, 1$, and a is of algebraic order four.

We require that the methods (14) should integrate exactly any linear combination of the functions:

$$\begin{gathered} \{1, x, x^2, x^3, \exp(\pm vx)\}, \\ \{1, x, \exp(\pm vx), x\exp(\pm vx)\}. \end{gathered} \tag{15}$$

To construct a method of the form (14) which integrates exactly the functions (15), we require that the method (14) integrates exactly (see [18, 21]),

$$\{1, x, \exp(\pm v_0 x), \exp(\pm v_1 x)\}, \tag{16}$$

and then put

$$\begin{gathered} v_0 = 0, \quad v_1 = v, \\ v_0 = v_1 = v. \end{gathered} \tag{17}$$

The method (14) integrates exactly the functions $1, x$. Demanding that (14) integrates (16) exactly, we obtain the following system of equations for b_i, $i = 0, 1$, and a,

$$2b_0 w_j^2 \cosh(w_j) - 2b_0 a w_j^4 + 2b_0 a w_j^4 \cosh(w_j) + b_1 w_j^2 = 2\cosh(w_j) - 2, \tag{18}$$

where $w_j = v_j h$, $j = 0, 1$.

Solving for b_i, $i = 0, 1$ we obtain

Case I. $v_0 = 0$, $v_1 = v$,

$$b_0 = -\frac{1}{2}\frac{w^2 - 2T_0}{w^2 T_0(1 + w^2 a)},$$
$$b_1 = \frac{-2T_0 + w^2\cosh(w) + w^4 a T_0}{w^2 T_0(1 + w^2 a)}, \tag{19}$$

where $T_0 = -1 + \cosh(w)$.

Case II. $v_0 = v_1 = v$,

$$b_0 = \frac{w\sinh(w) - 2T_0}{w^3(\sinh(w)T_1 + 2waT_0)}$$
$$b_1 = 2\frac{2\cosh(w)T_0 - w\sinh(w) + 4w^2 a T_0^2}{w^3(\sinh(w)T_1 + 2waT_0)}, \tag{20}$$

where $T_0 = -1 + \cosh(w)$ and $T_1 = 1 + w^2 a$.

5. STABILITY ANALYSIS

The periodic stability analysis of a numerical method is important for the determination of the interval of periodicity. The interval of periodicity defines the stepsize which can be used in order for the approximation of the solution of problems with high oscillatory or periodic solution to be of the same order as the algebraic and/or exponential order of the method. It is obvious that when we have a large interval of periodicity the we can have a large stepsize for the same accuracy. It is obvious, also, that when we have small interval of periodicity or zero interval of periodicity then we can have only very small stepsizes or we may have divergence of the method. The most important property is the P-stability (i.e., the interval of periodic stability of the proposed method is equal to $(0, \infty)$), because in this case we can use a very large stepsize for the same accuracy.

We investigate the numerical integration of the problem:

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y_0'. \tag{21}$$

To examine the stability properties of the methods for solving the initial-value problem (21) Lambert and Watson [13] introduce the scalar test equation

$$y'' = -w^2 y \tag{22}$$

and the *interval of periodicity*. When we apply a symmetric two-step method to the scalar test equation (22) we obtain a difference equation of the form

$$y_{n+1} - 2Q(s)y_n + y_{n-1} = 0, \tag{23}$$

where $s = wh$, h is the step length, $Q(s) = B(s)/A(s)$, where $B(s)$ and $A(s)$ are polynomials in s, and y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2 \ldots$. For explicit methods $A(s) = 1$.

The characteristic equation associated with (23) is

$$z^2 - 2Q(s)z + 1 = 0. \tag{24}$$

We have the following definitions.

DEFINITION 2 [35]. The method (23) with the characteristic equation (24) is unconditionally stable if $|z_1| \leq 1$ and $|z_2| \leq 1$ for all values of wh.

DEFINITION 3. Following Lambert and Watson [13] we say that the numerical method (23) has an interval of periodicity $(0, H_0^2)$, if, for all $s^2 \in (0, H_0^2)$, z_1 and z_2 satisfy

$$z_1 = e^{i\theta(s)}, \quad z_2 = e^{-i\theta(s)}, \tag{25}$$

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

DEFINITION 4 [13]. The method (23) is *P-stable* if its *interval of periodicity* is $(0, \infty)$.

Based on the above we have the following theorems (for the proofs see [28]).

THEOREM 1. *A method which has the characteristic equation* (24) *has an interval of periodicity* $(0, H_0^2)$, *if for all* $s^2 \in (0, H_0^2)$, $|Q(s)| < 1$. *For the implicit methods the above relation is equivalent to* $A(s) \pm B(s) > 0$.

If we apply the new method (14) to the scalar test equation (22) we obtain the difference equation (23) and the characteristic equation (24) with

$$A(s) = 1 + s^2 b_0 - s^4 b_0 a, \quad B(s) = 1 - \frac{1}{2} s^2 b_1 - s^4 b_0 a. \tag{26}$$

If we apply the coefficients b_0 and b_1 obtained above we have

Case I. $A(s) - B(s) = \frac{1}{2}s^2$,

$$A(s) + B(s) = 2 - \frac{1}{2}\frac{s^2(w^2 - 2\cosh(w) + 2)}{w^2(-1 + \cosh(w))(1 + w^2 a)} + \frac{s^4(w^2 - 2\cosh(w) + 2)a}{w^2(-1 + \cosh(w))(1 + w^2 a)} - \frac{1}{2}\frac{s^2(-2\cosh(w) + 2 + w^2\cosh(w) - w^4 a + w^4 a\cosh(w))}{w^2(-1 + \cosh(w))(1 + w^2 a)}. \tag{27}$$

Case II.

$$A(s) - B(s) = 2\frac{s^2(\cosh(w) - 1)^2(2w^2 a + 1)}{w^3(\sinh(w) - 2wa + 2wa\cosh(w) + w^2 a\sinh(w))}$$

$$A(s) + B(s) = 2 + \frac{s^2(w\sinh(w) - 2\cosh(w) + 2)}{w^3 T(\mathrm{w})} - 2\frac{s^4(w\sinh(w) - 2\cosh(w) + 2)a}{w^3 T(\mathrm{w})} - \frac{s^2\left(2\cosh(w)^2 - 2\cosh(w) - w\sinh(w) - 8w^2 a\cosh(w) + 4w^2 a + 4w^2 a\cosh(w)^2\right)}{w^3 T(\mathrm{w})}$$

$$T(\mathrm{w}) = \sinh(w) - 2wa + 2wa\cosh(w) + w^2 a\sinh(w). \tag{28}$$

Requiring $A(s) + B(s) > 0$ for all values of v and remarking that the stability polynomial $A(s) + B(s)$ for the two cases is a biquadratic polynomial we find the appropriate values of a by solving the equation $\mathrm{Dis} = 0$, where Dis is the discriminant of the biquadratic equation. So, we have the following values for the coefficient a:

Case I.

$$a=-\frac{4-8e^w+4(e^w)^2-4w+4w(e^w)^2+w^2+2w^2e^w+w^2(e^w)^2}{w^2\left(w^2(e^w)^2-2w^2e^w+w^2+4w(e^w)^2-4w-16e^w+8+8(e^w)^2\right)} \tag{29}$$

$$a=-\frac{4-8e^w+4(e^w)^2+4w-4w(e^w)^2+w^2+2w^2e^w+w^2(e^w)^2}{w^2\left(w^2(e^w)^2-2w^2e^w+w^2-4w(e^w)^2+4w-16e^w+8+8(e^w)^2\right)}. \tag{30}$$

The above formulae are subject to heavy cancellations for small values of $w=vh$ (for example, when $w<0.5$). In this case it is much more convenient to use series expansions for the coefficient a. For the above reason we choose the second value of a to avoid having w in the denominator in Taylor series expansions. An equivalent expression of this coefficient is given by

$$a=\frac{w^4T_2+16w^3\sinh(w)+4w^2T_3+16wT_4+32T_5}{-w^6T_5+64w^4T_6-64w^2T_5}, \tag{31}$$

where $T_2=1-\cosh(2w)$, $T_3=\cosh(2w)-5+4\cosh(w)$, $T_4=\sinh(2w)-2\sinh(w)$, $T_5=-\cosh(2w)-3+4\cosh(w)$, $T_6=1-\cosh(w)$.

The Taylor series expansion of this coefficient is given by

$$\begin{aligned}a=&-\frac{1}{12}+\frac{1}{180}w^2-\frac{103}{302400}w^4+\frac{61}{3024000}w^6-\frac{49337}{41912640000}w^8\\&+\frac{2231377}{32691859200000}w^{10}-\frac{36126667}{9153720576000000}w^{12}+\frac{1064060519}{4668397493760000000}w^{14}.\end{aligned} \tag{32}$$

Substituting the value of a given by (30) to the coefficients b_0 and b_1 given by (19) we obtain

$$\begin{aligned}b_0&=-\frac{1}{4}\frac{-w^2T_0+4w\sinh(w)-8T_0}{T_0w^2},\\b_1&=-\frac{1}{2}\frac{-w^2T_0-4w\sinh(w)+8T_0}{T_0w^2},\end{aligned} \tag{33}$$

where $T_0=-1+\cosh(w)$.

The Taylor series expansion of these coefficients are given by

$$\begin{aligned}b_0=&\frac{1}{12}+\frac{1}{360}w^2-\frac{1}{15120}w^4+\frac{1}{604800}w^6-\frac{1}{23950080}w^8+\frac{691}{653837184000}w^{10}\\&-\frac{1}{37362124800}w^{12}+\frac{3617}{5335311421440000}w^{14},\\b_1=&\frac{5}{6}-\frac{1}{180}w^2+\frac{1}{7560}w^4-\frac{1}{302400}w^6+\frac{1}{11975040}w^8-\frac{691}{326918592000}w^{10}\\&+\frac{1}{18681062400}w^{12}-\frac{3617}{2667655710720000}w^{14}.\end{aligned} \tag{34}$$

For the above coefficients we have that $A(s)\pm B(s)>0$; i.e. the method is *P-stable*.

Based on the above formulae, we can use the following algorithm

When $w\geq 0.5$ then (31) and (33) expansions can be used.

When $w<0.5$ then (32) and (34) expansions can be used.

Case II.

$$a = -\frac{1}{2w^2} \tag{35}$$

$$a = \frac{-2w^2 + 4w\sinh(w) + 1 - \cosh(2w)}{14w^2 + 4w^4 - 16w^2\cosh(w) + 2w^2\cosh(2w)}. \tag{36}$$

We choose the second value of a to avoid having w in the denominator. The Taylor series expansion of this coefficient is given by

$$a = -\frac{1}{12} + \frac{1}{90}w^2 - \frac{221}{151200}w^4 + \frac{877}{4536000}w^6 - \frac{119323}{4656960000}w^8 + \frac{1133023}{333590400000}w^{10} - \frac{3090911491}{6865290432000000}w^{12} + \frac{208956373909}{3501298120320000000}w^{14}. \tag{37}$$

Substituting the value of a given by (36) to the coefficients b_0 and b_1 given by (20) we obtain

$$\begin{aligned} b_0 &= \frac{16w^4 - 32w^3\sinh(w) - 16w^2T_5 - 8wT_7 + 2T_8}{8w^6 + 8w^4T_2 + w^2T_9} \\ b_1 &= \frac{-32w^4 + 64w^3\sinh(w) - 32w^2T_5 - 16wT_{10} + 4T_{11}}{8w^6 + 8w^4T_2 + w^2T_9}, \end{aligned} \tag{38}$$

where $T_2 = 1 - \cosh(2w)$, $T_5 = -\cosh(2w) - 3 + 4\cosh(w)$, $T_7 = \sinh(3w) + 13\sinh(w) - 8\sinh(2w)$, $T_8 = \cosh(4w) + 12\cosh(2w) - 13 - 8\cosh(3w) + 8\cosh(w)$, $T_9 = \cosh(4w) - 4\cosh(2w) + 3$, $T_{10} = 3\sinh(3w) + 7\sinh(w) - 8\sinh(2w)$, $T_{11} = 3\cosh(4w) + 4\cosh(2w) - 7 - 8\cosh(3w) + 8\cosh(w)$.

The Taylor series expansion of these coefficients are given by

$$\begin{aligned} b_0 &= \frac{1}{12} + \frac{1}{180}w^2 - \frac{1}{1512}w^4 + \frac{19}{907200}w^6 + \frac{13}{17740800}w^8 - \frac{8039}{81729648000}w^{10} \\ &\quad + \frac{27851}{7846046208000}w^{12} + \frac{408887}{8002967132160000}w^{14}, \\ b_1 &= \frac{5}{6} - \frac{1}{90}w^2 - \frac{11}{7560}w^4 + \frac{41}{453600}w^6 - \frac{17}{26611200}w^8 - \frac{15317}{81729648000}w^{10} \\ &\quad + \frac{1613}{150885504000}w^{12} - \frac{362987}{4001483566080000}w^{14}. \end{aligned} \tag{39}$$

For the above coefficients we have that $A(s) \pm B(s) > 0$; i.e. the method is *P-stable*.

Based on the above formulae, we can use the following algorithm:

When $w \geq 0.5$ then (36) and (38) expansions can be used.
When $w < 0.5$ then (37) and (39) expansions can be used.

The local truncation error is given by:

Case I.

$$\text{L.T.E.}(h) = h^6\left(-\frac{1}{240}\left(D^{(6)}\right)(y)(x) - \frac{1}{360}w^2\left(D^{(4)}\right)(y)(x) - \frac{1}{144}\left(D^{(4)}\right)(y)(x)\right). \tag{40}$$

Case II.

$$\text{L.T.E.}(h) = h^6\left(-\frac{1}{240}\left(D^{(6)}\right)(y)(x) - \frac{1}{180}w^2\left(D^{(4)}\right)(y)(x) + \frac{1}{360}w^4\left(D^{(2)}\right)(y)(x) - \frac{1}{144}\left(D^{(4)}\right)(y)(x)\right). \tag{41}$$

6. NUMERICAL ILLUSTRATIONS

In this section we present some numerical results to illustrate the performance of our new methods. Consider the numerical integration of the radial Schrödinger equation (1).

6.1. *Resonance Problem*

We will here investigate the case of positive energy $E = k^2$, corresponding to a scattering state. In this case, in the asymptotic region, the potential function $V(x)$ generally dies away faster than the term $l(l+1)/x^2$; Eq. (1) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right)y(x) = 0 \tag{42}$$

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 Eq. (1) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - B_{kx}n_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)], \end{aligned} \tag{43}$$

where δ_l is the *phase shift* which may be calculated from

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{44}$$

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, $y_0 = 0$. The value y_1 is computed using the Runge–Kutta–Nyström 12(10) method of Dormand *et al.* [36–37]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l from the above relation.

6.1.1. The Woods–Saxon potential. As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (1) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods–Saxon one,

$$V(x) = V_w(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{\left[a(1+z)^2\right]} \tag{45}$$

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

For positive energies one has the so-called "*resonance problem*" when *the positive eigenenergies lie under the potential barrier*. The problem considered here consists either of finding the *phase shift* $\delta(E) = \delta_l$ or of finding those E for $E \in [1, 1000]$, at which δ equals $\pi/2$. In our case we find the phase shifts for given energies. The obtained phase shift is then compared to the accurate value of the phase shift which is equal to $\pi/2$.

The boundary conditions for this problem are

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

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 methods of Raptis and Allison [19] (which is indicated as method [b]), Ixaru and Rizea [7] (which is indicated as method [c]), the method of Chawla *et al.* [32] (which is indicated as method [d]), the method of Chawla *et al.* [33] (which is indicated as method [e]), the new exponentially fitted method (Case I) (which is indeicated as method [f]) and the new exponentially fitted method (Case II) (which is indeicated as method [g]). We note here that the methods [b] and [c] integrate the same exponential functions as the methods produced in this paper and the methods [d] and [e] are fourth-order Numerov-type with minimal phase-lag or P-stable.

The phase shifts obtained for the seven methods, with stepsizes equal to $h = 1/2^n$, were compared with the accurate value of the phase shift which is equal to $\pi/2$. Figure 1 shows the errors $\text{Err} = -\log_{10}|\text{phase} - \text{shift}_{\text{calculated}} - \pi/2|$ of the highest eigenenergy $E_3 = 989.701916$ 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

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5], \\ (-E)^{1/2} & \text{for } x \in (6.5, 15]. \end{cases} \tag{46}$$

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].

6.1.2. Modified Woods-Saxon potential. In Fig. 2 some results errors for $\text{Err} = -\log_{10}|E_{\text{calculated}} - E_{\text{accurate}}|$ of the highest eigenenergy $E_3 = 1002.768393$ for several values of n, obtained with another potential in (1), using the methods mentioned above, are shown. We note here that the value $E_3 = 1002.768393$ is considered as the accurate one. We use this potential in order to see the accuracy of the proposed methods in the case which the potential has a singularity. The proposed potential is

$$V(x) = V_W(x) + \frac{D}{x}, \tag{47}$$

where V_W is the Woods–Saxon potential (45). 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

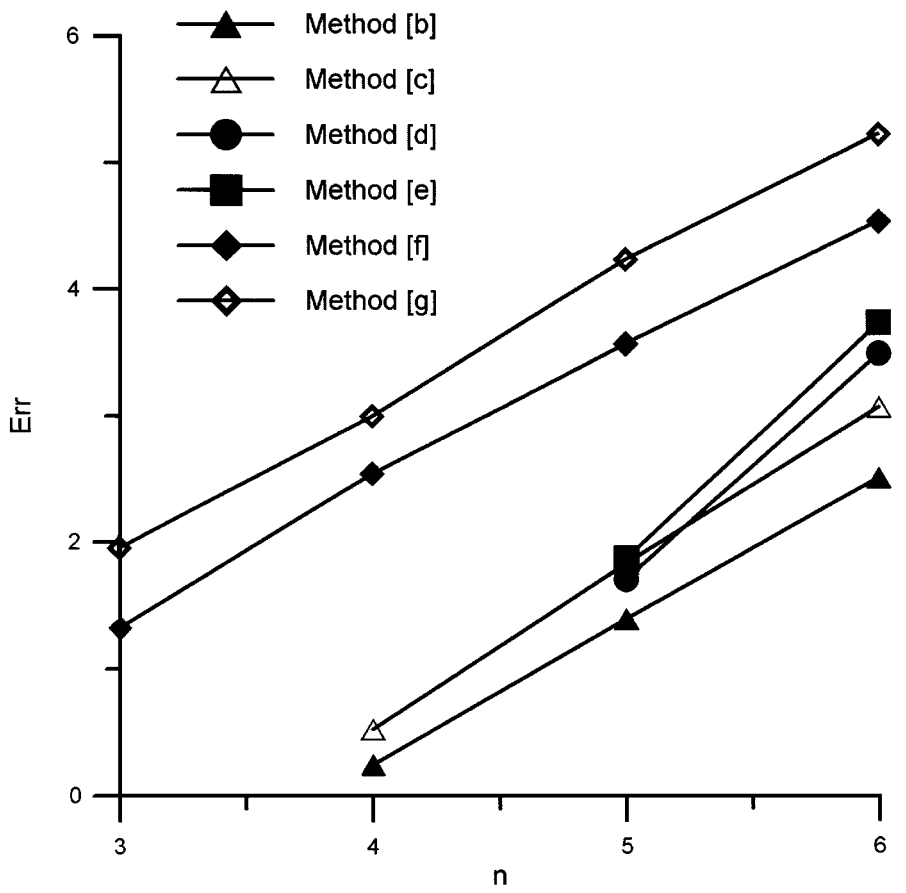

FIG. 1. Values of *Err* for several values of n for the resonance $E = 989.701916$. The non-existance of a value for a method indicates that Err is negative. Methods used: (i) Numerov's method (which is indicated as method [a]); (ii) the exponentially-fitted methods of Raptis and Allison [19] (which is indicated as method [b]); (iii) Ixaru and Rizea [7] (which is indicated as method [c]); (iv) the method of Chawla *et al.* [32] (which is indicated as method [d]); (v) the method of Chawla *et al.* [33] (which is indicated as method [e]); (vi) the new exponentially fitted method (Case I) (which is indicated as method [f]); and (vii) the new exponentially fitted method (Case II) (which is indicated as method [g]).

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

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

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

The positive eigenenergies are computed as the solutions of the transcendental equation which results by matching the logarithmic derivatives of the forward and backward

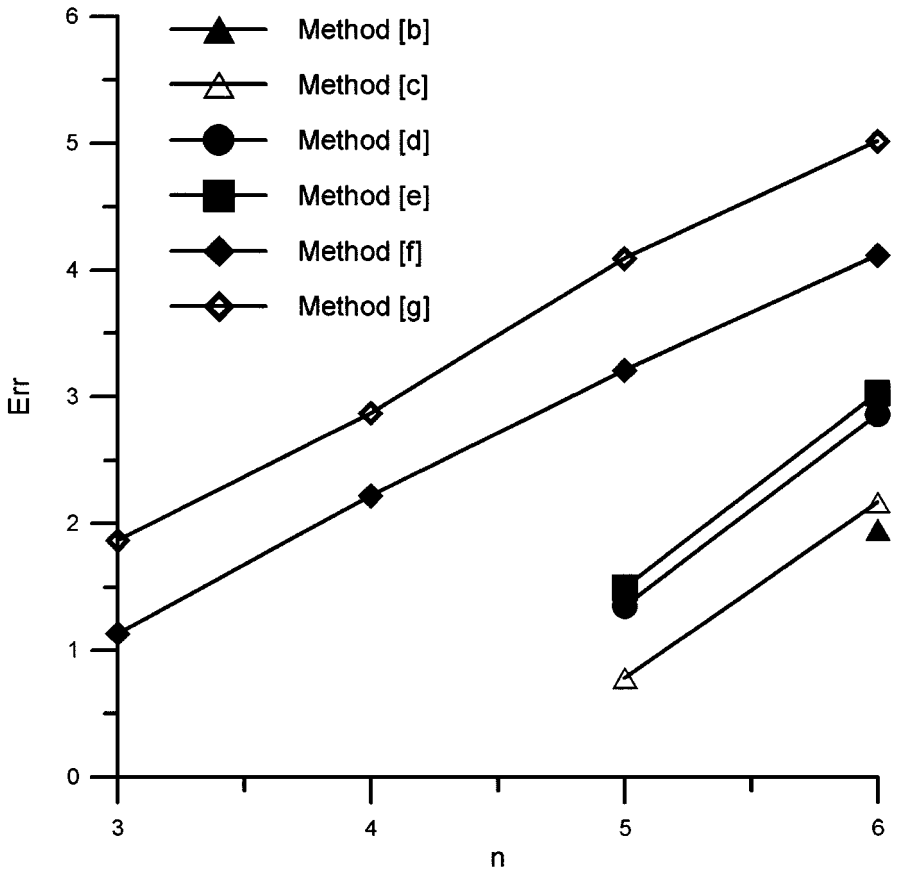

FIG. 2. Values of *Err* for several values of n for the positive eigenenergy $E = 1002.768393$. The nonexistance of a value for a method indicates that Err is negative. Methods used: (i) Numerov's method (which is indicated as method [a]); (ii) the exponentially fitted methods of Raptis and Allison [19] (which is indicated as method [b]); (iii) Ixaru and Rizea [7] (which is indicated as method [c]); (iv) the method of Chawla *et al*. [32] (which is indicated as method [d]); (v) the method of Chawla *et al*. [33] (which is indicated as method [e]); (vi) the new exponentially fitted method (Case I) (which is indeicated as method [f]; and (vii) the new exponentially fitted method (Case II) (which is indeicated as method [g]).

approximate solutions at the point a_3. The asymptotic solution in this case is the well-known Coulomb function. The values of the Coulomb function at the points $x = 15$ and $x = 15 - h$, required for the backward integration, are calculated using the method which is fully described in [7].

6.2. *The Bound-States Problem*

For negative energies we solve the so-called bound-states problem, i.e. Eq. (1) with $l = 0$ and boundary conditions given by

$$y(0) = 0,$$

$$y(x) \sim \exp(-\sqrt{-E}x) \quad \text{for large } x.$$

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

$$y(x_b) = \exp(-\sqrt{-E}x_b), \quad y(x_b - h) = \exp[-\sqrt{-E}(x_b - h)], \tag{48}$$

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 seven methods mentioned above were compared to this true solution. In Fig. 3 some results for errors $\mathrm{Err} = -\log_{10}|E_{\mathrm{calculated}} - E_{\mathrm{accurate}}|$ of the eigenenergy $E_0 = -49.457788728$ using stepsizes equal to $h = 1/2^n$ for several values of n are shown. In Fig. 4 some results for

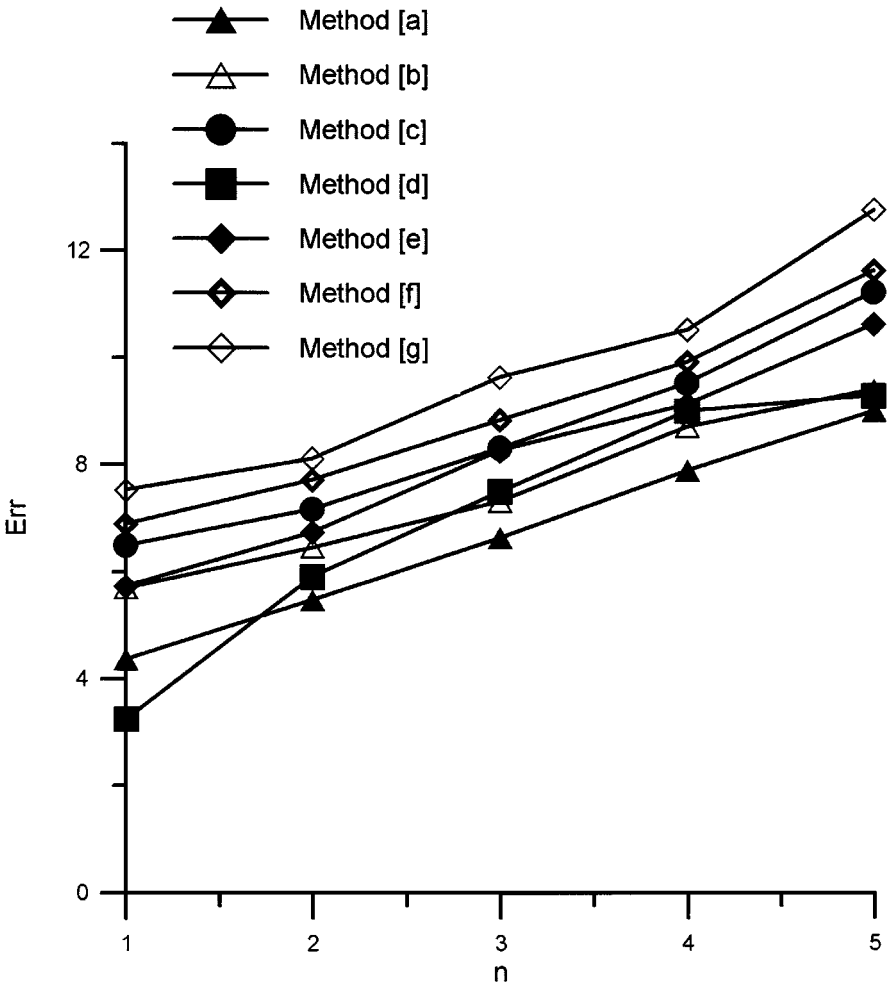

FIG. 3. Values of *Err* for several values of n for the eigenvalue $E = -49.457788728$. Methods used: (i) Numerov's method (which is indicated as method [a]); (ii) the exponentially fitted methods of Raptis and Allison [19] (which is indicated as method [b]); (iii) Ixaru and Rizea [7] (which is indicated as method [c]); (iv) the method of Chawla *et al.* [32] (which is indicated as method [d]); (v) the method of Chawla *et al.* [33] (which is indicated as method [e]); (vi) the new exponentially fitted method (Case I) (which is indicated as method [f]); and (vii) the new exponentially fitted method (Case II) (which is indicated as method [g]).

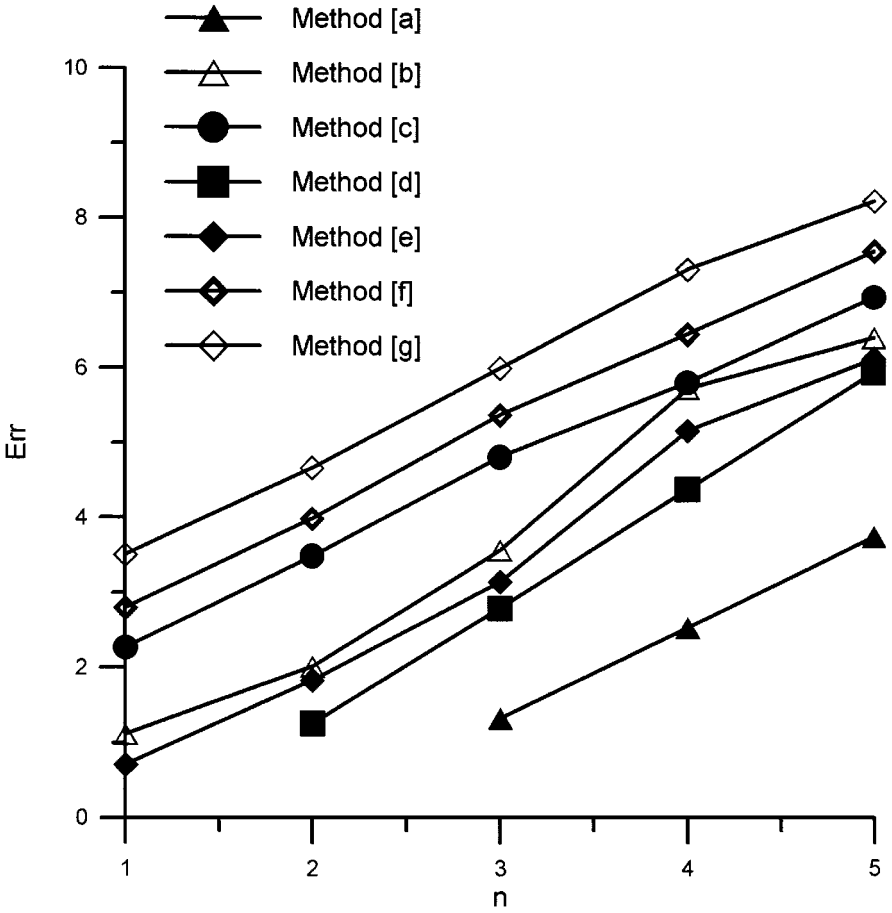

FIG. 4. Values of *Err* for several values of n for the eigenvalue $E = -8.676081670$. Methods used: (i) Numerov's method (which is indicated as method [a]); (ii) the exponentially fitted methods of Raptis and Allison [19] (which is indicated as method [b]); (iii) Ixaru and Rizea [7] (which is indicated as method [c]); (iv) the method of Chawla *et al.* [32] (which is indicated as method [d]); (v) the method of Chawla *et al.* [33] (which is indicated as method [e]); (vi) the new exponentially fitted method (Case I) (which is indeicated as method [f]); and (vii) the new exponentially fitted method (Case II) (which is indeicated as method [g]).

$\text{Err} = -\log_{10}|E_{\text{calculated}} - E_{\text{accurate}}|$ of the eigenenergy $E_{12} = -8.676081670$ using stepsizes equal to $h = 1/2^n$ for several values of n are also shown. We note here that the values $E_0 = -49.457788728$ and $E_{12} = -8.676081670$ are considered as the accurate ones.

In all the above examples we compare the value of Err, i.e. the values of absolute error. It is obvious that when we have a small absolute error, the value of Err is large. Based on this and on Figs. 1–4, we can observe that the new exponentially fitted P-stable methods developed in this paper are more accurate than the other similar well-known exponentially fitted ones, i.e. the method of Raptis and Allison [19] and the method of Ixaru and Rizea [7], and they are more accurate than the very popular methods of Chawla *et al.* [32–33]. More specifically, from the results presented in the Figs. 1–4 one can see the importance of the property of P-stability, since it can be seen that, even for high resonances or eigenvalues (in which cases the solution is highly oscillatory) and high stepsizes, the new methods are much more accurate than the other finite difference ones (most of which are diverged for high stepsizes).

7. CONCLUSIONS

In this paper a new approach for constructing exponentially fitted methods is developed. Using this new approach we can construct methods which exactly integrate functions of the form (3) and which are P-stable. With this new approach we must know only one approximation of the frequency of the problem for each interval of integration. Based on this new approach two P-stable exponentially fitted methods are obtained. Numerical and theoretical results show that these methods are much more accurate than similar well-known exponentially fitted ones, i.e. methods which integrate the same functions.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digit accuracy (IEEE standard).

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