Journal of Mathematical Chemistry 25 (1999) 65–84

A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation

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Received 22 June 1998

A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation is developed in this paper. An application to the resonance problem 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.

1. Introduction

The numerical solution of the Schrödinger equation has been the subject of great activity (see [1–3,8,13–19,23–34,37]), 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

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

Equations of this type occur very frequently in theoretical physics and chemistry, quantum physics and chemistry, chemical physics and physical chemistry (see, for example, [12–14,21]), and it is needed to be able to solve them both efficiently and reliably by numerical methods. In (1), the function $W(x) = l(l+1)/x^2 + V(x)$ is called the *effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k^2 is a real number denoting the *energy*, l is a given integer and V is a given function which denotes the potential. The boundary conditions are

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

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

It is known that a frutiful way for developing efficient methods for the solution of (1) is to use exponential fitting. Raptis and Allison [27] have derived a Numerov-type exponentially-fitted method. The computational results obtained in [27] indicated 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 [14]. 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

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

where v is the frequency of the problem, than to use classical exponential fitting methods. The reason for this is explained in [33]. We note here that the resonance problem is a stiff oscillatory problem. For the method obtained by Ixaru and Rizea [14] we have $m = 1$ and $p = 1$. Another low-order method of this type (with $m = 2$ and $p = 0$) was developed by Raptis [24]. Simos [30] 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 [23,25]. For this method we have $m = 3$ and $p = 0$. Simos [31] 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 [28] 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 [7] 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 $p = 5$, $m = 1$ and $p = 3$ and $m = 2$ and $p = 1$. The new methods are much more accurate than the corresponding exponentially-fitted methods of Ixaru et al. [14] and Raptis [24]. 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).

2. Exponential multistep methods

For the numerical solution of the initial value problem

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

the multistep methods of the form

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

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

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) is 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).

If $v_i = v$ for $i = 0, 1, \ldots, n,\ n \leqslant p + r - 1$, then the operator L vanishes for any linear combination of $\exp(vx), x\exp(vx), x^2\exp(vx), \ldots, x^n\exp(vx), \exp(v_{n+1}x), \ldots,$ $\exp(v_{p+r-1}x)$. Every exponential multistep method corresponds in a unique way, to an algebraic multistep method (by setting $v_i = 0$ for all i) (see [22,29]).

Lemma 1 (for proof, see [11,22]). Consider an operator L of the form (6). With $v \in \mathcal{C},\ h \in \mathcal{R},\ n \geqslant r$ if $v = 0$, and $n \geqslant 1$ otherwise, we have

$$\begin{aligned} L\left[x^m \exp(vx)\right] &= 0, \quad m = 0, 1, \ldots, n - 1, \\ L\left[x^n \exp(vx)\right] &\neq 0 \end{aligned} \tag{7}$$

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

Proposition 1 (for proof, see [29]). Consider an operator L with

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

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

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

3. The derivation of exponentially-fitted methods for general problems

Let us consider the derivation 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).

Based on lemma 1 we obtain the equations

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

or, equivalently,

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

where $n \leqslant k$ 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, based on 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 following 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 this system of equations (i) has a unique solution when $w_i \neq \pm w_j$, and (ii) leads to undetermined expressions of the form $(\frac{0}{0})$ when $w_i = \pm w_j$ for some i and j.

Consider that $X(w)$ and $Y(w)$ ($w = vh$) are the matrices of the unknown coefficients in the systems of equations (12) and (13), respectively. Consider now case (i). In order to make the matrices $X(w)$ (or $Y(w)$) singular, their columns would be linearly dependent. The elements in a row consist of terms like $\cosh M w_j$, $\sinh N w_j$ 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 (12) or (13) 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'Hospital's rule* must be used.

4. The family of exponentially-fitted method

Consider the following family of methods:

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

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

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

$$\begin{aligned}
&\big\{1, x, x^2, x^3, x^4, x^5, \exp(\pm vx)\big\},\\
&\big\{1, x, x^2, x^3, \exp(\pm vx), x\exp(\pm vx)\big\},\\
&\big\{1, x\exp(\pm vx), x\exp(\pm vx), x^2\exp(\pm vx)\big\}.
\end{aligned} \tag{15}$$

To construct a method of the form (14) which integrates exactly the functions (15), we require that the method (14) integrates exactly (see [26,29])

$$\big\{1, x, \exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x)\big\} \tag{16}$$

and then put

$$\begin{aligned}
&v_0 = v_1 = 0 \quad \text{and} \quad v_2 = v,\\
&v_0 = 0 \quad \text{and} \quad v_1 = v_2 = v,\\
&v_0 = v_1 = v_2 = v.
\end{aligned} \tag{17}$$

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, b:

$$\begin{aligned}
&2b_0 w_j^2 \cosh(w_j) + b_1 w_j^2 - 2b_1 b w_j^4 \cosh(w_j) + 2b_1 ba w_j^6\\
&\quad - 2b_1 ba w_j^6 \cosh(w_j) + 2b_1 b w_j^4 = 2\cosh(w_j) - 2,
\end{aligned} \tag{18}$$

where $w_j = v_j h,\ j = 0, 1, 2$.

Solving for $b_i,\ i=0,1$, and b we obtain:

Case I. $v_0=v_1=0,\ v_2=v$:

$$b_0=\frac{1}{12},\qquad b_1=\frac{5}{6},$$
$$b=\frac{1}{10}\frac{-12\cosh(w)+12+5w^2+w^2\cosh(w)}{w^4(-1+\cosh(w))(1+aw^2)}. \tag{19}$$

Case II. $v_0=0,\ v_1=v_2=v$:

$$\begin{aligned}
b_0=&-\frac{1}{4}\big(2w^2\cosh(w)-4w^4a+w^3\sinh(w)-2w^2+4w^4\cosh(w)a+w^5\sinh(w)a\\
&-12aw^2+16\cosh(w)-8\cosh(w)^2+24aw^2\cosh(w)-12\cosh(w)^2aw^2-8\big)\\
&\big/\big(w^2\big(1-2\cosh(w)+\cosh(w)^2-4aw^2\cosh(w)+2\cosh(w)^2aw^2+2aw^2\big)\big),\\
b_1=&\frac{1}{2}\big(w^3\sinh(w)-12aw^2+16\cosh(w)-8\cosh(w)^2-8-12\cosh(w)^2aw^2\\
&+w^5\sinh(w)a+4w^4\cosh(w)^2a-4w^4\cosh(w)a+24aw^2\cosh(w)\\
&-2w^2\cosh(w)+2w^2\cosh(w)^2\big)\big/\big(w^2\big(1-2\cosh(w)+\cosh(w)^2\\
&-4aw^2\cosh(w)+2\cosh(w)^2aw^2+2aw^2\big)\big),\\
b=&-\frac{1}{2}\big(8\cosh(w)-4-4\cosh(w)^2+w^3\sinh(w)\big)\big/\big(w^2\big(w^3\sinh(w)-12aw^2\\
&+16\cosh(w)-8\cosh(w)^2-8-12\cosh(w)^2aw^2+w^5\sinh(w)a\\
&+4w^4\cosh(w)^2a-4w^4\cosh(w)a+24aw^2\cosh(w)-2w^2\cosh(w)\\
&+2w^2\cosh(w)^2\big)\big).
\end{aligned} \tag{20}$$

Case III. $v_0=v_1=v_2=v$:

$$\begin{aligned}
b_0=&\big(2w^2\cosh(w)+3w^4a\cosh(w)-8\cosh(w)-24aw^2\cosh(w)+24w^2a+4w^2\\
&+8-2w\sinh(w)+6w^4a+3w^3a\sinh(w)\big)\big/\big(\big(2w^3\cosh(w)a+w\cosh(w)\\
&+4w^3a+2w+6w^2\sinh(w)a+\sinh(w)\big)w^3\big),\\
b_1=&-2\big(-8\cosh(w)^2-24\cosh(w)^2aw^2+2w^2\cosh(w)+24aw^2\cosh(w)\\
&+3w^4a\cosh(w)+8\cosh(w)-2w\sinh(w)+4w^2+3w^3a\sinh(w)+6w^4a\big)\\
&\big/\big(\big(2w^3\cosh(w)a+w\cosh(w)+4w^3a+2w+6w^2\sinh(w)a+\sinh(w)\big)w^3\big),\\
b=&-\frac{1}{2}\big(3\sinh(w)\cosh(w)+\cosh(w)^2w-3\sinh(w)-w\cosh(w)-2w\sinh(w)^2\big)\\
&\times\big(2w^3\cosh(w)a+w\cosh(w)+4w^3a+2w+6w^2\sinh(w)a+\sinh(w)\big)\\
&\big/\big(w\big(-2w\sinh(w)^2+\cosh(w)^2w-4w^3\sinh(w)^2a-2w^3\cosh(w)a\\
&+2w^3\cosh(w)^2a-6w^2\cosh(w)a\sinh(w)+6w^2\sinh(w)a+\sinh(w)
\end{aligned}$$

$$- w\cosh(w) - \sinh(w)\cosh(w)\big)\big(-8\cosh(w)^2 - 24\cosh(w)^2 a w^2 + 2w^2\cosh(w) + 24 a w^2\cosh(w) + 3w^4 a\cosh(w) + 8\cosh(w) - 2w\sinh(w) + 4w^2 + 3w^3 a\sinh(w) + 6w^4 a\big)\big). \tag{21}$$

5. Stability analysis

We investigate the numerical integration of the problem

$$y'' = f(x, y), \quad y(x_0) = y_0,\ y'(x_0) = y'_0. \tag{22}$$

To examine the stability properties of the methods for solving the initial-value problem (22), Lambert and Watson [20] introduce the scalar test equation

$$y'' = -w^2 y \tag{23}$$

and the *interval of periodicity*. When we apply a symmetric two-step method to the scalar test equation (23), we obtain a difference equation of the form

$$y_{n+1} - 2Q(s)y_n + y_{n-1} = 0, \tag{24}$$

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 (24) is

$$z^2 - 2Q(s)z + 1 = 0. \tag{25}$$

We have the following definitions.

Definition 2 ([35]). The method (24) with the characteristic equation (25) is unconditionally stable if $|z_1| \leqslant 1$ and $|z_2| \leqslant 1$ for all values of wh.

Definition 3. Following Lambert and Watson [20] we say that the numerical method (24) 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

$$z_1 = \mathrm{e}^{\mathrm{i}\theta(s)} \quad \text{and} \quad z_2 = \mathrm{e}^{-\mathrm{i}\theta(s)}, \tag{26}$$

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

Definition 4 ([20]). The method (24) is *P-stable* if its *interval of periodicity* is $(0, \infty)$.

Based on the above we have the following theorems (for the proofs, see [34]).

Theorem 1. A method, which has the characteristic equation (25), 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 (23), we obtain the difference equation (24) and the characteristic equation (25) with

$$A(s) = 1 + s^2 b_0 + s^4 b_1 b - s^6 b_1 b a, \qquad B(s) = 1 - \frac{1}{2} s^2 b_1 + s^4 b_1 b - s^6 b_1 b a. \quad (27)$$

If we apply the coefficients b_0, b_1 and b obtained above we have:

Case I.

$$\begin{aligned} A(s) - B(s) &= \frac{1}{2} s^2, \\ A(s) + B(s) &= 2 - \frac{1}{3} s^2 + \frac{1}{6} \frac{s^4(-12\cosh(w) + 12 + 5w^2 + w^2\cosh(w))}{w^4(-1+\cosh(w))(1+aw^2)} \\ &\quad - \frac{1}{6} \frac{s^6(-12\cosh(w) + 12 + 5w^2 + w^2\cosh(w))a}{w^4(-1+\cosh(w))(1+aw^2)}. \end{aligned} \quad (28)$$

Case II.

$$\begin{aligned} A(s) - B(s) &= \frac{1}{2} s^2, \\ A(s) + B(s) &= 2 - \frac{1}{4} s^2 \big(2w^2\cosh(w) - 4w^4 a + w^3\sinh(w) - 2w^2 + 4w^4\cosh(w)a \\ &\quad + w^5\sinh(w)a - 12aw^2 + 16\cosh(w) - 8\cosh(w)^2 + 24aw^2\cosh(w) \\ &\quad - 12\cosh(w)^2 aw^2 - 8\big) \big/ \big(w^2 T_0\big) \\ &\quad - \frac{1}{2} \frac{s^4(8\cosh(w) - 4 - 4\cosh(w)^2 + w^3\sinh(w))}{w^4 T_0} \\ &\quad + \frac{1}{2} \frac{s^6(8\cosh(w) - 4 - 4\cosh(w)^2 + w^3\sinh(w))a}{w^4 T_0} \\ &\quad - \frac{1}{4} s^2 \big(w^3\sinh(w) - 12aw^2 + 16\cosh(w) - 8\cosh(w)^2 - 8 \\ &\quad - 12\cosh(w)^2 aw^2 + w^5\sinh(w)a + 4w^4\cosh(w)^2 a - 4w^4\cosh(w)a \\ &\quad + 24aw^2\cosh(w) - 2w^2\cosh(w) + 2w^2\cosh(w)^2\big) \big/ \big(w^2 T_0\big), \\ T_0 &:= 1 - 2\cosh(w) + \cosh(w)^2 - 4aw^2\cosh(w) + 2\cosh(w)^2 aw^2 + 2aw^2. \end{aligned} \quad (29)$$

Case III.

$$\begin{aligned} &A(s) - B(s) \\ &\quad = 8 \frac{s^2(-2\cosh(w) - 6aw^2\cosh(w) + 3w^2 a + 1 + \cosh(w)^2 + 3\cosh(w)^2 aw^2)}{(2w^3\cosh(w)a + w\cosh(w) + 4w^3 a + 2w + 6w^2\sinh(w)a + \sinh(w))w^3}, \\ &A(s) + B(s) = 2 + s^2\big(2w^2\cosh(w) + 3w^4 a\cosh(w) - 8\cosh(w) - 24aw^2\cosh(w) \\ &\qquad + 24w^2 a + 4w^2 + 8 - 2w\sinh(w) + 6w^4 a + 3w^3 a\sinh(w)\big) \\ &\qquad \big/ \big(\big(2w^3\cosh(w)a + w\cosh(w) + 4w^3 a + 2w + 6w^2\sinh(w)a \end{aligned}$$

$$+\sinh(w)\big)w^3\big) + 2s^4\big(-3\sinh(w)\cosh(w) - \cosh(w)^2 w + 3\sinh(w)$$
$$+ w\cosh(w) + 2w\sinh(w)^2\big)\big/\big(w^4\big(2w\sinh(w)^2 - \cosh(w)^2 w$$
$$+ 4w^3\sinh(w)^2 a + 2w^3\cosh(w)a - 2w^3\cosh(w)^2 a$$
$$+ 6w^2\cosh(w)a\sinh(w) - 6w^2\sinh(w)a - \sinh(w) + w\cosh(w)$$
$$+ \sinh(w)\cosh(w)\big)\big) - 2s^6\big(-3\sinh(w)\cosh(w) - \cosh(w)^2 w$$
$$+ 3\sinh(w) + w\cosh(w) + 2w\sinh(w)^2\big)a\big/\big(w^4\big(2w\sinh(w)^2$$
$$- \cosh(w)^2 w + 4w^3\sinh(w)^2 a + 2w^3\cosh(w)a - 2w^3\cosh(w)^2 a$$
$$+ 6w^2\cosh(w)a\sinh(w) - 6w^2\sinh(w)a - \sinh(w) + w\cosh(w)$$
$$+ \sinh(w)\cosh(w)\big)\big) + s^2\big(-8\cosh(w)^2 - 24\cosh(w)^2 a w^2$$
$$+ 2w^2\cosh(w) + 24aw^4\cosh(w) + 3w^4 a\cosh(w) + 8\cosh(w)$$
$$- 2w\sinh(w) + 4w^2 + 3w^3 a\sinh(w) + 6w^4 a\big)\big/\big(\big(2w^3\cosh(w)a$$
$$+ w\cosh(w) + 4w^3 a + 2w + 6w^2\sinh(w)a + \sinh(w)\big)w^3\big). \tag{30}$$

Requiring $A(s) + B(s) > 0$ for all values of v and remarking that the stability polynomial $A(s) + B(s)$ for all the cases can be written as

$$A(s) + B(s) = 2 + s^2\big(c_1 + c_2 s^2 + c_4 s^4\big), \tag{31}$$

we find the appropriate values of a by solving the equation Dis $= 0$, where Dis is the discriminant of the polynomial $c_1 + c_2 s^2 + c_4 s^4$. So, we have the following values for the coefficient a:

Case I.

$$a = \left(-\frac{1}{2}w\mathrm{e}^w + \frac{1}{2}w + \frac{1}{4}\sqrt{6w^2(\mathrm{e}^w)^2 + 12w^2\mathrm{e}^w + 6w^2 + 48\mathrm{e}^w - 24(\mathrm{e}^w)^2 - 24}\right)$$
$$\Big/\big((\mathrm{e}^w - 1)w^3\big). \tag{32}$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use series expansions for the coefficient a. The Taylor series expansion of this coefficient is given by

$$a = \frac{1}{160} - \frac{463}{1612800}w^2 + \frac{1583}{129024000}w^4 - \frac{2962027}{5722472448000}w^6$$
$$+ \frac{1984790747}{89270570188800000}w^8 - \frac{295929081941}{299949115834368000000}w^{10}$$
$$+ \frac{55591933485043}{1223792392604221440000000}w^{12}$$
$$- \frac{2482759929905892097}{1145861293043184618700800000000}w^{14} + \cdots. \tag{33}$$

Substituting the value of a given by (32) to the coefficient b given by (19) we obtain

$$b = \frac{2}{5}\big(-12e^{w}\cosh(w) + 12e^{w} + 5w^2e^{w} + e^{w}w^2\cosh(w) + 12\cosh(w) - 12 - 5w^2 - w^2\cosh(w)\big)\big/\big(w^3\big(-2we^{w} + 2w - \sqrt{6w^2e^{(2w)} + 12w^2e^{w} + 6w^2 - 24e^{2w} - 24 + 48e^{w}} + 2\cosh(w)we^{w} - 2\cosh(w)w + \cosh(w)\sqrt{6w^2e^{(2w)} + 12w^2e^{w} + 6w^2 - 24e^{(2w)} - 24 + 48e^{w}}\,\big)\big). \tag{34}$$

The Taylor series expansion of this coefficient is given by

$$b = \frac{1}{200} - \frac{463}{2016000}w^2 + \frac{1583}{161280000}w^4 - \frac{2962027}{7153090560000}w^6 + \frac{1984790747}{111588212736000000}w^8 - \frac{295929081941}{374936394792960000000}w^{10} + \frac{55591933485043}{1529740490755276800000000}w^{12} - \frac{2482759929905892097}{1432326616303980773376000000000}w^{14} + \cdots. \tag{35}$$

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

Case II.

$$a = \frac{1}{2}\frac{-8\cosh(w) + 4 + 4\cosh(w)^2 - w^3\sinh(w)}{w^2(w^3\sinh(w) - 2w^2 + 2w^2\cosh(w)^2 - 12 - 12\cosh(w)^2 + 24\cosh(w))}. \tag{36}$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use series expansions for the coefficient a. The Taylor series expansion of this coefficient is given by

$$a = \frac{1}{160} - \frac{463}{806400}w^2 + \frac{2143}{64512000}w^4 - \frac{81413}{56770560000}w^6 + \frac{496640621}{111588212736000000}w^8 - \frac{509863901}{892705701888000000}w^{10} - \frac{104076245053}{231778862235648000000 0}w^{12} + \frac{17695186777754263}{383658915081423421440000000 0}w^{14} + \cdots. \tag{37}$$

Substituting the value of a given by (36) to the coefficients b_i, $i = 0, 1$, and b given by (19) we obtain

$$b_0 = -\frac{1}{16}\big(-32w^2\cosh(w)^3 + 144\cosh(w)^3 + 8w^4\cosh(w)^2 - 432\cosh(w)^2 + 96w^2\cosh(w) - 24w^3\sinh(w)\cosh(w) + \cosh(w)w^6 + 4w^5\cosh(w)\sinh(w) + 432\cosh(w) + 24w^3\sinh(w) - 64w^2 - 144 - 8w^4 + w^6 + 4w^5\sinh(w)\big)$$

$$/\big(w^2\big(-4\cosh(w)^3+w^2\cosh(w)^3-w^2\cosh(w)^2+12\cosh(w)^2-12\cosh(w) -w^2\cosh(w)+w^2+4\big)\big),$$

$$b_1=\frac{1}{8}\big(8w^4\cosh(w)^3+144\cosh(w)^3-64w^2\cosh(w)^3-432\cosh(w)^2 +96w^2\cosh(w)^2+4w^5\cosh(w)\sinh(w)+\cosh(w)w^6-8w^4\cosh(w) +432\cosh(w)-24w^3\sinh(w)\cosh(w)+24w^3\sinh(w)-32w^2-144 +4w^5\sinh(w)+w^6\big)/\big(w^2\big(-4\cosh(w)^3+w^2\cosh(w)^3-w^2\cosh(w)^2 +12\cosh(w)^2-12\cosh(w)-w^2\cosh(w)+w^2+4\big)\big),$$

$$b=-\big(-8\cosh(w)^3w^2+48\cosh(w)^3+8\cosh(w)^2w^2-144\cosh(w)^2+144\cosh(w) -16w^3\sinh(w)\cosh(w)+w^6\cosh(w)+2w^5\cosh(w)\sinh(w)+8w^2\cosh(w) -8w^2-48+16w^3\sinh(w)+w^6+2w^5\sinh(w)\big)/\big(\big(-64\cosh(w)^3w^2 +8w^4\cosh(w)^3+144\cosh(w)^3+96\cosh(w)^2w^2-432\cosh(w)^2+432\cosh(w) +4w^5\cosh(w)\sinh(w)-24w^3\sinh(w)\cosh(w)+w^6\cosh(w)-8w^4\cosh(w) -32w^2+24w^3\sinh(w)-144+4w^5\sinh(w)+w^6\big)w^2\big). \tag{38}$$

The Taylor series expansions of these coefficients are given by

$$b_0=\frac{1}{12}-\frac{463}{2419200}w^4+\frac{1583}{96768000}w^6-\frac{2924279}{2682408960000}w^8 +\frac{287402161}{4184557977600000}w^{10}-\frac{15059972261}{3515028701184000000}w^{12} +\frac{24822582683}{93125435719680000000}w^{14}+\cdots,$$

$$b_1=\frac{5}{6}+\frac{463}{1209600}w^4-\frac{1583}{48384000}w^6+\frac{2924279}{1341204480000}w^8 -\frac{287402161}{2092278988800000}w^{10}+\frac{15059972261}{1757514350592000000}w^{12} -\frac{24822582683}{46562717859840000000}w^{14}+\cdots,$$

$$b=\frac{1}{200}-\frac{463}{1008000}w^2+\frac{1513}{50400000}w^4-\frac{6550231}{3725568000000}w^6 +\frac{1233025133}{12454041600000000}w^8-\frac{53071754041}{9763968614400000000}w^{10} +\frac{35982534552827}{124490599833600000000000}w^{12} -\frac{594557721928816259}{40348744074067968000000000000}w^{14}+\cdots. \tag{39}$$

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

Case III.

$$a = \frac{1}{2}\big(8(e^w)^4 - 8w^2(e^w)^3 + 8w(e^w)^3 - 32w^2(e^w)^2 - 16(e^w)^2 - 8w^2e^w - 8we^w + 8$$
$$- 4\big(10we^w - 30w(e^w)^3 - 2w^3(e^w)^6 - 8w^3(e^w)^5 + w^4(e^w)^2 + w^4(e^w)^6$$
$$+ 18w^4(e^w)^4 + 8w^4(e^w)^5 + 4(e^w)^8 + 4 + 8(e^w)^3w^4 + 2w^3(e^w)^2 + 8w^3(e^w)^3$$
$$- 2w^2(e^w)^7 + 2w^2(e^w)^5 + 2w^2(e^w)^3 + 5w^2(e^w)^6 - 10w^2(e^w)^4 - 2w^2e^w$$
$$+ 5w^2(e^w)^2 + 24(e^w)^4 - 16(e^w)^6 - 16(e^w)^2 + 30w(e^w)^5 - 10w(e^w)^7\big)^{1/2}\big)$$
$$\big/\big(\big(12w^3(e^w)^3 + 12w^3e^w + 48w^3(e^w)^2 + 12w^2(e^w)^3 - 12w^2e^w - 24w(e^w)^4$$
$$+ 48w(e^w)^2 - 24w\big)w\big). \tag{40}$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use series expansions for the coefficient a. The Taylor series expansion of this coefficient is given by

$$a = \frac{1}{160} - \frac{463}{537600}w^2 + \frac{901}{14336000}w^4 - \frac{7291861}{3179151360000}w^6 - \frac{261918823}{2705168793600000}w^8$$
$$+ \frac{287661416507}{11109226512384000000}w^{10} - \frac{369665045999663}{135976932511580160000000}w^{12}$$
$$+ \frac{745886359408066345O3}{38195376434772820623360000000O}w^{14} + \cdots. \tag{41}$$

Substituting the value of a given by (40) to the coefficients b_i, $i = 0, 1$, and b given by (19) we obtain

$$b_0 = \frac{3}{2}\big(32\cosh(w)we^{(3w)} + 12w^2 + 20w\sinh(w)e^{(2w)} - 10w\sinh(w)e^{(4w)} + 32we^w$$
$$- 16\cosh(w) + 6w^2\cosh(w) + 6w^3\sinh(w)e^{(3w)} - 2w^4\cosh(w)e^{(3w)}$$
$$- 6w^3\cosh(w)e^{(3w)} + 2w^2\sinh(w)e^{(3w)} - 10w\sinh(w) + 8\sqrt{T_0} + 16$$
$$+ 24w^3\sinh(w)e^{(2w)} - 16\cosh(w)e^{(4w)} - 4w^4e^w + 12w^3e^w + 32\cosh(w)e^{(2w)}$$
$$- 32\cosh(w)we^w - 2w^4\cosh(w)e^w + 6w^3\cosh(w)e^w + w^2\cosh(w)\sqrt{T_0}$$
$$+ 6w^3\sinh(w)e^w - 2w^2\sinh(w)e^w + w\sinh(w)\sqrt{T_0} + 2w^2\sqrt{T_0}$$
$$- 8\cosh(w)\sqrt{T_0} - 32we^{(3w)} - 12w^2\cosh(w)e^{(2w)} + 6w^2\cosh(w)e^{(4w)}$$
$$- 16w^4e^{(2w)} + 16e^{(4w)} - 32e^{(2w)} - 12w^3e^{(3w)} - 4e^{(3w)}w^4 + 12w^2e^{(4w)}$$
$$- 24w^2e^{(2w)} - 8w^4\cosh(w)e^{(2w)}\big)\big/\big(w^3\big(10w^2e^w + 8w - 8w^3e^{(2w)} - 2w^3e^{(3w)}$$
$$- 10w^2e^{(3w)} - 16we^{(2w)} + 4w\cosh(w) - 2w^3e^w + 8we^{(4w)} - 5w^2\cosh(w)e^{(3w)}$$
$$+ 5\cosh(w)w^2e^w - w^3\cosh(w)e^{(3w)} - w^3\cosh(w)e^w + 3w^2\sinh(w)e^{(3w)}$$
$$+ 3w^2\sinh(w)e^w - 4w^3\cosh(w)e^{(2w)} + 4w\cosh(w)e^{(4w)} - 8w\cosh(w)e^{(2w)}$$
$$+ w\cosh(w)\sqrt{T_0} - 9w\sinh(w)e^{(3w)} + 12w^2\sinh(w)e^{(2w)} + 9\sinh(w)we^w$$
$$+ 2w\sqrt{T_0} + 3\sinh(w)\sqrt{T_0}\,\big)\big),$$

$$
\begin{aligned}
T_0 :=\ & 10w\mathrm{e}^{w} + 4 - 2w^2\mathrm{e}^{w} - 2w^3\mathrm{e}^{(6w)} - 30w\mathrm{e}^{(3w)} + w^4\mathrm{e}^{(2w)} + 24\mathrm{e}^{(4w)} + 8w^4\mathrm{e}^{(5w)}\\
& - 16\mathrm{e}^{(2w)} + w^4\mathrm{e}^{(6w)} + 18w^4\mathrm{e}^{(4w)} + 8w^3\mathrm{e}^{(3w)} + 2w^3\mathrm{e}^{(2w)} + 8\mathrm{e}^{(3w)}w^4 + 4\mathrm{e}^{(8w)}\\
& - 8w^3\mathrm{e}^{(5w)} - 16\mathrm{e}^{(6w)} - 2w^2\mathrm{e}^{(7w)} + 2w^2\mathrm{e}^{(5w)} + 2w^2\mathrm{e}^{(3w)} + 5w^2\mathrm{e}^{(6w)}\\
& - 10w^2\mathrm{e}^{(4w)} + 5w^2\mathrm{e}^{(2w)} + 30w\mathrm{e}^{(5w)} - 10w\mathrm{e}^{(7w)},
\end{aligned}
$$

$$
\begin{aligned}
b_1 =\ & -3\big(- 32\cosh(w)w\mathrm{e}^{(3w)} + 12w^2 + 20w\sinh(w)\mathrm{e}^{(2w)} - 10w\sinh(w)\mathrm{e}^{(4w)}\\
& + 16\cosh(w) - 16\cosh(w)^2 + 6w^2\cosh(w) + 6w^3\sinh(w)\mathrm{e}^{(3w)}\\
& - 2w^4\cosh(w)\mathrm{e}^{(3w)} - 6w^3\cosh(w)\mathrm{e}^{(3w)} + 2w^2\sinh(w)\mathrm{e}^{(3w)} - 10w\sinh(w)\\
& + 24w^3\sinh(w)\mathrm{e}^{(2w)} + 16\cosh(w)\mathrm{e}^{(4w)} - 4w^4\mathrm{e}^{w} + 12w^3\mathrm{e}^{w} - 8\cosh(w)^2\sqrt{T_1}\\
& - 32\cosh(w)\mathrm{e}^{(2w)} + 32\cosh(w)w\mathrm{e}^{w} - 2w^4\cosh(w)\mathrm{e}^{w} + 6w^3\cosh(w)\mathrm{e}^{w}\\
& + w^2\cosh(w)\sqrt{T_1} + 6w^3\sinh(w)\mathrm{e}^{w} - 2w^2\sinh(w)\mathrm{e}^{w} + w\sinh(w)\sqrt{T_1}\\
& + 32\cosh(w)^2\mathrm{e}^{(2w)} - 16\cosh(w)^2\mathrm{e}^{(4w)} + 32\cosh(w)^2w\mathrm{e}^{(3w)} + 2w^2\sqrt{T_1}\\
& + 8\cosh(w)\sqrt{T_1} - 12w^2\cosh(w)\mathrm{e}^{(2w)} + 6w^2\cosh(w)\mathrm{e}^{(4w)} - 16w^4\mathrm{e}^{(2w)}\\
& - 12w^3\mathrm{e}^{(3w)} - 4\mathrm{e}^{(3w)}w^4 - 32\cosh(w)^2w\mathrm{e}^{w} + 12w^2\mathrm{e}^{(4w)} - 24w^2\mathrm{e}^{(2w)}\\
& - 8w^4\cosh(w)\mathrm{e}^{(2w)}\big)\big/\big(w^3\big(10w^2\mathrm{e}^{w} + 8w - 8w^3\mathrm{e}^{(2w)} - 2w^3\mathrm{e}^{(3w)} - 10w^2\mathrm{e}^{(3w)}\\
& - 16w\mathrm{e}^{(2w)} + 4w\cosh(w) - 2w^3\mathrm{e}^{w} + 8w\mathrm{e}^{(4w)} - 5w^2\cosh(w)\mathrm{e}^{(3w)}\\
& + 5\cosh(w)w^2\mathrm{e}^{w} - w^3\cosh(w)\mathrm{e}^{(3w)} - w^3\cosh(w)\mathrm{e}^{w} + 3w^2\sinh(w)\mathrm{e}^{(3w)}\\
& + 3w^2\sinh(w)\mathrm{e}^{w} - 4w^3\cosh(w)\mathrm{e}^{(2w)} + 4w\cosh(w)\mathrm{e}^{(4w)} - 8w\cosh(w)\mathrm{e}^{(2w)}\\
& + w\cosh(w)\sqrt{T_1} - 9w\sinh(w)\mathrm{e}^{(3w)} + 12w^3\sinh(w)\mathrm{e}^{(2w)} + 9\sinh(w)w\mathrm{e}^{w}\\
& + 2w\sqrt{T_1} + 3\sinh(w)\sqrt{T_1}\,\big)\big),
\end{aligned}
$$

$$
\begin{aligned}
T_1 :=\ & 10w\mathrm{e}^{w} + 4 - 2w^2\mathrm{e}^{w} - 2w^3\mathrm{e}^{(6w)} - 30w\mathrm{e}^{(3w)} + w^4\mathrm{e}^{(2w)} + 24\mathrm{e}^{(4w)} + 8w^4\mathrm{e}^{(5w)}\\
& - 16\mathrm{e}^{(2w)} + w^4\mathrm{e}^{(6w)} + 18w^4\mathrm{e}^{(4w)} + 8w^3\mathrm{e}^{(3w)} + 2w^3\mathrm{e}^{(2w)} + 8\mathrm{e}^{(3w)}w^4 + 4\mathrm{e}^{(8w)}\\
& - 8w^3\mathrm{e}^{(5w)} - 16\mathrm{e}^{(6w)} - 2w^2\mathrm{e}^{(7w)} + 2w^2\mathrm{e}^{(5w)} + 2w^2\mathrm{e}^{(3w)} + 5w^2\mathrm{e}^{(6w)}\\
& - 10w^2\mathrm{e}^{(4w)} + 5w^2\mathrm{e}^{(2w)} + 30w\mathrm{e}^{(5w)} - 10w\mathrm{e}^{(7w)},
\end{aligned}
$$

$$
\begin{aligned}
b =\ & -\frac{1}{2}\big(-3\sinh(w)\cosh(w) - \cosh(w)^2w + 3\sinh(w) + w\cosh(w) + 2w\sinh(w)^2\big)\\
& \times\left(w\cosh(w) + \frac{w^2\cosh(w)T_2}{T_3} + 2\frac{w^2T_2}{T_3} + 2w + 3\frac{w\sinh(w)T_2}{T_3} + \sinh(w)\right)\\
& \Bigg/\Bigg(w\Bigg(2w\sinh(w)^2 - \cosh(w)^2w + 2\frac{w^2\sinh(w)^2T_2}{T_3} + \frac{w^2\cosh(w)T_2}{T_3}\\
& - \frac{w^2\cosh(w)^2T_2}{T_3} + 3\frac{w\cosh(w)T_2\sinh(w)}{T_3} - 3\frac{w\sinh(w)T_2}{T_3} - \sinh(w)\\
& + w\cosh(w) + \sinh(w)\cosh(w)\Bigg)\Bigg(-8\cosh(w)^2 - 12\frac{\cosh(w)^2T_2w}{T_3}
\end{aligned}
$$

$$+ 2w^2\cosh(w) + 12\frac{T_2 w\cosh(w)}{T_3} + \frac{3}{2}\frac{w^3T_2\cosh(w)}{T_3} + 8\cosh(w) - 2w\sinh(w) + 4w^2 + \frac{3}{2}\frac{w^2T_2\sinh(w)}{T_3} + 3\frac{w^3T_2}{T_3}\bigg)\bigg),$$

$$T_2 := 8(e^w)^4 - 8w^2(e^w)^3 + 8w(e^w)^3 - 32w^2(e^w)^2 - 16(e^w)^2 - 8w^2e^w - 8we^w + 8 - 4\big(10we^w - 30w(e^w)^3 - 2w^3(e^w)^6 - 8w^3(e^w)^5 + w^4(e^w)^2 + w^4(e^w)^6 + 18w^4(e^w)^4 + 8w^4(e^w)^5 + 4(e^w)^8 + 4 + 8(e^w)^3w^4 + 2w^3(e^w)^2 + 8w^3(e^w)^3 - 2w^2(e^w)^7 + 2w^2(e^w)^5 + 2w^2(e^w)^3 + 5w^2(e^w)^6 - 10w^2(e^w)^4 - 2w^2e^w + 5w^2(e^w)^2 + 24(e^w)^4 - 16(e^w)^6 - 16(e^w)^2 + 30w(e^w)^5 - 10w(e^w)^7\big)^{1/2},$$

$$T_3 := 12w^3(e^w)^3 + 12w^3e^w + 48w^3(e^w)^2 + 12w^2(e^w)^3 - 12w^2e^w - 24w(e^w)^4 + 48w(e^w)^2 - 24w. \qquad (42)$$

The Taylor series expansions of these coefficients are given by

$$b_0 = \frac{1}{12} - \frac{463}{806400}w^4 + \frac{48641}{580608000}w^6 - \frac{39041609}{4768727040000}w^8 + \frac{26589631841}{446352850944000000}w^{10} - \frac{4035312085333}{14997455791718400000}w^{12} - \frac{43370585700139}{6798846625579008000000}w^{14} + \cdots,$$

$$b_1 = \frac{5}{6} + \frac{463}{403200}w^4 + \frac{6919}{290304000}w^6 - \frac{19466071}{2384363520000}w^8 + \frac{23296561399}{223176425472000000}w^{10} - \frac{7070580531227}{7498727895859200000}w^{12} + \frac{2799639972287}{441483547115520000000}w^{14} + \cdots,$$

$$b = \frac{1}{200} - \frac{463}{672000}w^2 + \frac{5431}{89600000}w^4 - \frac{12716387}{2838528000000}w^6 + \frac{270621097441}{929901772800000000}w^8 - \frac{338138001379}{23144221900800000000}w^{10} + \frac{3647766243428891}{212463957049344000000000000}w^{12} + \frac{5103176966188546746119}{596802756793325322240000000000000}w^{14} + \cdots. \qquad (43)$$

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

Table 1
Properties of some two-step exponentially-fitted methods.

Method	Algebraic order	Interval of periodicity	Integrated exponential functions
Numerov's method	4	(0,6)	$1, x, x^2, x^3, x^4, x^5$
Derived by Raptis and Allison [27]	4	$(0, \infty) - S$	$m = 0,\ p = 3$
Derived by Ixaru and Rizea [14]	4	$(0, \infty) - S$	$m = 1,\ p = 1$
Derived by Raptis [24]	4	$(0, \infty) - S$	$m = 2,\ p = 0$
Derived by Raptis and Cash [28]*	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 [32]*	6	$(0, \infty) - S$	$m = 2,\ p = 0$
Method of TMS – case I**	4	$(0, \infty) - S$	$m = 0,\ p = 7$
Method of TMS – case II**	4	$(0, \infty) - S$	$m = 1,\ p = 5$
Method of TMS – case III**	4	$(0, \infty) - S$	$m = 2,\ p = 3$
New method – case I	4	$(0, \infty)$	$m = 0,\ p = 5$
New method – case II	4	$(0, \infty)$	$m = 1,\ p = 3$
New method – case III	4	$(0, \infty)$	$m = 2,\ p = 1$

$S = \{H^2\colon\ H = sq\pi,\ q = 1, 2, \ldots\}$. The quantities m and p are defined by (3).
* Hybrid two-step method. ** TMS = Thomas, Mitsou and Simos [36].

The new methods are of algebraic order four and are P-stable while the interval of periodicity of the other well-known exponentially-fitted methods listed in table 1 is $(0, \infty) - S$, where S is a set of distinct points. The hybrid methods listed in table 1 have algebraic order six. However, the new methods are P-stable. For the above reason, the methods perform better with large step lengths.

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 Schrödinger equation (1).

6.1. Resonance problem

In the asymptotic region, equation (1) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{44}$$

for x greater than some value X.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the *spherical Bessel* and *Neumann functions*, respectively. Thus the solution of equation (1) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D\left[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)\right], \end{aligned} \tag{45}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)}, \tag{46}$$

for x_1 and x_2 distinct points in the asymptotic region (for which we have that x_1 is the right-hand and 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. [9,10]. 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:

$$V(r) = V_w(r) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)]^2} \tag{47}$$

with $z = \exp[(r - R_0)/a],\ u_0 = -50,\ a = 0.6$ and $R_0 = 7.0$.

The problem considered here consists of either finding the *phase shift* $\delta(E) = \delta_l$ or finding those E, for $E \in [1, 1000]$, at which δ is equal to $\pi/2$. 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 $\pi/2$.

For positive energies one has the so-called resonance problem. This problem consists of either finding the *phase shift* $\delta(E) = \delta_l$ or finding those E, for $E \in [1, 1000]$, at which δ is equal to $\pi/2$. We actually solve the latter problem, using the technique fully described in [1], known as the "*resonance problem*" when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are

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

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 [27] (which is indicated as method [b]) and Ixaru and Rizea [14] (which is indicated as method [c]), the method of Chawla et al. [4] (which is indicated as method [d]), the method of Chawla et al. [5] (which is indicated as method [e]), the method of Thomas, Mitsou and Simos (case III) [36] (which is indicated as method [f]), the new exponentially-fitted method (case I) (which is indicated as method [g]), the new exponentially-fitted method (case II) (which is indicated as method [h]) and the new exponentially-fitted method (case III) (which is indicated as method [i]).

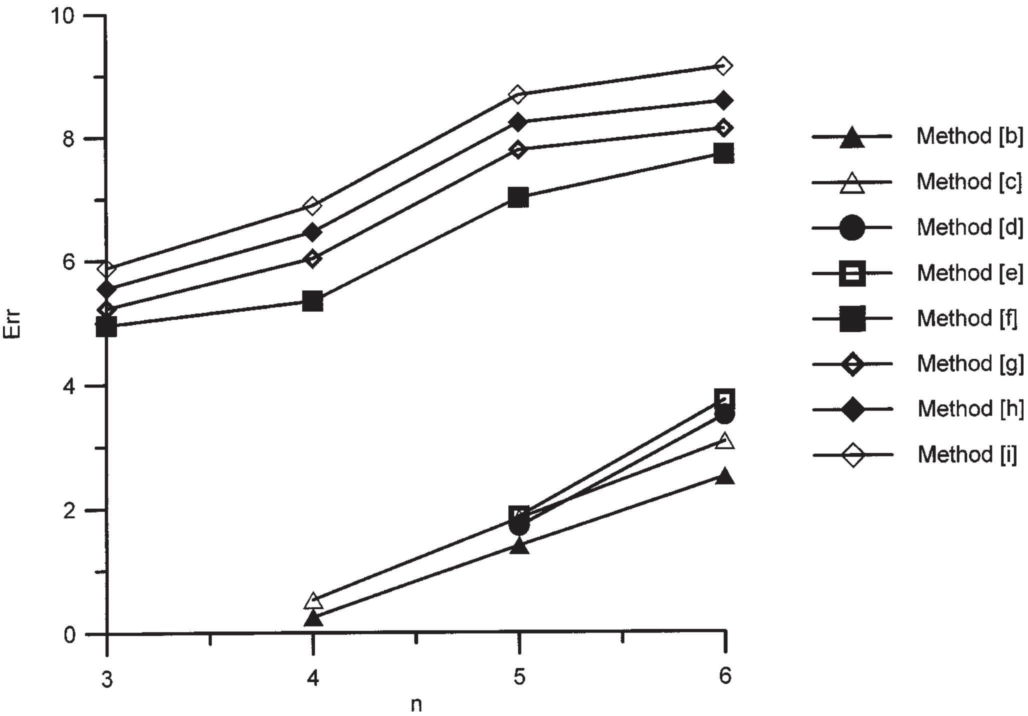

Figure 1. Values of Err for several values of n for the resonance $E = 989.7019159$. The nonexistance of a value for a method indicates that Err is negative.

The numerical results obtained for the four methods, 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.

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 [14]. That is, we choose

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5], \\ (-E)^{1/2} & \text{for } x \in [6.5, 15]. \end{cases} \tag{48}$$

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 [14, p. 25].

6.1.2. 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

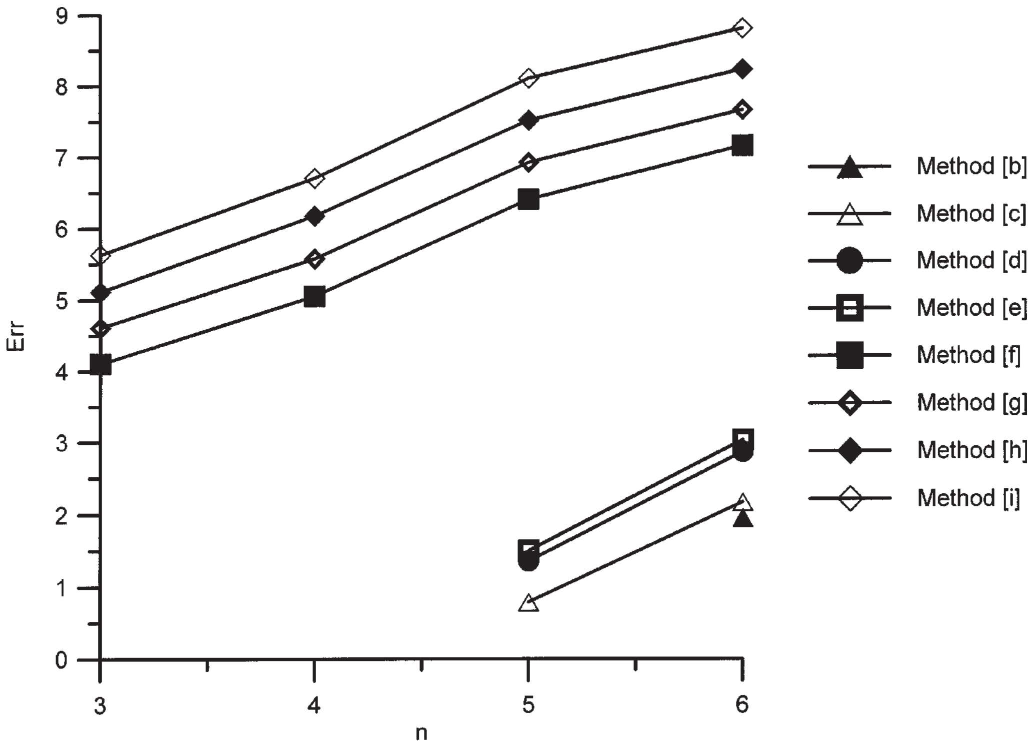

Figure 2. Values of Err for several values of n for the resonance $E = 1002.768393$. The nonexistance of a value for a method indicates that Err is negative.

potential in (1) using the methods mentioned above are shown. This potential is

$$V(x) = V_W(x) + \frac{D}{x}, \tag{49}$$

where V_W is the Woods–Saxon potential (47). For the purpose of our numerical experiments, we use the same parameters as in [14], i.e., $D = 20$, $l = 2$.

Since $V(x)$ is singular at the origin, we use the special strategy of [14]. We start the integration from a point $\varepsilon > 0$ and the initial values $y(\varepsilon)$ and $y(\varepsilon + h)$ for the integration scheme are obtained using a perturbative method (see [13]). As in [14], 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 [14]. That is, we choose

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

where a_i, $i = 1(1)3$, are fully defined in [14].

In all cases the new exponentially-fitted P-stable methods developed in this paper are more accurate than the other similar well-known exponentially-fitted ones.

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 digits accuracy (IEEE standard).

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