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New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation

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A family of P-stable high algebraic order exponentially-fitted methods for the numerical solution of the Schrödinger equation is developed in this paper. Numerical illustration to the resonance problem of the radial Schrödinger equation indicates that the new proposed methods are generally more efficient than the previously developed exponentially-fitted methods of the same kind.

KEY WORDS: Schrödinger equation, exponential fitting, P-stability, finite difference, multistep methods, scattering problems

1. Introduction

The radial form of the Schrödinger equation has the form:

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

In many scientific areas such as theoretical physics and chemistry, quantum physics and chemistry, chemical physics and physical chemistry there is a demand for the numerical solution of (1) (see, for example, [1–4]. 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:

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

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

The numerical solution of the Schrödinger equation is an area of great activity (see [1,2,5–39,63] for the last decades. The scope of this activity is the development of a fast and reliable method that approximates the solution of the Schrödinger equation.

In the literature two kind of methods are used for the numerical solution of problems of the form (1). The first category consists of methods with constant coefficients while the second category consists of methods with coefficients dependent from the frequency of the problem. It is known that methods of the second category are much more accurate than methods of the first category. Exponential fitting is one of the most known procedures for the construction of methods of the second category. Well known exponentially-fitted methods are the methods developed by Raptis and Allison [18] and Ixaru and Rizea [2]. The approach of Ixaru and Rizea [2] is interesting since they have proved 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 mathematical reason for this was explained in [24]. We note here that the resonance problem is a stiff oscillatory problem. For the method obtained by Ixaru and Rizea [2] we have $m = 1$ and $p = 1$. Another low order method of this type (with $m = 2$ and $p = 0$) was developed by Raptis [15]. In [35,40] and [36] a complete review for the exponentially-fitted methods is given. Recently Coleman and Ixaru [41] have derived P-stable exponentially-fitted methods. Their paper is very interesting because they have introduced a procedure for the production of P-stable exponentially-fitted method. They also produce a very simple and low order P-stable exponentially-fitted method. But their procedure may lead to methods that require the knowledge of two frequencies for the same problem which for many real problems is impossible. Recently Simos [32] and Avdelas et al. [42] have developed families of P-stable *low* algebraic order methods. Recently, also, Vigo-Aguiar and Simos have developed an eighth order P-stable exponentially-fitted method.

The purpose of this paper is to derive *a family* of P-stable eight algebraic order methods fitted to (3) and in particular to derive methods with $m = 0$ and $p = 7$, $m = 1$ and $p = 5$ and $m = 2$ and $p = 3$. The obtained methods are applied to coupled system of differential equations of the Schrödinger type. The results show the efficiency of the new proposed methods.

2. Exponential multistep methods

For the numerical integration of the initial value problem

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

consider that 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 $[A, B]$ are used.

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

$$\left\{1, x, x^2, \ldots, x^{p+r-1}\right\} \tag{7}$$

(or

$$\left\{\exp(v_0 x), \exp(v_1 x), \ldots, \exp(v_{p+r-1} x)\right\}, \tag{8}$$

where v_i, $i = 0, 1, \ldots, p+r-1$, are real or complex numbers).

Remark 1 (See [20,43]). 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

$$\left\{\exp(vx), x\exp(vx), x^2\exp(vx), \ldots, x^n\exp(vx), \exp(v_{n+1}x), \ldots, \exp(v_{p+r-1}x)\right\}. \tag{9}$$

Remark 2 (See [20,43]). 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 [43,44]). 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, then we have

$$L\left[x^m \exp(vx)\right] = 0, \quad m = 0, 1, \ldots, n-1, \qquad L\left[x^n \exp(vx)\right] \neq 0 \tag{10}$$

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 [20,27]). Consider an operator L with

$$L\left[\exp(\pm v_j x)\right] = 0, \quad j = 0, 1, \ldots, k \leqslant \frac{p+r-1}{2} \tag{11}$$

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 study the case $r = 2$.

3. A procedure for the derivation of exponentially-fitted methods for general problems

In this section we will study the derivation of an exponentially-fitted multistep method (5) which exactly integrates the set of functions $\{\exp(\pm v_j x)\}_{j=0}^{k}$. The obtained method can be used for the numerical solution of the general problem (4).

Based on lemma 1 we obtain the equations

$$\rho\big[\exp(\pm v_j h)\big] - (\pm v_j h)^r \sigma\big[\exp(\pm v_j h)\big] = 0 \tag{12}$$

or, equivalently,

$$\sum_{i=0}^{k}\big[a_i \exp(\pm v_j h) - (\pm v_j h)^r b_i \exp(\pm v_j h)\big] = 0, \quad j = 0, 1, \ldots, n, \tag{13}$$

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:

$$a_i = (-1)^r a_{k-i}, \quad b_i = b_{k-i}, \qquad i = 0, 1, \ldots, k. \tag{14}$$

We now let $a_k = 1$, which is the case adopted for all families of known multistep methods. Then (13) and (14) give the following system of equations

$$2\sum_{i=1}^{k/2-1} a_i \sinh\left[\left(\frac{k}{2} - i\right)w_j\right] + a_{k/2} - w_j^r\left[2\sum_{i=0}^{k/2-1} b_i \cosh\left[\left(\frac{k}{2} - i\right)w_j\right] + b_{k/2}\right]$$
$$= -2\sinh\left(\frac{kw_j}{2}\right), \quad \text{for } r = 1, 3, 5, \ldots, \tag{15}$$

$$2\sum_{i=1}^{k/2-1} a_i \cosh\left[\left(\frac{k}{2} - i\right)w_j\right] + a_{k/2} - w_j^r\left[2\sum_{i=0}^{k/2-1} b_i \cosh\left[\left(\frac{k}{2} - i\right)w_j\right] + b_{k/2}\right]$$
$$= -2\cosh\left(\frac{kw_j}{2}\right), \quad \text{for } r = 2, 4, 6, \ldots, \tag{16}$$

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

We now prove that the system of equations (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 us consider that $X(w)$ and $Y(w)$ $(w = vh)$ be the matrices of the unknown coefficients in the systems of equations (15) and (16), respectively. We study now the 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 $\cosh Kw_j$, $\sinh Lw_j$ and powers of w_j. We note here that 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 over any set of $k+1$ distinct points. 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 (15) and (16) has a unique solution.

We study now the 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 (15) or (16) 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. We note here that in these cases L'Hospital's rule is applied as follows. We calculate the kth derivative of numerator and denominator (where $k = 0, 1, \ldots$) until we find a k for which we have S_1/S_2 where $S_1 \neq 0$ and $S_2 \neq 0$. With the above procedure we solve the problem of undetermined expressions of the form $0/0$.

4. The new family of eighth algebraic order P-stable methods

Consider the following family of implicit methods:

$$\bar{y}_{n\pm1/2} = \frac{1}{2}(y_n + y_{n\pm1}) - h^2\left(a y''_n + \left(\frac{1}{8} - a\right) y''_{n\pm1}\right) + O\left(h^3\right), \tag{17}$$

$$\tilde{y}_{n\pm1/2} = \frac{1}{2}(y_n + y_{n\pm1}) - \frac{h^2}{96}\left(y''_{n\pm1} + 10\bar{y}''_{n\pm1/2} + y_n\right) + O\left(h^5\right), \tag{18}$$

$$\check{y}_{n\pm1/2} = \frac{1}{2}(y_n + y_{n\pm1}) - \frac{h^2}{1920}\left(19y''_{n\pm1} + 204\tilde{y}''_{n\pm1/2} + 14y_n + 4\tilde{y}''_{n\mp1/2} - y''_{n\mp1}\right) + O\left(h^7\right), \tag{19}$$

$$\bar{y}_{n\pm1/5} = \frac{1}{5}(4y_n + y_{n\pm1}) - \frac{h^2}{468750}\left(1411y''_{n\pm1} + 26096\tilde{y}''_{n\pm1/2} + 11246y''_n - 1424\tilde{y}''_{n\mp1/2} + 171y''_{n\mp1}\right) + O\left(h^7\right), \tag{20}$$

$$y_{n+1} = 2y_n - y_{n-1} - h^2\left[q_0 y''_{n+1} + q_1 y''_n + q_0 y''_{n-1} + q_2\left(\check{y}''_{n+1/2} + \check{y}''_{n-1/2}\right) + q_3\left(\bar{y}''_{n+1/5} + \bar{y}''_{n-1/5}\right)\right], \tag{21}$$

where $y''_n = f(x_n, y_n)$, $\bar{y}''_{n\pm1/2} = f(x_{n\pm1/2}, \bar{y}''_{n\pm1/2})$, $\bar{y}''_{n\pm1/5} = f(x_{n\pm1/5}, \bar{y}''_{n\pm1/5})$, $\tilde{y}''_{n\pm1/2} = f(x_{n\pm1/2}, \tilde{y}''_{n\pm1/2})$, $\check{y}''_{n\pm1/2} = f(x_{n\pm1/2}, \check{y}''n \pm 1/2)$.

In order the above method to integrate exactly any linear combination of the functions:

Case I.

$$\left\{1, x, x^2, x^3, x^4, x^5, x^6, x^7, \exp(\pm vx)\right\}. \tag{22}$$

Case II.

$$\left\{1, x, x^2, x^3, x^4, x^5, \exp(\pm vx), x\exp(\pm vx)\right\}. \tag{23}$$

Case III.

$$\left\{1, x, x^2, x^3, \exp(\pm vx), x\exp(\pm vx), x^2\exp(\pm vx)\right\}. \tag{24}$$

We obtain the following systems of equations:

Case I.

$$\begin{aligned}
&2q_0 + q_1 + 2q_2 + 2q_3 = 1,\\
&300q_0 + 75q_2 + 12q_3 = 25,\\
&30000q_0 + 1875q_2 + 48q_3 = 1000,\\
&w^2\left[2q_0\cosh(w) + 2q_3\cosh\left(\frac{1}{5}w\right) + 2q_2\cosh\left(\frac{1}{2}w\right) + q_1\right] = 2\cosh(w) - 2,
\end{aligned} \tag{25}$$

where $w = vh$.

Case II.

$$\begin{aligned}
&2q_0 + q_1 + 2q_2 + 2q_3 = 1,\\
&300q_0 + 75q_2 + 12q_3 = 25,\\
&w^2\left[2q_0\cosh(w) + 2q_3\cosh\left(\frac{1}{5}w\right) + 2q_2\cosh\left(\frac{1}{2}w\right) + q_1\right] = 2\cosh(w) - 2,\\
&-2\sinh(w) = -\frac{1}{5}w\Big[20q_0\cosh(w) + 10q_0 w\sinh(w) + 10q_1\\
&\qquad +20q_2\cosh\left(\frac{1}{2}w\right) + 5q_2 w\sinh\left(\frac{1}{2}w\right)\\
&\qquad +20q_3\cosh\left(\frac{1}{5}w\right) + 2q_3 w\sinh\left(\frac{1}{5}w\right)\Big],
\end{aligned} \tag{26}$$

where $w = vh$.

Case III.

$$\begin{aligned}
&2q_0 + q_1 + 2q_2 + 2q_3 = 1,\\
&w^2\left[2q_0\cosh(w) + 2q_3\cosh\left(\frac{1}{5}w\right) + 2q_2\cosh\left(\frac{1}{2}w\right) + q_1\right] = 2\cosh(w) - 2,\\
&-2\sinh(w) = -\frac{1}{5}w\Big[20q_0\cosh(w) + 10q_0 w\sinh(w) + 10q_1\\
&\qquad +20q_2\cosh\left(\frac{1}{2}w\right) + 5q_2 w\sinh\left(\frac{1}{2}w\right)\\
&\qquad +20q_3\cosh\left(\frac{1}{5}w\right) + 2q_3 w\sinh\left(\frac{1}{5}w\right)\Big],
\end{aligned} \tag{27}$$

$$2\cos(w) = -2q_0 w^2\cos(w) - \frac{2}{25}q_3 w^2\cos\left(\frac{1}{5}w\right) + 4q_0\cos(w) + 4q_2\cos\left(\frac{1}{2}w\right) - \frac{1}{2}q_2 w^2\cos\left(\frac{1}{2}w\right) + 2q_1 + 4q_3\cos\left(\frac{1}{5}w\right) - 4q_2 w\sin\left(\frac{1}{2}w\right) - \frac{8}{5}q_3 w\sin\left(\frac{1}{5}w\right) - 8q_0 w\sin(w),$$

where $w = vh$.

Solving the above systems of equations for q_i, $i = 0(1)3$, we obtain the values of parameters presented in appendix A.

In order to avoid cancellations for small values of w, the Taylor series expansions presented in appendix B can be used.

It is easy for one to see that when $w = \mathrm{i}\phi$, where $\mathrm{i} = \sqrt{-1}$, then the methods developed above integrate exactly any linear combination of the functions:

Case I.

$$\{1, x, x^2, x^3, x^4, x^5, x^6, x^7, \cos(\phi x), \sin(\phi x)\}. \tag{28}$$

Case II.

$$\{1, x, x^2, x^3, x^4, x^5, \cos(\phi x), \sin(\phi x), x\cos(\phi x), x\sin(\phi x)\}. \tag{29}$$

Case III.

$$\{1, x, x^2, x^3, \cos(\phi x), \sin(\phi x), x\cos(\phi x), x\sin(\phi x), x^2\cos(\phi x), x^2\sin(\phi x)\}. \tag{30}$$

5. Stability analysis

In this section we investigate the numerical solution of the problem [60–63]:

$$y'' = f(x, y), \qquad y(x_0) = y_0,\ y'(x_0) = y'_0. \tag{31}$$

Lambert and Watson [46] introduce the scalar test equation

$$y'' = -q^2 y \tag{32}$$

in order to examine the stability properties of the methods for solving the initial-value problem (31). They have also defined the *interval of periodicity*. When we apply a symmetric two-step method to the scalar test equation (32) we obtain a difference equation of the form

$$y_{n+1} - 2Q(H)y_n + y_{n-1} = 0, \tag{33}$$

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

The characteristic equation associated with (33) is

$$z^2 - 2Q(H)z + 1 = 0. \tag{34}$$

We have the following definitions.

Definition 2 [45]. The method (33) with the characteristic equation (34) is unconditionally stable if $|z_1| \leqslant 1$ and $|z_2| \leqslant 1$ for all values of wh.

Definition 3. Following Lambert and Watson [46] we say that the numerical method (33) has an interval of periodicity $(0, H_0^2)$, if, for all $H^2 \in (0, H_0^2)$, z_1 and z_2 satisfy:

$$z_1 = \mathrm{e}^{\mathrm{i}\theta(H)} \quad \text{and} \quad z_2 = \mathrm{e}^{-\mathrm{i}\theta(H)}, \tag{35}$$

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

Definition 4 [46,60]. The method (33) is P-*stable* if its *interval of periodicity* is $(0, \infty)$.

Based on the above we have the following theorems (for the proofs see [26]).

Theorem 1. A method which has the characteristic equation (34), has an interval of periodicity $(0, H_0^2)$, if for all $H^2 \in (0, H_0^2)$, $|Q(H)| < 1$. For implicit methods the above relation is equivalent to $A(H) \pm B(H) > 0$.

Our proposed family of methods have a free parameter a which will be used in order to obtain P-stable methods. If we apply the new methods (with coefficients obtained for the trigonometrically-fitted method) to the scalar test equation (32) we get a difference equation of the form (33) and a characteristic equation (34) with $A(H)$ and $B(H)$ given as follows:

$$\begin{aligned} A(H) = {} & 1 - \frac{13}{1152}H^8 q_2 a - \frac{257}{46875}H^8 q_3 a + \frac{1}{2}q_2 H^2 + \frac{61}{960}q_2 H^4 + \frac{13}{1920}q_2 H^6 \\ & + \frac{1}{5}q_3 H^2 + \frac{6959}{234375}q_3 H^4 + \frac{257}{78125}q_3 H^6 + H^2 q_0 + \frac{13}{9216}H^8 q_2 \\ & + \frac{257}{375000}H^8 q_3, \\ B(H) = {} & -\frac{13}{1152}H^8 q_2 a - \frac{257}{46875}H^8 q_3 a + 1 - \frac{1}{2}q_2 H^2 - \frac{59}{960}q_2 H^4 - \frac{4}{5}q_3 H^2 \\ & - \frac{11791}{234375}q_3 H^4 - \frac{1}{2}H^2 q_1 - \frac{13}{1920}q_2 H^6 - \frac{257}{78125}q_3 H^6, \end{aligned} \tag{36}$$

where $H = qh$.

So, we have

$$\begin{aligned} A(H) + B(H) = {} & 2 - \frac{13}{576}H^8 q_2 a - \frac{514}{46875}H^8 q_3 a + \frac{1}{480}q_2 H^4 - \frac{3}{5}q_3 H^2 \\ & - \frac{4832}{234375}q_3 H^4 + H^2 q_0 + \frac{13}{9216}H^8 q_2 + \frac{257}{375000}H^8 q_3 \\ & - \frac{1}{2}H^2 q_1, \end{aligned} \tag{37}$$

$$A(H) - B(H) = q_2 H^2 + \frac{1}{8} q_2 H^4 + \frac{13}{960} q_2 H^6 + q_3 H^2 + \frac{2}{25} q_3 H^4 + \frac{514}{78125} q_3 H^6 + H^2 q_0 + \frac{13}{9216} H^8 q_2 + \frac{257}{375000} H^8 q_3 + \frac{1}{2} H^2 q_1. \tag{38}$$

Substituting the coefficients of the method obtained above to the stability polynomials (37) and (38) we observe that the polynomial $A(H) - B(H) \geqslant 0$ for all $H \in (0, \infty)$. About polynomial $A(H) + B(H)$ we observe that if we require that the coefficient of H^8 to be greater or equal to [1000 − the coefficient of H^6 − the coefficient of H^4 − the coefficient of H^2], then $A(H) + B(H) \geqslant 0$ for all $H \in (0, \infty)$. Based on the above remark we find the following value of a:

Case I.

$$\begin{aligned} a = -\frac{1}{80}\Bigg(& -12101950502400 w^2 \cos\left(\frac{1}{10}w\right)^4 + 6913820812800 w^2 \cos\left(\frac{1}{10}w\right)^2 \\ & + 493440 w^2 \cos\left(\frac{1}{2}w\right) - 2764643819520 w^2 \cos\left(\frac{1}{10}w\right) \\ & + 15490496643072 w^2 \cos\left(\frac{1}{10}w\right)^{10} - 38726241607680 w^2 \cos\left(\frac{1}{10}w\right)^8 \\ & + 33885461406720 w^2 \cos\left(\frac{1}{10}w\right)^6 + 6465 w^2 \cos(w) - 1015625 w^2 \cos\left(\frac{1}{5}w\right) \\ & + 26535168000 \cos\left(\frac{1}{10}w\right)^2 + 594387763200 \cos\left(\frac{1}{10}w\right)^6 \\ & - 212281344000 \cos\left(\frac{1}{10}w\right)^4 + 271720120320 \cos\left(\frac{1}{10}w\right)^{10} \\ & - 679300300800 \cos\left(\frac{1}{10}w\right)^8 - 8846860222464 w^2 \cos\left(\frac{1}{10}w\right)^5 \\ & + 11058575278080 w^2 \cos\left(\frac{1}{10}w\right)^3 - 1062477120 - 4908391586008 w^2 \\ & + 1070400 \cos(w)\Bigg) \\ & \Bigg/ \Bigg(214080 - 98688 w^2 \cos\left(\frac{1}{2}w\right) - 210184 w^2 - 214080 \cos(w) \\ & - 1293 w^2 \cos(w) + 203125 w^2 \cos\left(\frac{1}{5}w\right)\Bigg)\Bigg). \end{aligned} \tag{39}$$

Case II.

$$a = \frac{1}{80}\Bigg(948282216 \sin\left(\frac{17}{10}w\right) - 913480716 \sin\left(\frac{2}{5}w\right) - 6764101620 \sin\left(\frac{3}{5}w\right)$$

$$
\begin{aligned}
&- 2053053864\sin\left(\frac{4}{5}w\right) + 2148816648w\cos(w) + 2575076364w\cos\left(\frac{4}{5}w\right)\\
&+ 1722556932w\cos\left(\frac{3}{5}w\right) + 1296297216w\cos\left(\frac{6}{5}w\right)\\
&- 5167670796w\cos\left(\frac{1}{5}w\right) - 3018854148w\cos\left(\frac{2}{5}w\right)\\
&+ 648148608w\cos\left(\frac{13}{10}w\right) - 2796965256w\cos\left(\frac{3}{10}w\right)\\
&+ 648148608w\cos\left(\frac{1}{2}w\right) + 3445113864w\cos\left(\frac{7}{10}w\right)\\
&+ 2353187472w\cos\left(\frac{9}{10}w\right) + 2592594432w\cos\left(\frac{11}{10}w\right)\\
&- 3649484688w\cos\left(\frac{1}{10}w\right) + 478813920\sin\left(\frac{1}{10}w\right)\\
&+ 1816849492924w^3\cos\left(\frac{1}{10}w\right) + 173618833930w^3\cos\left(\frac{7}{10}w\right)\\
&- 1381384364292w^3\cos\left(\frac{1}{2}w\right) - 1121610782398w^3\cos\left(\frac{3}{10}w\right)\\
&- 8438777160\sin\left(\frac{3}{10}w\right) - 9830837160\sin\left(\frac{1}{2}w\right)\\
&+ 950912898956w^3\cos\left(\frac{9}{10}w\right) - 345499150464w^3\cos\left(\frac{11}{10}w\right)\\
&- 172749575232w^3\cos\left(\frac{6}{5}w\right) + 345894268054w^3\cos(w)\\
&+ 605453260251w^3\cos\left(\frac{4}{5}w\right) + 87520628627w^3\cos\left(\frac{3}{5}w\right)\\
&- 2504553136193w^3\cos\left(\frac{2}{5}w\right) + 607067792415w^3\cos\left(\frac{1}{5}w\right)\\
&- 86374787616w^3\cos\left(\frac{13}{10}w\right) - 2796965256w + 2401068864\sin\left(\frac{6}{5}w\right)\\
&+ 1038148965038w^3 + 648148608\sin(w) - 3979981620\sin\left(\frac{1}{5}w\right)\\
&+ 1896564432\sin\left(\frac{8}{5}w\right) + 4267269972\sin\left(\frac{7}{5}w\right) + 2844846648\sin\left(\frac{3}{2}w\right)\\
&+ 3097098864\sin\left(\frac{13}{10}w\right) - 887555568\sin\left(\frac{11}{10}w\right) - 408741648\sin\left(\frac{9}{10}w\right)
\end{aligned}
$$

$$- 6289960512 \sin\left(\frac{7}{10}w\right) + 474141108 \sin\left(\frac{9}{5}w\right)\bigg)$$
$$\bigg/ \bigg(397128 \sin\left(\frac{17}{10}w\right) - 3776280 \sin\left(\frac{2}{5}w\right) - 2783460 \sin\left(\frac{3}{5}w\right)$$
$$- 613512 \sin\left(\frac{4}{5}w\right) + 801384w \cos(w) + 906012w \cos\left(\frac{4}{5}w\right)$$
$$+ 696756w \cos\left(\frac{3}{5}w\right) + 592128w \cos\left(\frac{6}{5}w\right) - 2090268w \cos\left(\frac{1}{5}w\right)$$
$$- 1288884w \cos\left(\frac{2}{5}w\right) + 296064w \cos\left(\frac{13}{10}w\right) - 1097448w \cos\left(\frac{3}{10}w\right)$$
$$+ 296064w \cos\left(\frac{1}{2}w\right) + 1393512w \cos\left(\frac{7}{10}w\right) + 714576w \cos\left(\frac{9}{10}w\right)$$
$$+ 1184256w \cos\left(\frac{11}{10}w\right) - 1306704w \cos\left(\frac{1}{10}w\right) + 939360 \sin\left(\frac{1}{10}w\right)$$
$$+ 692492w^3 \cos\left(\frac{1}{10}w\right) + 314690w^3 \cos\left(\frac{7}{10}w\right) + 620364w^3 \cos\left(\frac{1}{2}w\right)$$
$$+ 803866w^3 \cos\left(\frac{3}{10}w\right) - 3386280 \sin\left(\frac{3}{10}w\right) - 4166280rm \sin\left(\frac{1}{2}w\right)$$
$$+ 59548w^3 \cos\left(\frac{9}{10}w\right) + 98688w^3 \cos\left(\frac{11}{10}w\right) + 49344w^3 \cos\left(\frac{6}{5}w\right)$$
$$+ 66782w^3 \cos(w) + 174783w^3 \cos\left(\frac{4}{5}w\right) + 455191w^3 \cos\left(\frac{3}{5}w\right)$$
$$+ 786131w^3 \cos\left(\frac{2}{5}w\right) + 822195w^3 \cos\left(\frac{1}{5}w\right) + 24672w^3 \cos\left(\frac{13}{10}w\right)$$
$$- 1097448w + 808512 \sin\left(\frac{6}{5}w\right) + 383254w^3 + 296064 \sin(w)$$
$$- 1223460 \sin\left(\frac{1}{5}w\right) + 794256 \sin\left(\frac{8}{5}w\right) + 1787076 \sin\left(\frac{7}{5}w\right)$$
$$+ 1191384 \sin\left(\frac{3}{2}w\right) + 1198512 \sin\left(\frac{13}{10}w\right) - 765744 \sin\left(\frac{11}{10}w\right)$$
$$+ 173616 \sin\left(\frac{9}{10}w\right) - 2584896 \sin\left(\frac{7}{10}w\right) + 198564 \sin\left(\frac{9}{5}w\right)\bigg). \tag{40}$$

Case III.

$$a = -\bigg(-3013411080 \sin(w) + 43172993808w^4 \sin\left(\frac{1}{10}w\right)$$
$$- 345600000w^2 \sin\left(\frac{3}{5}w\right) + 2700945720w - 230400000w^2 \sin\left(\frac{2}{5}w\right)$$

$$
\begin{aligned}
&+ 129518981424w^4 \sin\left(\frac{3}{10}w\right) + 1966268736\sin\left(\frac{13}{10}w\right)\\
&+ 3348371520\sin\left(\frac{3}{2}w\right) + 359987369040w^4 \sin\left(\frac{1}{2}w\right)\\
&+ 5250063168\sin\left(\frac{9}{10}w\right) + 50288375232w^4 \sin\left(\frac{7}{10}w\right)\\
&+ 64729781424w^4 \sin\left(\frac{9}{10}w\right) + 2052371520\sin\left(\frac{1}{10}w\right)\\
&+ 79171187616w^4 \sin\left(\frac{11}{10}w\right) - 43221600000w^4 \sin\left(\frac{3}{2}w\right)\\
&+ 93612593808w^4 \sin\left(\frac{13}{10}w\right) + 3608165952\sin\left(\frac{11}{10}w\right)\\
&+ 2917857600\sin\left(\frac{1}{2}w\right) + 6891960384\sin\left(\frac{7}{10}w\right) + 6157114560\sin\left(\frac{3}{10}w\right)\\
&- 68412384w\cos\left(\frac{23}{10}w\right) - 136824768w\cos\left(\frac{21}{10}w\right) - 205237152w\cos\left(\frac{19}{10}w\right)\\
&- 273649536w\cos\left(\frac{17}{10}w\right) - 5671151712w\cos\left(\frac{7}{10}w\right)\\
&- 5577824160w\cos\left(\frac{1}{2}w\right) - 6139424160w\cos\left(\frac{3}{10}w\right)\\
&- 810334368w\cos\left(\frac{13}{10}w\right) - 2430606816w\cos\left(\frac{11}{10}w\right)\\
&- 4050879264w\cos\left(\frac{9}{10}w\right) + 410474304\sin\left(\frac{23}{10}w\right) + 632188144w\cos\left(\frac{8}{5}w\right)\\
&+ 1237288466w\cos\left(\frac{7}{5}w\right) + 1842388788w\cos\left(\frac{6}{5}w\right) + 3318130360w\cos(w)\\
&+ 2998407576w\cos\left(\frac{4}{5}w\right) + 8095087974w\cos\left(\frac{1}{5}w\right)\\
&+ 6396194508w\cos\left(\frac{2}{5}w\right) + 4697301042w\cos\left(\frac{3}{5}w\right)\\
&- 6139424160w\cos\left(\frac{1}{10}w\right) - 903661920w\cos\left(\frac{3}{2}w\right) + 27087822w\cos\left(\frac{9}{5}w\right)\\
&+ 462410000w\cos(2w) + 820948608\sin\left(\frac{21}{10}w\right) + 1231422912\sin\left(\frac{19}{10}w\right)\\
&- 230400000w^2\sin(w) - 460800000w^2\sin\left(\frac{4}{5}w\right) - 115200000w^2\sin\left(\frac{1}{5}w\right)
\end{aligned}
$$

$$+ 259200000w^2 \sin\left(\frac{3}{10}w\right) + 720000000w^2 \sin\left(\frac{1}{2}w\right)$$
$$+ 100800000w^2 \sin\left(\frac{7}{10}w\right) + 129600000w^2 \sin\left(\frac{9}{10}w\right)$$
$$+ 158400000w^2 \sin\left(\frac{11}{10}w\right) + 1641897216 \sin\left(\frac{17}{10}w\right)$$
$$+ 86400000w^2 \sin\left(\frac{1}{10}w\right) - 86400000w^2 \sin\left(\frac{3}{2}w\right) + 187200000w^2 \sin\left(\frac{13}{10}w\right)$$
$$- 4058672898 \sin\left(\frac{7}{5}w\right) - 2416775682 \sin\left(\frac{8}{5}w\right) - 774878466 \sin\left(\frac{9}{5}w\right)$$
$$- 1734037500 \sin(2w) - 5700570114 \sin\left(\frac{6}{5}w\right) - 5712645114 \sin\left(\frac{4}{5}w\right)$$
$$- 230399597500w^4 \sin\left(\frac{4}{5}w\right) - 115199798750w^4 \sin(w)$$
$$- 172799698125w^4 \sin\left(\frac{3}{5}w\right) - 4070747898 \sin\left(\frac{3}{5}w\right) - 2428850682 \sin\left(\frac{2}{5}w\right)$$
$$- 115199798750w^4 \sin\left(\frac{2}{5}w\right) - 57599899375w^4 \sin\left(\frac{1}{5}w\right)$$
$$- 786953466 \sin\left(\frac{1}{5}w\right)\Bigg)\Bigg)$$
$$\Bigg/\Bigg(158851200 \sin(w) + 986880w^4 \sin\left(\frac{1}{10}w\right) - 111100800w$$
$$+ 2960640w^4 \sin\left(\frac{3}{10}w\right) - 106583040 \sin\left(\frac{13}{10}w\right) - 59212800 \sin\left(\frac{3}{2}w\right)$$
$$+ 4934400w^4 \sin\left(\frac{1}{2}w\right) - 201323520 \sin\left(\frac{9}{10}w\right) + 3947520w^4 \sin\left(\frac{7}{10}w\right)$$
$$+ 2960640w^4 \sin\left(\frac{9}{10}w\right) - 59212800 \sin\left(\frac{1}{10}w\right) + 1973760w^4 \sin\left(\frac{11}{10}w\right)$$
$$+ 986880w^4 \sin\left(\frac{13}{10}w\right) - 153953280 \sin\left(\frac{11}{10} - 296064000 \sin\left(\frac{1}{2}w\right)\right.$$
$$- 248693760 \sin\left(\frac{7}{10}w\right) - 177638400 \sin\left(\frac{3}{10}w\right) + 1973760w \cos\left(\frac{23}{10}w\right)$$
$$+ 3947520w \cos\left(\frac{21}{10}w\right) + 5921280w \cos\left(\frac{19}{10}w\right) + 7895040w \cos\left(\frac{17}{10}w\right)$$
$$+ 183559680w \cos\left(\frac{7}{10}w\right) + 226982400w \cos\left(\frac{1}{2}w\right) + 226982400w \cos\left(\frac{3}{10}w\right)$$

$$
\begin{aligned}
&+ 53291520w\cos\left(\frac{13}{10}w\right) + 96714240w\cos\left(\frac{11}{10}w\right) + 140136960w\cos\left(\frac{9}{10}w\right)\\
&- 11842560\sin\left(\frac{23}{10}w\right) - 21180160w\cos\left(\frac{8}{5}w\right) - 38270240w\cos\left(\frac{7}{5}w\right)\\
&- 55360320w\cos\left(\frac{6}{5}w\right) - 115350400w\cos(w) - 141920640w\cos\left(\frac{4}{5}w\right)\\
&- 272331360w\cos\left(\frac{1}{5}w\right) - 228861120w\cos\left(\frac{2}{5}w\right) - 185390880w\cos\left(\frac{3}{5}w\right)\\
&+ 226982400w\cos\left(\frac{1}{10}w\right) + 9868800w\cos\left(\frac{3}{2}w\right) - 4090080w\cos\left(\frac{9}{5}w\right)\\
&- 10400000w\cos(2w) - 23685120\sin\left(\frac{21}{10}w\right) - 35527680\sin\left(\frac{19}{10}w\right)\\
&- 47370240\sin\left(\frac{17}{10}w\right) + 122610720\sin\left(\frac{7}{5}w\right) + 75240480\sin\left(\frac{8}{5}w\right)\\
&+ 27870240\sin\left(\frac{9}{5}w\right) + 39000000\sin(2w) + 169980960\sin\left(\frac{6}{5}w\right)\\
&+ 247980960\sin\left(\frac{4}{5}w\right) - 2600000w^4\sin\left(\frac{4}{5}w\right) - 1300000w^4\sin(w)\\
&- 1950000w^4\sin\left(\frac{3}{5}w\right) + 200610720\sin\left(\frac{3}{5}w\right) + 153240480\sin\left(\frac{2}{5}w\right)\\
&- 1300000w^4\sin\left(\frac{2}{5}w\right) - 650000w^4\sin\left(\frac{1}{5}w\right) + 105870240\sin\left(\frac{1}{5}w\right)\Bigg)\Bigg). \qquad (41)
\end{aligned}
$$

The appropriate Taylor series expansion for the above coefficient is given by:

Case I.

$$
\begin{aligned}
a = &-\frac{76225509269}{280240} + \frac{1406566565019}{490840360}w^2 - \frac{173767548977000433}{6877655124320000}w^4\\
&+ \frac{438472275070694441156979}{250561229365126784000000}w^6 - \frac{4961149998575631870628004770 7}{386195034045057214714880000000000}w^8\\
&+ \frac{10180353531546773208275242635718 13}{1082272963407868338516979712000000000 00}w^{10}\\
&- \frac{76192626305970613919305147840934029960 85609}{111247520606480104199508281107282329600000000000000 00}w^{12} + \cdots. \qquad (42)
\end{aligned}
$$

Case II.

$$
a = -\frac{76225509269}{280240} + \frac{1406566565019}{245420180}w^2 - \frac{149580232987644463}{859706890540000}w^4
$$

$$+\frac{335094963121440778537459}{689043380754098656000000}w^6-\frac{301911963486115791994773531 8957}{21723470665034468327712000000000}w^8$$
$$+\frac{277265642691023575522870045474489 36241}{70313921591404946118025025664000000000000}w^{10}$$
$$-\frac{34796499388155120010954469288341551359837122097}{3102762879415109156189410652757796224000000000000000}w^{12}+\cdots. \quad (43)$$

Case III.

$$a=-\frac{76225509269}{280240}+\frac{4219699695057}{490840360}w^2-\frac{3068622944772465813}{6877655124320000}w^4$$
$$+\frac{586608454656437737360904 11}{275617352301639462400000 0}w^6$$
$$-\frac{11843448132759818944657086141 8741}{11585851021351716441446400000000 0}w^8$$
$$+\frac{36801017731373224088936073628273152 63347}{75001516364165275859226694041600000000000 0}w^{10}$$
$$-\frac{31187449739543321712252330460952197272272936138731}{1323845495217113239974148545176659722240000000000000 0}w^{12}+\cdots. \quad (44)$$

Applying the Taylor series expansions of $y_{n\pm1}$, $y_{n\pm1/2}$, $y_{n\pm1/5}$, $y''_{n\pm1/2}$, $y''_{n\pm1/5}$, $y''_{n\pm1}$ about x_n in (17)–(21) we have the following result for the local truncation error (*LTE*) of the family of exponentially-fitted methods (17)–(21):

Case I.

$$LTE=-\frac{139h^{10}}{1016064000}\left(y_n^{(10)}-w^2y_n^{(8)}\right). \quad (45)$$

Case II.

$$LTE=-\frac{139\,h^{10}}{1016064000}\left(y_n^{(10)}-2w^2y_n^{(8)}+w^4y_n^{(6)}\right). \quad (46)$$

Case III.

$$LTE=-\frac{139h^{10}}{1016064000}\left(y_n^{(10)}-3w^2y_n^{(8)}-3w^4y_n^{(6)}+w^6y_n^{(4)}\right). \quad (47)$$

For comparison purposes in table 1 we list the properties of two-step hybrid exponentially-fitted method developed in this paper, together with the corresponding properties of some similar two-step exponentially-fitted methods presented previously in the literature. We present the properties of the methods: MI: Numerov's method; MII: derived by Raptis and Allison; MIII: derived by Raptis and Cash; MIV: method of Thomas, Mitsou and Simos – case I; MV: method of Simos and Williams; MVI: method of Simos and Williams [24]; MVII: the method developed in [37]; MVIII: the new developed method (case I); MIX: the new developed method (case II) and MX: the

Table 1
Properties of some two-step exponentially-fitted methods. $S = \{T^2\colon\ T = q\pi,\ q = 1, 2, \ldots\}$. A.O. = the algebraic order of the method. Inter. period. = the interval of periodicity of the method.

Method	A.O.	Inter. period.	Integrated exponential functions
MI	4	(0,6)	$\{1, x, x^2, x^3, x^4, x^5\}$
MII	4	$(0, \infty) - S$	$\{1, x, x^2, x^3, \exp(\pm wx)\}$
MIII	6	$(0, \infty) - S$	$\{1, x, x^2, x^3, x^4, x^5, \exp(\pm wx)\}$
MIV	4	$(0, \infty) - S$	$\{1, x, x^2, x^3, x^4, x^5, x^6, x^7, \exp(\pm wx)\}$
MV	4	$(0, \infty) - S$	$\{1, x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9, \exp(\pm wx)\}$
MVI	6	$(0, \infty)$	$\{1, x, x^2, x^3, x^4, x^5, \exp(\pm wx)\}$
MVII	8	$(0, \infty)$	$\{1, x, x^2, x^3, x^4, x^5, x^6, x^7, \exp(\pm wx)\}$
MVIII	8	$(0, \infty)$	$\{1, x, x^2, x^3, x^4, x^5, x^6, x^7, \exp(\pm wx)\}$
MIX	8	$(0, \infty)$	$\{1, x, x^2, x^3, x^4, x^5, \exp(\pm wx), x\exp(\pm wx)\}$
MX	8	$(0, \infty)$	$\{1, x, x^2, x^3, \exp(\pm wx), x\exp(\pm wx), x^2\exp(\pm wx)\}$

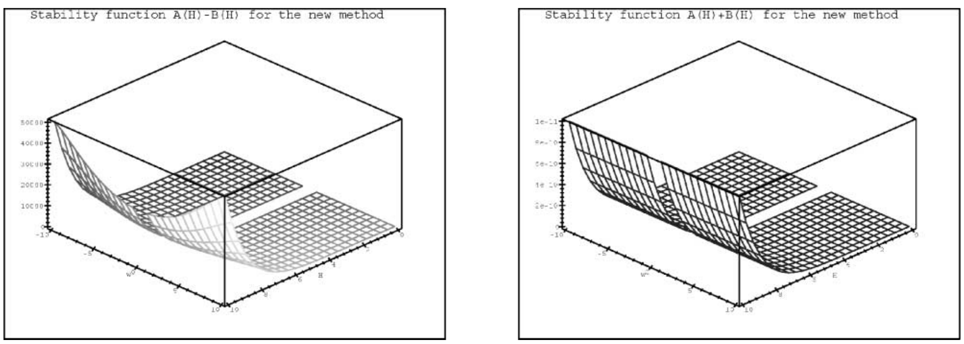

Figure 1. Stability functions $A(H) \pm B(H)$ for the new proposed method (case I).

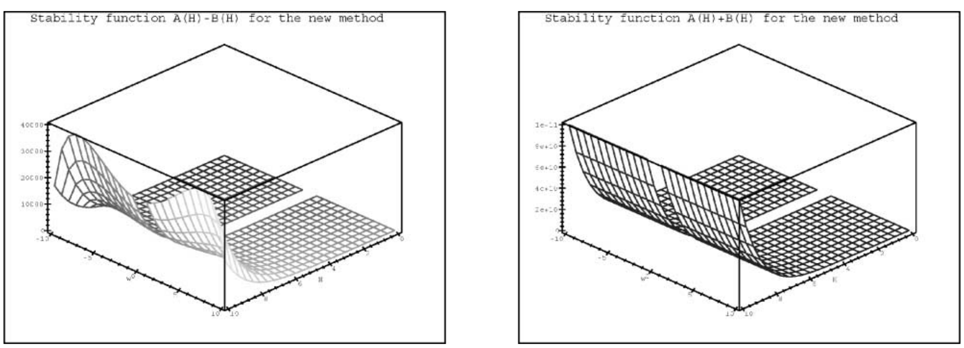

Figure 2. Stability functions $A(H) \pm B(H)$ for the new proposed method (case II).

new developed method (case III). We note that all the methods presented in the table are implicit.

In figures 1–3 we present the stability functions $A(H) \pm B(H)$ for the new family of methods (cases I–III). From these figures it is obvious that the new methods are P-stable

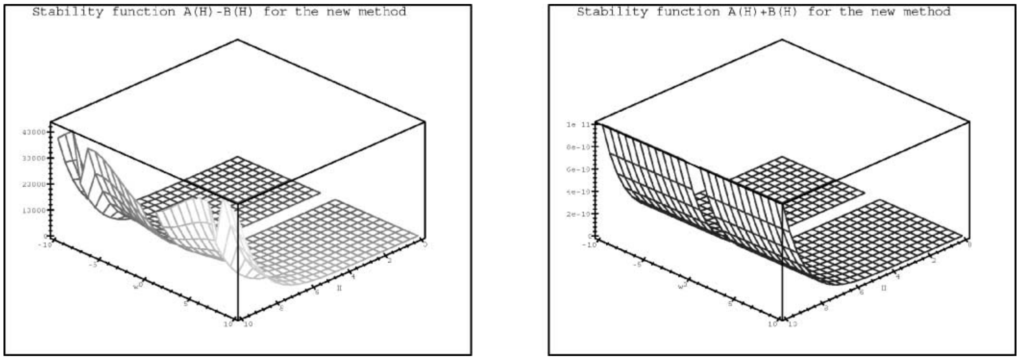

Figure 3. Stability functions $A(H) \pm B(H)$ for the new proposed method (case III).

and there is a zone near to $w = 0$ in which the stability functions are not defined due to cancellations of the coefficients of the method.

6. Error estimation

In the literature there are several methods for the estimation of the local truncation error (*LTE*) for the numerical solution of systems of initial-value problems (see, for example, [47]).

The local error estimation procedure in this work is based on an embedded pair of numerical methods and on the fact that when the algebraic order is minimal then the approximation of the solution for the problems with an oscillatory or periodic solution is better.

In this section we will define three variable-step procedures. The first is based on the case I of the P-stable exponentially-fitted method developed above. The second is based on the case II of the P-stable exponentially-fitted method developed above. Finally, the third is based on the case III of the P-stable exponentially-fitted method developed above.

We have the following definition.

Definition 5. We define the *local error* estimate in the lower order solution y^L_{n+1} by the quantity

$$LEE = \left| y^H_{n+1} - y^L_{n+1} \right|. \tag{48}$$

We note here that y^H_{n+1} is the solution obtained with: (1) the P-stable exponentially-fitted method of algebraic order eight (case I) developed in this paper (for the first variable-step procedure), (2) the P-stable exponentially-fitted method of algebraic order eight (case II) developed in this paper (for the second variable-step procedure) and (3) the P-stable exponentially-fitted method of algebraic order eight (case III) developed in this paper (for the third variable-step procedure) and y^L_{n+1} is the solution obtained with (1) the P-stable hybrid exponentially-fitted method of sixth algebraic order developed by Simos and Williams [48] (for the first variable-step procedure); (2) the hybrid exponentially-fitted method of sixth algebraic order developed by Thomas and Simos [11] (case II) (for the second variable-step procedure) and (3) the hybrid exponentially-fitted method of sixth algebraic order developed by Thomas and Simos [11] (case III) (for the third variable-step procedure).

Remark 3. Under the assumption that h is sufficiently small, the *local error* in y_{n+1}^H can be neglected compared with that in y_{n+1}^L.

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

$$h_{n+1} = h_n \left(\frac{acc}{LEE} \right)^{1/q}, \tag{49}$$

where q is the algebraic order.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in [49], the step control procedure which we have actually used is:

$$\begin{aligned} &\text{if } LEE < acc,\ h_{n+1} = 2h_n; \\ &\text{if } 100acc > LEE \geqslant acc,\ h_{n+1} = h_n; \\ &\text{if } LEE \geqslant 100acc,\ h_{n+1} = \frac{h_n}{2} \text{ and repeat the step.} \end{aligned} \tag{50}$$

We note, here, that the local error estimate is in the lower order solution y_{n+1}^L. However, if this error estimate is acceptable, i.e., less than *acc*, we adopt the widely used procedure of performing local extrapolation. Thus, although we are actually controlling an estimate of the local error in lower phase-lag order solution y_{n+1}^L, it is the higher order solution y_{n+1}^H which we actually accept at each point.

7. Numerical illustrations

In the present section we will investigate the efficiency of the previously described variable-step techniques by applying them to the numerical solution of coupled differential equations arising from the Schrödinger equation.

7.1. *Coupled differential equations*

The close-coupled differential equations of the Schrödinger type have the form

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{51}$$

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

We have investigated the case in which all channels are open. So, the boundary conditions are (see, for details, [14]):

$$y_{ij} = 0 \quad \text{at } x = 0, \tag{52}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x), \tag{53}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. The proposed methods are P-stable (i.e., have intervals of periodicity $(0, \infty)$). This property is essential to avoid numerical instabilities. Such methods are thus very suitable for problems involving closed channels.

Using the detailed analysis developed in [50] and defining a matrix K' and diagonal matrices M, N by:

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

we find that the asymptotic condition (53) may be written:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}'. \tag{54}$$

A classical example of a problem that can be transformed to a set of close-coupled differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [50], the entrance channel by the quantum numbers by (j, l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we find that

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_{j'j}^2 - \frac{l'(l+1)}{x^2}\right] y_{j'l'}^{Jjl}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l';\ J|V|j''l'';\ J\rangle y_{j''l''}^{Jjl}(x), \tag{55}$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\left\{j(j+1) - j'\left(j'+1\right)\right\}\right], \tag{56}$$

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

Following the analysis of [50], the potential V may be written

$$V\left(x, \hat{\mathbf{k}}_{j'j} \cdot \hat{\mathbf{k}}_{jj}\right) = V_0(x) P_0\left(\hat{\mathbf{k}}_{j'j} \cdot \hat{\mathbf{k}}_{jj}\right) + V_2(x) P_2\left(\hat{\mathbf{k}}_{j'j} \cdot \hat{\mathbf{k}}_{jj}\right), \tag{57}$$

and the coupling matrix element is

$$\left\langle j'l'; J\middle|V\middle|j''l''; J\right\rangle = \delta_{j'j''}\delta_{l'l''} V_0(x) - f_2\left(j'l', j''l''; J\right) V_2(x), \tag{58}$$

where the f_2 coefficients can be obtained from formulae given by Berstein et al. [51], $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i, $i = 0, 2$ are Legendre polynomials (see, for details, [51]). The boundary conditions may then be written (see [50])

$$y_{j'l'}^{Jjl}(x) = 0 \quad \text{at } x = 0, \tag{59}$$

$$y_{j'l}^{Jj'l}(x) \sim \delta_{jj'}\delta_{ll'} \exp\left[-\mathrm{i}\left(k_{jj}x - \frac{l\pi}{2}\right)\right] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \times \exp\left[\mathrm{i}\left(k_{j'j}x - \frac{l'\pi}{2}\right)\right], \quad \text{as } x \to \infty, \tag{60}$$

where the scattering matrix $\mathbf{S}$ is related to the $\mathbf{K}$ matrix of (53) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathrm{i}\mathbf{K})(\mathbf{I} - \mathrm{i}\mathbf{K})^{-1}. \tag{61}$$

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

In our numerical test, we choose the $\mathbf{S}$ matrix given by the following parameters:

$$\frac{2\mu}{\hbar^2} = 1000.0, \qquad \frac{\mu}{I} = 2.351, \qquad E = 1.1,$$

$$V_0(x) = \frac{1}{x^{12}} - \frac{2}{x^6}, \qquad V_2(x) = 0.2283 V_0(x).$$

Following [50], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of *four, nine* and *sixteen coupled differential equations*, respectively. Following Berstein [52] and Allison [50] a reduction of the interval $[0, \infty)$ to $[x_0, \infty]$ is made. The wave functions are then zero in this region and consequently the boundary condition (59) may be written

$$y_{j'l'}^{Jjl}(x_0) = 0. \tag{62}$$

For the numerical solution we have used (i) the iterative Numerov method of Allison [50], (ii) the variable-step method of Raptis and Cash [49], (iii) the variable-step method of Simos [53], (iv) the variable-step exponentially-fitted method of Simos and Williams [54], (v) the explicit variable-step method developed in [28], (vi) the variable-step Bessel and Neumann fitted method developed in [55], (vii) the variable-step fourth algebraic order method developed in [56], (viii) the variable-step sixth algebraic order method developed in [56], (ix) the variable-step eighth algebraic order method developed in [33], (x) the method RKN12 described in [57, page 298]. This method is based on the Runge–Kutta–Nyström method of order 12(10) developed by Dormand et al. [58] (for Runge–Kutta–Nyström methods see also [59]), (xi) the new variable-step P-stable exponentially-fitted method (procedure 1) developed in this paper, (xii) the new variable-step P-stable exponentially-fitted method (procedure 2) developed in this paper and (xiii) the new variable-step P-stable exponentially-fitted method (procedure 3) developed in this paper. In table 2, we present the real computation time required by these

Table 2

RTC (Real time of computation (in seconds)) to calculate $|S|^2$ for the variable-step methods (i)–(xiii). $acc = 10^{-6}$; hmax is the maximum step size; *MErr* is the maximum absolute error.

Method	N	hmax	RTC	*MErr*
Iterative Numerov [50]	4	0.014	3.25	$1.2 \cdot 10^{-3}$
	9	0.014	23.51	$5.7 \cdot 10^{-2}$
	16	0.014	99.15	$6.8 \cdot 10^{-1}$
Variable-step method of Raptis and Cash [49]	4	0.056	1.55	$8.9 \cdot 10^{-4}$
	9	0.056	8.43	$7.4 \cdot 10^{-3}$
	16	0.056	43.32	$8.6 \cdot 10^{-2}$
Variable-step method of Simos [53]	4	0.056	1.05	$8.0 \cdot 10^{-4}$
	9	0.056	5.25	$6.7 \cdot 10^{-3}$
	16	0.056	27.15	$8.1 \cdot 10^{-2}$
Variable-step method of Simos and Williams [54]	4	0.448	0.24	$5.2 \cdot 10^{-4}$
	9	0.448	0.96	$4.4 \cdot 10^{-3}$
	16	0.448	5.04	$6.4 \cdot 10^{-2}$
Variable-step method of Simos et al. [28]	4	0.448	0.29	$6.1 \cdot 10^{-4}$
	9	0.448	1.59	$5.6 \cdot 10^{-3}$
	16	0.448	6.44	$7.2 \cdot 10^{-2}$
Variable-step method of Simos and Williams [55]	4	0.448	0.18	$4.5 \cdot 10^{-4}$
	9	0.448	0.92	$3.8 \cdot 10^{-3}$
	16	0.224	5.32	$4.2 \cdot 10^{-2}$
Variable-step methods of order four of Avdelas and Simos [56]	4	0.112	1.37	$8.4 \cdot 10^{-4}$
	9	0.112	7.72	$7.0 \cdot 10^{-3}$
	16	0.112	33.11	$8.4 \cdot 10^{-2}$
Variable-step methods of order six of Avdelas and Simos [56]	4	0.224	1.03	$8.1 \cdot 10^{-4}$
	9	0.224	6.91	$6.7 \cdot 10^{-3}$
	16	0.224	14.05	$7.1 \cdot 10^{-2}$
Variable-step methods of order eight of Avdelas and Simos [33]	4	0.896	0.07	$5.5 \cdot 10^{-5}$
	9	0.896	0.39	$3.5 \cdot 10^{-4}$
	16	0.896	2.72	$4.4 \cdot 10^{-3}$
RKN12	4	0.224	0.78	$9.6 \cdot 10^{-5}$
	9	0.224	4.93	$9.8 \cdot 10^{-4}$
	16	0.224	13.25	$9.5 \cdot 10^{-3}$
Variable-step procedure 1 of this paper	4	0.896	0.03	$2.1 \cdot 10^{-8}$
	9	0.896	0.21	$9.2 \cdot 10^{-8}$
	16	0.896	1.72	$3.4 \cdot 10^{-7}$
Variable-step procedure 2 of this paper	4	0.896	0.02	$7.8 \cdot 10^{-9}$
	9	0.896	0.17	$9.4 \cdot 10^{-9}$
	16	0.896	1.32	$6.5 \cdot 10^{-8}$
Variable-step procedure 3 of this paper	4	0.896	0.01	$1.2 \cdot 10^{-9}$
	9	0.896	0.11	$1.3 \cdot 10^{-9}$
	16	0.896	0.94	$7.6 \cdot 10^{-9}$

methods to calculate the square of the modulus of the **S** matrix for sets of 4, 9 and 16 coupled differential equations. In the same table the maximum absolute error is also presented. In table 2, N indicates the number of equations of the set of coupled differential equations.

8. Remarks and conclusions

In this paper a variable-step technique for the numerical solution of the Schrödinger equation and related problems is described.

From the results presented above we arrive to the following conclusions.

1. The variable-step fourth and sixth algebraic order methods of Avdelas and Simos [56] are more efficient (more accurate and more rapid) than the iterative Numerov of Allison [50], the variable-step method of Raptis and Cash [49] and the variable-step method of Simos [53].

2. The method of Simos and Williams [54] and the method of Simos et al. [28] are more efficient than the iterative Numerov of Allison [50], the variable-step method of Raptis and Cash [49], the variable-step method of Simos [53], the variable-step fourth and sixth algebraic order methods of Avdelas and Simos [56]. The method of Simos and Williams [55] is more efficient than the method of Simos [28].

3. The method RKN12 described in [57, p. 298] is more efficient than the iterative Numerov of Allison [50], the variable-step method of Raptis and Cash [49] and the variable-step method of Simos [53].

4. The variable-step eighth algebraic order method of Avdelas and Simos [33] is more efficient than the iterative Numerov of Allison [50], the variable-step method of Raptis and Cash [49], the variable-step method of Simos [53], the method of Simos and Williams [54], the method of Simos et al. [28], the variable-step fourth and sixth algebraic order methods of Avdelas and Simos [56], the method of Simos and Williams [55] and the method RKN12 described in [57, p. 298].

5. Finally the new variable-step P-stable exponentially-fitted techniques are the most efficient ones.

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

Appendix A.

Case I.

$$q_0 = \frac{-84\cosh(w) + 84 - 125w^2\cosh(\frac{1}{5}w) + 48w^2\cosh(\frac{1}{2}w) + 119w^2}{-84w^2\cosh(w) - 7500w^2\cosh(\frac{1}{5}w) + 1536w^2\cosh(\frac{1}{2}w) + 6048w^2},$$

$$q_1 = \frac{-119w^2\cosh(w) - 1625w^2\cosh(\frac{1}{5}w) - 1280w^2\cosh(\frac{1}{2}w) + 6048\cosh(w) - 6048}{-42w^2\cosh(w) - 3750w^2\cosh(\frac{1}{5}w) + 768w^2\cosh(\frac{1}{2}w) + 3024w^2},$$

$$q_2 = \frac{-12w^2\cosh(w) - 500w^2\cosh(\frac{1}{5}w) + 320w^2 + 384\cosh(w) - 384}{-21w^2\cosh(w) - 1875w^2\cosh(\frac{1}{5}w) + 384w^2\cosh(\frac{1}{2}w) + 1512\,w^2},$$

$$q_3 = \frac{125w^2\cosh(w) + 2000w^2\cosh(\frac{1}{2}w) + 1625w^2 - 7500\cosh(w) + 7500}{-84w^2\cosh(w) - 7500w^2\cosh(\frac{1}{5}w) + 1536w^2\cosh(\frac{1}{2}w) + 6048w^2}. \tag{63}$$

Case II.

$$\begin{aligned}
q_0 = \Bigg(&6w^3 - 204\sinh\left(\frac{9}{10}w\right) + 96\sinh\left(\frac{1}{2}w\right) + 12w\cosh\left(\frac{4}{5}w\right) - 48\sinh\left(\frac{6}{5}w\right)\\
&+ 72w\cosh\left(\frac{2}{5}w\right) + 15w^3\cosh\left(\frac{3}{5}w\right) - 48\sinh\left(\frac{7}{5}w\right) + 12w\cosh\left(\frac{3}{5}w\right)\\
&- 48w\cosh\left(\frac{3}{10}w\right) - 48w\cosh\left(\frac{1}{2}w\right) - 504\sinh\left(\frac{1}{10}w\right) + 72w\cosh\left(\frac{1}{5}w\right)\\
&- 48\sinh\left(\frac{3}{5}w\right) - 108w\cosh\left(\frac{1}{10}w\right) + 12w\cosh(w) - 48w\cosh\left(\frac{7}{10}w\right)\\
&+ 12w\cosh\left(\frac{6}{5}w\right) - 48\sinh(w) + 132w\cosh\left(\frac{9}{10}w\right) - 10w^3\cosh\left(\frac{1}{10}w\right)\\
&- 48\sinh\left(\frac{4}{5}w\right) + 12w^3\cosh\left(\frac{1}{5}w\right) + 36w + 300\sinh\left(\frac{11}{10}w\right)\\
&- 120w\cosh\left(\frac{11}{10}w\right) + 96\sinh\left(\frac{7}{10}w\right) + 12w\cosh\left(\frac{7}{5}w\right) - 23w^3\cosh\left(\frac{2}{5}w\right)\\
&+ 96\sinh\left(\frac{3}{10}w\right)\Bigg)\\
&\Bigg/\Bigg(192w^3\cosh\left(\frac{3}{5}w\right) + 12w^3\cosh\left(\frac{4}{5}w\right) - 48w^3\cosh\left(\frac{3}{10}w\right)\\
&- 48w^3\cosh\left(\frac{1}{2}w\right) - 48w^3\cosh\left(\frac{7}{10}w\right) + 12w^3\cosh\left(\frac{7}{5}w\right)\\
&+ 132w^3\cosh\left(\frac{9}{10}w\right) - 120w^3\cosh\left(\frac{11}{10}w\right) + 12w^3\cosh(w) + 72w^3\cosh\left(\frac{1}{5}w\right)\\
&- 348w^3\cosh\left(\frac{2}{5}w\right) + 36w^3 + 12w^3\cosh\left(\frac{6}{5}w\right) + 132w^3\cosh\left(\frac{1}{10}w\right)\Bigg),
\end{aligned}$$

$$\begin{aligned}
q_1 = \Bigg(&87w^3 + 648\sinh\left(\frac{9}{10}w\right) + 1548\sinh\left(\frac{1}{2}w\right) + 288w\cosh\left(\frac{4}{5}w\right)\\
&- 50w^3\cosh\left(\frac{1}{2}w\right) - 50w^3\cosh\left(\frac{7}{10}w\right) - 1152\sinh\left(\frac{6}{5}w\right) + 1728w\cosh\left(\frac{2}{5}w\right)\\
&- 20w^3\cosh\left(\frac{9}{10}w\right) + 56w^3\cosh\left(\frac{3}{5}w\right) - 19w^3\cosh\left(\frac{4}{5}w\right) - 50w^3\cosh\left(\frac{3}{10}w\right)
\end{aligned}$$

$$
\begin{aligned}
&- 19w^3\cosh\left(\frac{7}{5}w\right) - 20w^3\cosh\left(\frac{11}{10}w\right) - 1152\sinh\left(\frac{7}{5}w\right) + 288w\cosh\left(\frac{3}{5}w\right) \\
&- 19w^3\cosh(w) - 1152w\cosh\left(\frac{3}{10}w\right) - 1152w\cosh\left(\frac{1}{2}w\right) - 252\sinh\left(\frac{1}{10}w\right) \\
&+ 1728w\cosh\left(\frac{1}{5}w\right) - 1152\sinh\left(\frac{3}{5}w\right) - 1332w\cosh\left(\frac{1}{10}w\right) + 288w\cosh(w) \\
&+ 252\sinh\left(\frac{19}{10}w\right) - 19w^3\cosh\left(\frac{6}{5}w\right) - 1152w\cosh\left(\frac{7}{10}w\right) + 288w\cosh\left(\frac{6}{5}w\right) \\
&- 1152\sinh(w) + 252\sinh\left(\frac{3}{2}w\right) + 252\sinh\left(\frac{13}{10}w\right) - 612w\cosh\left(\frac{9}{10}w\right) \\
&- 50w^3\cosh\left(\frac{1}{10}w\right) + 252\sinh\left(\frac{17}{10}w\right) - 1152\sinh\left(\frac{4}{5}w\right) + 174w^3\cosh\left(\frac{1}{5}w\right) \\
&+ 864w + 1152\sinh\left(\frac{11}{10}w\right) - 360w\cosh\left(\frac{11}{10}w\right) + 1548\sinh\left(\frac{7}{10}w\right) \\
&+ 288w\cosh\left(\frac{7}{5}w\right) - w^3\cosh\left(\frac{2}{5}w\right) + 1548\sinh\left(\frac{3}{10}w\right)\bigg) \\
&\bigg/\bigg(96w^3\cosh\left(\frac{3}{5}w\right) + 6w^3\cosh\left(\frac{4}{5}w\right) - 24w^3\cosh\left(\frac{3}{10}w\right) - 24w^3\cosh\left(\frac{1}{2}w\right) \\
&- 24w^3\cosh\left(\frac{7}{10}w\right) + 6w^3\cosh\left(\frac{7}{5}w\right) + 66w^3\cosh\left(\frac{9}{10}w\right) - 60w^3\cosh\left(\frac{11}{10}w\right) \\
&+ 6w^3\cosh(w) + 36w^3\cosh\left(\frac{1}{5}w\right) - 174w^3\cosh\left(\frac{2}{5}w\right) + 18w^3 \\
&+ 6w^3\cosh\left(\frac{6}{5}w\right) + 66w^3\cosh\left(\frac{1}{10}w\right)\bigg),
\end{aligned}
$$

$$
\begin{aligned}
q_2 = &\bigg(31w^3\cosh\left(\frac{3}{10}w\right) + 18w^3\cosh\left(\frac{1}{2}w\right) + 11w^3\cosh\left(\frac{7}{10}w\right) + 120w\cosh\left(\frac{1}{10}w\right) \\
&+ 10w^3\cosh\left(\frac{9}{10}w\right) - 12\sinh\left(\frac{17}{10}w\right) - 120\sinh\left(\frac{11}{10}w\right) - 72\sinh\left(\frac{13}{10}w\right) \\
&- 36\sinh\left(\frac{3}{2}w\right) + 96\sinh\left(\frac{7}{10}w\right) + 120\sinh\left(\frac{9}{10}w\right) + 156\sinh\left(\frac{3}{10}w\right) \\
&+ 108\sinh\left(\frac{1}{2}w\right) - 120w\cosh\left(\frac{9}{10}w\right) - 60w\cosh\left(\frac{7}{10}w\right) + 60w\cosh\left(\frac{3}{10}w\right) \\
&+ 240\sinh\left(\frac{1}{10}w\right) + 50w^3\cosh\left(\frac{1}{10}w\right)\bigg) \\
&\bigg/\bigg(90w^3\cosh\left(\frac{1}{10}w\right) - 9w^3\cosh(w) - 27w^3 - 18w^3\cosh\left(\frac{4}{5}w\right)
\end{aligned}
$$

$$
\begin{aligned}
&- 30w^3\cosh\left(\frac{3}{5}w\right) - 90w^3\cosh\left(\frac{2}{5}w\right) - 63w^3\cosh\left(\frac{1}{5}w\right) + 27w^3\cosh\left(\frac{7}{10}w\right)\\
&+ 36w^3\cosh\left(\frac{1}{2}w\right) + 57w^3\cosh\left(\frac{3}{10}w\right) + 30w^3\cosh\left(\frac{9}{10}w\right)\\
&- 3w^3\cosh\left(\frac{6}{5}w\right)\bigg),
\end{aligned}
$$

$$
\begin{aligned}
q_3 = \bigg(&-75w^3 - 1500\sinh\left(\frac{9}{10}w\right) - 1500\sinh\left(\frac{1}{2}w\right) - 300w\cosh\left(\frac{4}{5}w\right)\\
&+ 50w^3\cosh\left(\frac{1}{2}w\right) + 50w^3\cosh\left(\frac{7}{10}w\right) + 1200\sinh\left(\frac{6}{5}w\right) - 1800w\cosh\left(\frac{2}{5}w\right)\\
&+ 50w^3\cosh\left(\frac{9}{10}w\right) + 25w^3\cosh\left(\frac{3}{5}w\right) + 25w^3\cosh\left(\frac{4}{5}w\right) + 50w^3\cosh\left(\frac{3}{10}w\right)\\
&+ 25w^3\cosh\left(\frac{7}{5}w\right) + 1200\sinh\left(\frac{7}{5}w\right) - 300w\cosh\left(\frac{3}{5}w\right) + 25w^3\cosh(w)\\
&+ 1200w\cosh\left(\frac{3}{10}w\right) + 1200w\cosh\left(\frac{1}{2}w\right) - 1500\sinh\left(\frac{1}{10}w\right)\\
&- 1800w\cosh\left(\frac{1}{5}w\right) + 1200\sinh\left(\frac{3}{5}w\right) + 1200w\cosh\left(\frac{1}{10}w\right) - 300w\cosh(w)\\
&- 300\sinh\left(\frac{19}{10}\right) + 25w^3\cosh\left(\frac{6}{5}w\right) + 1200w\cosh\left(\frac{7}{10}w\right) - 300w\cosh\left(\frac{6}{5}w\right)\\
&+ 1200\sinh(w) - 300\sinh\left(\frac{3}{2}w\right) - 300\sinh\left(\frac{13}{10}w\right) + 1200w\cosh\left(\frac{9}{10}w\right)\\
&+ 50w^3\cosh\left(\frac{1}{10}w\right) - 300\sinh\left(\frac{17}{10}w\right) + 1200\sinh\left(\frac{4}{5}w\right) - 150w^3\cosh\left(\frac{1}{5}w\right)\\
&- 900w - 300\sinh\left(\frac{11}{10}w\right) - 1500\sinh\left(\frac{7}{10}w\right) - 300w\cosh\left(\frac{7}{5}w\right)\\
&- 150w^3\cosh\left(\frac{2}{5}w\right) - 1500\sinh\left(\frac{3}{10}w\right)\bigg)\\
&\bigg/\bigg(192w^3\cosh\left(\frac{3}{5}w\right) + 12w^3\cosh\left(\frac{4}{5}w\right) - 48w^3\cosh\left(\frac{3}{10}w\right)\\
&- 48w^3\cosh\left(\frac{1}{2}w\right) - 48w^3\cosh\left(\frac{7}{10}w\right) + 12w^3\cosh\left(\frac{7}{5}w\right)\\
&+ 132w^3\cosh\left(\frac{9}{10}w\right) - 120w^3\cosh\left(\frac{11}{10}w\right) + 12w^3\cosh(w) + 72w^3\cosh\left(\frac{1}{5}w\right)\\
&- 348w^3\cosh\left(\frac{2}{5}w\right) + 36w^3 + 12w^3\cosh\left(\frac{6}{5}w\right) + 132w^3\cosh\left(\frac{1}{10}w\right)\bigg).
\end{aligned}
\tag{64}
$$

Case III.

$$
\begin{aligned}
q_0 = -\Big(&-240w + 384w\cosh\Big(\frac{1}{10}w\Big) - 414w\cosh\Big(\frac{3}{5}w\Big) + 416w\cosh\Big(\frac{3}{10}w\Big)\\
&- 272w\cosh\Big(\frac{6}{5}w\Big) - 480w\cosh\Big(\frac{1}{5}w\Big) + 544w\cosh\Big(\frac{7}{10}w\Big) + 8w^4\sinh\Big(\frac{1}{5}w\Big)\\
&+ 3w^4\sinh\Big(\frac{3}{5}w\Big) - 240w\cosh(w) + 1260\sinh\Big(\frac{3}{5}w\Big) + 78w\cosh\Big(\frac{8}{5}w\Big)\\
&- 208w\cosh\Big(\frac{4}{5}w\Big) - 558w\cosh\Big(\frac{2}{5}w\Big) + 9w^4\sinh\Big(\frac{2}{5}w\Big) + 1020\sinh\Big(\frac{2}{5}w\Big)\\
&+ 480w\cosh\Big(\frac{1}{2}w\Big) - 66w\cosh\Big(\frac{7}{5}w\Big) + 432w\cosh\Big(\frac{9}{10}w\Big) + 144w\cosh\Big(\frac{11}{10}w\Big)\\
&+ 60\sinh\Big(\frac{7}{5}w\Big) + 480\sinh\Big(\frac{6}{5}w\Big) - 180\sinh\Big(\frac{8}{5}w\Big) - 240\sinh\Big(\frac{11}{10}w\Big)\\
&- 960\sinh\Big(\frac{7}{10}w\Big) - 720\sinh\Big(\frac{9}{10}w\Big) - 480\sinh\Big(\frac{1}{10}w\Big) + 480\sinh\Big(\frac{4}{5}w\Big)\\
&- 960\sinh\Big(\frac{1}{2}w\Big) - 960\sinh\Big(\frac{3}{10}\Big) + 14w^2\sinh\Big(\frac{7}{5}w\Big) + 480\sinh(w)\\
&- 12w^2\sinh\Big(\frac{8}{5}w\Big) - 32w^2\sinh\Big(\frac{11}{10}w\Big) - 112w^2\sinh\Big(\frac{7}{10}w\Big)\\
&- 16w^2\sinh\Big(\frac{1}{10}w\Big) + 48w^2\sinh\Big(\frac{6}{5}w\Big) + 32w^2\sinh\Big(\frac{4}{5}w\Big) + 40w^2\sinh(w)\\
&+ 114w^2\sinh\Big(\frac{3}{5}w\Big) - 96w^2\sinh\Big(\frac{9}{10}w\Big) + 48w^2\sinh\Big(\frac{1}{5}w\Big) - 48w^2\sinh\Big(\frac{3}{10}w\Big)\\
&- 80w^2\sinh\Big(\frac{1}{2}w\Big) + 136w^2\sinh\Big(\frac{2}{5}w\Big)\Big)\\
&\Big/\Big(48w^4\sinh\Big(\frac{3}{10}w\Big) + 112w^4\sinh\Big(\frac{7}{10}w\Big) + 16w^4\sinh\Big(\frac{1}{10}w\Big)\\
&+ 96w^4\sinh\Big(\frac{9}{10}w\Big) - 48w^4\sinh\Big(\frac{6}{5}w\Big) - 14w^4\sinh\Big(\frac{7}{5}w\Big) + 12w^4\sinh\Big(\frac{8}{5}w\Big)\\
&+ 32w^4\sinh\Big(\frac{11}{10}w\Big) - 32w^4\sinh\Big(\frac{4}{5}w\Big) - 114w^4\sinh\Big(\frac{3}{5}w\Big) - 136w^4\sinh\Big(\frac{2}{5}w\Big)\\
&+ 80w^4\sinh\Big(\frac{1}{2}w\Big) - 40w^4\sinh(w) - 48w^4\sinh\Big(\frac{1}{5}w\Big)\Big),
\end{aligned}
$$

$$
\begin{aligned}
q_1 = \Big(&150w\cosh\Big(\frac{11}{5}w\Big) + 50w\cosh\Big(\frac{12}{5}w\Big) + 159w^4\sinh\Big(\frac{4}{5}w\Big) + 250w\cosh(2w)\\
&- 2592w\cosh\Big(\frac{13}{10}w\Big) - 384w\cosh\Big(\frac{19}{10}w\Big) + 51w^4\sinh\Big(\frac{6}{5}w\Big)
\end{aligned}
$$

$$
\begin{aligned}
&+ 18w^4\sinh\left(\frac{7}{5}w\right) - 928w\cosh\left(\frac{17}{10}w\right) + 105w^4\sinh(w) - 1760w\cosh\left(\frac{3}{2}w\right) \\
&- 128w\cosh\left(\frac{21}{10}w\right) + 350w\cosh\left(\frac{9}{5}w\right) + 6w^4\sinh\left(\frac{8}{5}w\right) - 2100\sinh\left(\frac{9}{5}w\right) \\
&+ 7920\sinh\left(\frac{13}{10}w\right) - 300\sinh\left(\frac{12}{5}w\right) + 480\sinh\left(\frac{21}{10}w\right) - 900\sinh\left(\frac{11}{5}w\right) \\
&- 1500\sinh(2w) + 3120\sinh\left(\frac{17}{10}w\right) + 1440\sinh\left(\frac{19}{10}w\right) + 5510w \\
&- 13312w\cosh\left(\frac{1}{10}w\right) + 9986w\cosh\left(\frac{3}{5}w\right) - 12128w\cosh\left(\frac{3}{10}w\right) \\
&+ 3528w\cosh\left(\frac{6}{5}w\right) + 11020w\cosh\left(\frac{1}{5}w\right) - 7392w\cosh\left(\frac{7}{10}w\right) \\
&+ 84w^4\sinh\left(\frac{1}{5}w\right) - 6000\sinh\left(\frac{1}{5}w\right) + 171w^4\sinh\left(\frac{3}{5}w\right) + 5760w\cosh(w) \\
&- 12540\sinh\left(\frac{3}{5}w\right) + 528w\cosh\left(\frac{8}{5}w\right) + 7992w\cosh\left(\frac{4}{5}w\right) \\
&+ 10942w\cosh\left(\frac{2}{5}w\right) + 141w^4\sinh\left(\frac{2}{5}w\right) - 10980\sinh\left(\frac{2}{5}w\right) \\
&- 9760w\cosh\left(\frac{1}{2}w\right) + 1534w\cosh\left(\frac{7}{5}w\right) - 5408w\cosh\left(\frac{9}{10}w\right) \\
&- 3808w\cosh\left(\frac{11}{10}w\right) - 4140\sinh\left(\frac{7}{5}w\right) - 6120\sinh\left(\frac{6}{5}w\right) - 2880\sinh\left(\frac{8}{5}w\right) \\
&+ 9360\sinh\left(\frac{11}{10}w\right) + 8880\sinh\left(\frac{7}{10}w\right) + 9840\sinh\left(\frac{9}{10}w\right) + 1440\sinh\left(\frac{1}{10}w\right) \\
&- 10920\sinh\left(\frac{4}{5}w\right) + 6480\sinh\left(\frac{1}{2}w\right) + 4080\sinh\left(\frac{3}{10}w\right) + 14w^2\sinh\left(\frac{7}{5}w\right) \\
&- 8520\sinh(w) - 12w^2\sinh\left(\frac{8}{5}w\right) - 32w^2\sinh\left(\frac{11}{10}w\right) - 112w^2\sinh\left(\frac{7}{10}w\right) \\
&- 16w^2\sinh\left(\frac{1}{10}w\right) + 48w^2\sinh\left(\frac{6}{5}w\right) + 32w^2\sinh\left(\frac{4}{5}w\right) + 40w^2\sinh(w) \\
&+ 114w^2\sinh\left(\frac{3}{5}w\right) - 96w^2\sinh\left(\frac{9}{10}w\right) + 48w^2\sinh\left(\frac{1}{5}w\right) - 48w^2\sinh\left(\frac{3}{10}w\right) \\
&+ 5520\sinh\left(\frac{3}{2}w\right) - 80w^2\sinh\left(\frac{1}{2}w\right) + 136w^2\sinh\left(\frac{2}{5}w\right)\Bigg). \\
&\Bigg/\Bigg((24w^4\sinh\left(\frac{3}{10}w\right) + 56w^4\sinh\left(\frac{7}{10}w\right) + 8w^4\sinh\left(\frac{1}{10}w\right)
\end{aligned}
$$

$$+ 48w^4\sinh\left(\frac{9}{10}w\right) - 24w^4\sinh\left(\frac{6}{5}w\right) - 7w^4\sinh\left(\frac{7}{5}w\right) + 6w^4\sinh\left(\frac{8}{5}w\right)$$
$$+ 16w^4\sinh\left(\frac{11}{10}w\right) - 16w^4\sinh\left(\frac{4}{5}w\right) - 57w^4\sinh\left(\frac{3}{5}w\right) - 68w^4\sinh\left(\frac{2}{5}w\right)$$
$$+ 40w^4\sinh\left(\frac{1}{2}w\right) - 20w^4\sinh(w) - 24w^4\sinh\left(\frac{1}{5}w\right)\Bigg),$$

$$q_2 = -\Bigg(720 - 56w\sinh\left(\frac{9}{5}w\right) + 200w\sinh\left(\frac{7}{5}w\right) - 552w\sinh\left(\frac{1}{5}w\right)$$
$$- 92w^4\cosh\left(\frac{1}{5}w\right) + 240\cosh(2w) - 32w^4\cosh\left(\frac{4}{5}w\right) - 480w\sinh\left(\frac{2}{5}w\right)$$
$$- 360w\sinh\left(\frac{3}{5}w\right) + 360\cosh\left(\frac{9}{5}w\right) + 304w\sinh\left(\frac{6}{5}w\right) - 64w\sinh(2w)$$
$$+ 128w\sinh(w) - 192w\sinh\left(\frac{4}{5}w\right) - 60w^4\cosh\left(\frac{3}{5}w\right) + 80w\sinh\left(\frac{8}{5}w\right)$$
$$- 8w^4\cosh(w) - 48w^4 - 80w^4\cosh\left(\frac{2}{5}w\right) - 360\cosh\left(\frac{3}{5}w\right) - 360\cosh\left(\frac{6}{5}w\right)$$
$$+ 1080\cosh\left(\frac{1}{5}w\right) - 960\cosh(w) + 120\cosh\left(\frac{8}{5}w\right) - 1080\cosh\left(\frac{4}{5}w\right)$$
$$+ 360\cosh\left(\frac{2}{5}w\right) - 120\cosh\left(\frac{7}{5}w\right)\Bigg)$$
$$\Bigg/\Bigg(96w^4 + 184w^4\cosh\left(\frac{1}{5}w\right) + 120w^4\cosh\left(\frac{3}{5}w\right) + 160w^4\cosh\left(\frac{2}{5}w\right)$$
$$- 210w^4\cosh\left(\frac{1}{10}w\right) - 186w^4\cosh\left(\frac{3}{10}w\right) - 25w^4\cosh\left(\frac{11}{10}w\right)$$
$$+ 6w^4\cosh\left(\frac{3}{2}w\right) - w^4\cosh\left(\frac{13}{10}w\right) - 45w^4\cosh\left(\frac{9}{10}w\right) - 61w^4\cosh\left(\frac{7}{10}w\right)$$
$$- 118w^4\cosh\left(\frac{1}{2}w\right) + 64w^4\cosh\left(\frac{4}{5}w\right) + 16w^4\cosh(w)\Bigg),$$

$$q_3 = -\Bigg(150w\cosh\left(\frac{11}{5}w\right) + 50w\cosh\left(\frac{12}{5}w\right) + 175w^4\sinh\left(\frac{4}{5}w\right) + 250w\cosh(2w)$$
$$- 2800w\cosh\left(\frac{13}{10}w\right) - 400w\cosh\left(\frac{19}{10}w\right) + 75w^4\sinh\left(\frac{6}{5}w\right)$$
$$+ 25w^4\sinh\left(\frac{7}{5}w\right) - 1200w\cosh\left(\frac{17}{10}w\right) + 125w^4\sinh(w) - 2000w\cosh\left(\frac{3}{2}w\right)$$
$$+ 350w\cosh\left(\frac{9}{5}w\right) - 2100\sinh\left(\frac{9}{5}w\right) + 8400\sinh\left(\frac{13}{10}w\right) - 300\sinh\left(\frac{12}{5}w\right)$$

$$- 900\sinh\left(\frac{11}{5}w\right) - 1500\sinh(2w) + 3600\sinh\left(\frac{17}{10}w\right) + 1200\sinh\left(\frac{19}{10}w\right)$$
$$+ 5750w - 14800w\cosh\left(\frac{1}{10}w\right) + 10400w\cosh\left(\frac{3}{5}w\right) - 12400w\cosh\left(\frac{3}{10}w\right)$$
$$+ 3800w\cosh\left(\frac{6}{5}w\right) + 11500w\cosh\left(\frac{1}{5}w\right) - 7600w\cosh\left(\frac{7}{10}w\right)$$
$$+ 100w^4\sinh\left(\frac{1}{5}w\right) - 6000\sinh\left(\frac{1}{5}w\right) + 225w^4\sinh\left(\frac{3}{5}w\right) + 6000w\cosh(w)$$
$$- 13800\sinh\left(\frac{3}{5}w\right) + 450w\cosh\left(\frac{8}{5}w\right) + 8200w\cosh\left(\frac{4}{5}w\right)$$
$$+ 11500w\cosh\left(\frac{2}{5}w\right) + 200w^4\sinh\left(\frac{2}{5}w\right) - 12000\sinh\left(\frac{2}{5}w\right)$$
$$- 10000w\cosh\left(\frac{1}{2}w\right) + 1600w\cosh\left(\frac{7}{5}w\right) - 5200w\cosh\left(\frac{9}{10}w\right)$$
$$- 3600w\cosh\left(\frac{11}{10}w\right) - 4200\sinh\left(\frac{7}{5}w\right) - 6600\sinh\left(\frac{6}{5}w\right) - 2700\sinh\left(\frac{8}{5}w\right)$$
$$+ 10800\sinh\left(\frac{11}{10}w\right) + 8400\sinh\left(\frac{7}{10}w\right) + 10800\sinh\left(\frac{9}{10}w\right)$$
$$+ 1200\sinh\left(\frac{1}{10}w\right) - 11400\sinh\left(\frac{4}{5}w\right) + 6000\sinh\left(\frac{1}{2}w\right) + 3600\sinh\left(\frac{3}{10}w\right)$$
$$- 9000\sinh(w) + 6000\sinh\left(\frac{3}{2}w\right)\Bigg)$$
$$\Bigg/\Bigg(48w^4\sinh\left(\frac{3}{10}w\right) + 112w^4\sinh\left(\frac{7}{10}w\right) + 16w^4\sinh\left(\frac{1}{10}w\right)$$
$$+ 96w^4\sinh\left(\frac{9}{10}w\right) - 48w^4\sinh\left(\frac{6}{5}w\right) - 14w^4\sinh\left(\frac{7}{5}w\right) + 12w^4\sinh\left(\frac{8}{5}w\right)$$
$$+ 32w^4\sinh\left(\frac{11}{10}w\right) - 32w^4\sinh\left(\frac{4}{5}w\right) - 114w^4\sinh\left(\frac{3}{5}w\right) - 136w^4\sinh\left(\frac{2}{5}w\right)$$
$$+ 80w^4\sinh\left(\frac{1}{2}w\right) - 40w^4\sinh(w) - 48w^4\sinh\left(\frac{1}{5}w\right)\Bigg). \qquad (65)$$

Appendix B

Case I.

$$q_0 = \frac{379}{30240} - \frac{139}{2032128}w^2 + \frac{220579}{1877686272000}w^4 + \frac{128267173}{136695560601600000}w^6$$
$$- \frac{256860666221}{344472812716032000000000}w^8 + \frac{140823496782299}{98381435311698739200000000000}w^{10}$$

$$+\frac{595569598884963343}{523389235858237292544000000000000}w^{12}+\cdots,$$

$$q_1=\frac{36}{35}+\frac{139}{14112}w^2-\frac{220579}{13039488000}w^4-\frac{128267173}{949274726400000}w^6+\frac{256860666221}{23921723105280000000}w^8-\frac{140823496782299}{683204411886796800000000}w^{10}-\frac{595569598884963343}{363464747123775897600000000000000}w^{12}+\cdots,$$

$$q_2=\frac{2264}{6615}+\frac{139}{111132}w^2-\frac{220579}{102685968000}w^4-\frac{128267173}{7475538470400000}w^6+\frac{256860666221}{188383569454080000000}w^8-\frac{140823496782299}{5380234743608524800000000}w^{10}-\frac{595569598884963343}{2862228488359973519360000000000000}w^{12}+\cdots,$$

$$q_3=-\frac{15625}{42336}-\frac{86875}{14224896}w^2+\frac{1102895}{105150431232}w^4+\frac{128267173}{1530990278737920}w^6-\frac{256860666221}{38580955024195584000}w^8+\frac{140823496782299}{1101872075491025879040000}w^{10}+\frac{595569598884963343}{586195944161225767649280000000000}w^{12}+\cdots. \qquad (66)$$

Case II.

$$q_0=\frac{379}{30240}-\frac{139}{1016064}w^2+\frac{594701}{469421568000}w^4-\frac{1348906997}{128152088064000000}w^6+\frac{175266371597}{21529555079475200000000}w^8-\frac{460792156268131}{76860496337264640000000000}w^{10}+\frac{58106196692431471}{13629928017141596160000000000000}w^{12}+\cdots,$$

$$q_1=\frac{36}{35}+\frac{139}{7056}w^2+\frac{158533}{1086624000}w^4+\frac{115090849}{296648352000000}w^6+\frac{2034470273}{1359188812800000000}w^8-\frac{13795332311}{7321720806400000000000}w^{10}+\frac{7790255724625687}{2839568336904499200000000000000}w^{12}+\cdots,$$

$$q_2=\frac{2264}{6615}+\frac{139}{55566}w^2+\frac{26003}{3208936500}w^4+\frac{1192362319}{14016634632000000}w^6-\frac{27032213147}{117739730908800000000}w^8+\frac{215310882251987}{840661678688832000000000000}w^{10}-\frac{77648057049083}{460115239776192000000000000}w^{12}+\cdots,$$

$$q_3=-\frac{15625}{42336}-\frac{86875}{7112448}w^2-\frac{2163935}{26287607808}w^4-\frac{15416717}{57412135452672}w^6$$

$$
\begin{aligned}
&- \frac{14473351219}{24113096890122240000} w^8 - \frac{135033244403}{13243654753497907200000} w^{10} \\
&- \frac{168633964182961}{15265519379198587699200000000} w^{12} + \cdots .
\end{aligned} \tag{67}
$$

Case III.

$$
\begin{aligned}
q_0 = {} & \frac{379}{30240} - \frac{139}{677376} w^2 + \frac{86329}{25035816960} w^4 - \frac{119917785763}{2050433409024000000} w^6 \\
& + \frac{1273995009769}{1275825232281600000000} w^8 - \frac{280861831255173989}{1639690588528312320000000000} w^{10} \\
& + \frac{1542231819234872079647}{52338923585823729254400000000000} w^{12} + \cdots , \\
q_1 = {} & \frac{36}{35} + \frac{139}{4704} w^2 + \frac{84919}{173859840} w^4 + \frac{2258239369}{527374848000000} w^6 \\
& + \frac{2178255629279}{7973907701760000000} w^8 + \frac{810914534325599}{10351581998284800000000000} w^{10} \\
& + \frac{196746783118603001}{23755865825083392000000000000} w^{12} + \cdots , \\
q_2 = {} & \frac{2264}{6615} + \frac{139}{37044} w^2 + \frac{42107}{1369146240} w^4 + \frac{2660818663}{112133077056000000} w^6 \\
& + \frac{291611764993}{20931507717120000000} w^8 - \frac{17694431599745311}{8967057906014208000000000} w^{10} \\
& + \frac{9043817728667197223}{2602077166908850176000000000000} w^{12} + \cdots , \\
q_3 = {} & -\frac{15625}{42336} - \frac{86875}{4741632} w^2 - \frac{9758635}{35050143744} w^4 - \frac{9674010119}{4592970836213760} w^6 \\
& - \frac{52926418073}{3297517523435520000} w^8 - \frac{7702985156291}{33390062893667450880000} w^{10} \\
& - \frac{61921369658318772577}{5861959441612257676492800000000} w^{12} + \cdots .
\end{aligned} \tag{68}
$$

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