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An accurate eighth order exponentially-fitted method for the efficient solution of the Schrödinger equation

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Abstract

An accurate eighth algebraic order exponentially-fitted method is developed for the numerical solution of radial Schrödinger equation and of the coupled differential equations of the Schrödinger type. The free parameters of the new scheme are defined in order to integrate exactly exponential functions. Numerical and theoretical results indicate that the new method is much more efficient than other classical and exponentially fitted methods. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

There is a great activity in last decade for the numerical solution of the radial Schrödinger equation and coupled differential equations of the Schrödinger type. The aim of this activity is the construction of an efficient and reliable algorithm that approximates the solution (see [1] and references therein).

The radial Schrödinger equation can be written as

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

Differential equations of the above type occur very frequently in many problems in theoretical physics and chemistry, in chemical physics, in physical chemistry, in astrophysics, in electronics and elsewhere (see, for example, [2]). For the above reason it is needed the construction of an efficient and reliable numerical method. In (1) the function

$$W(r) = l(l+1)/r^2 + V(r)$$

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denotes *the effective potential*, which satisfies $W(r) \to 0$ as $r \to \infty$, 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 r, determined by physical considerations.

An explanation about the not efficiency of boundary and initial value methods is given in [3].

One of the most popular and well known methods for the numerical solution of (1) is **Numerov's method**. The reason is given in [3]. In [4,5] high order numerical methods for the eigenvalue problem of the radial Schrödinger equation are developed for some special potentials $V(x)$ which are even functions.

In [6] the Runge–Kutta type or hybrid methods, which are an alternative approach for deriving higher order methods, are introduced.

In [7] (and references therein) another approach for developing efficient methods for the numerical solution of (1), which is the exponential fitting (see [7] and references therein), is introduced. This approach is appropriate because for large values of r and positive k^2 the solution of (1) is *periodic*. Many authors have investigated the idea of exponential fitting, since Raptis and Allison [8]. Ixaru and Rizea [7] have produced a method which integrates 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. For the method obtained by Ixaru and Rizea [7] we have $m = 1$ and $p = 1$. Raptis [9] develop an exponentially-fitted method with $m = 2$ and $p = 0$. Simos [10] 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 [11,12]. For this method we have $m = 3$ and $p = 0$. Simos [13] 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 [14] 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 [15]. The method of Cash, Raptis and Simos [16] is also based on the formula proposed in [15] and is fitted to (3) with $m = 1$ and $p = 3$. All the above methods are of algebraic order four and six.

The purpose of this paper is to derive an eighth algebraic order method fitted to (3) and in particular to derive an exponentially-fitted method with $m = 4$ and $p = 0$. Based on the new developed method and the sixth-order exponentially-fitted method of Simos [17] a variable-step procedure is introduced. We have applied the new methods to the solution of coupled differential equations arising from the Schrödinger equation. The results indicate that the approach is more efficient than the well known iterative Numerov method of Allison [18], the exponentially-fitted variable-step method of Raptis and Cash [14] and the classical (with constant coefficients) variable-step method of Simos [19].

2. Exponential multistep methods

For the numerical solution of the initial value problem

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

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.

The method (5) is associated with the operator

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

where z is a continuously differentiable function.

Definition 1. The multistep method (5) called algebraic (or exponential) of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p+r-1}$ (or $\exp(v_0x), \exp(v_1x), \ldots, \exp(v_{p+r-1}x)$ where $v_i,\ i=0,1,\ldots,p+r-1$ are real or complex numbers).

Remark 1 (see [20]). 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

$$\left\{\exp(vx), x\exp(vx), x^2\exp(vx), \ldots, x^n\exp(vx), \exp(v_{n+1}x), \ldots, \exp(v_{p+r-1}x)\right\}. \tag{7}$$

Remark 2 (see [20]). 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 [20] and [21]). *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*

$$L\left[x^m\exp(vx)\right]=0,\quad m=0,1,\ldots,n-1,\qquad L\left[x^n\exp(vx)\right]\neq 0 \tag{8}$$

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 [22] and [23]). *Consider an operator L with*

$$L\left[\exp(\pm v_i x)\right]=0,\quad j=0,1,\ldots,k\leqslant\frac{p+r-1}{2} \tag{9}$$

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 new exponentially-fitted method

Consider the following method:

$$y_{n+1}+q_1y_n+y_{n-1}=h^2\left[t_0(f_{n+1}+f_{n-1})+t_1f_n+t_2(f_{n+s}+f_{n-s})+t_3(f_{n+q}+f_{n-q})\right]. \tag{10}$$

This method for appropriate values of $t_i,\ i=0(1)3$, for $s=\sqrt{21}/3$ and arbitrary values of q is of algebraic order eight (see for details [19]).

We require that the methods (10) should integrate exactly any linear combination of the functions:

$$\left\{\exp(\pm vx), x\exp(\pm vx), x^2\exp(\pm vx), x^3\exp(\pm vx), x^4\exp(\pm vx)\right\}. \tag{11}$$

To construct a method of the form (10) which integrates exactly the functions (11), we require that the method (10) integrates exactly (see [22] and [23]):

$$\left\{\exp(\pm v_0x), \exp(\pm v_1x), \exp(\pm v_2x), \exp(\pm v_3x), \exp(\pm v_4x)\right\} \tag{12}$$

and then put:

$$v_0 = v_1 = v_2 = v_3 = v_4 = v. \tag{13}$$

Demanding that (10) integrates (12) exactly, we obtain the following system of equations for q_1 and for $t_i,\ i = 0(1)3$

$$2t_2 w_j^2 \cosh(w_j s) + 2\cosh(w_j) t_0 w_j^2 - q_1 + t_1 w_j^2 + 2t_3 w_j^2 \cosh(w_j q) = 2\cosh(w_j) \tag{14}$$

where $w_j = v_j h,\ j = 0(1)4$.

Solving for q_1 and for $t_i,\ i = 0(1)3$ and putting $s = \sqrt{21}/3$ and $q = \frac{1}{2}$, we obtain the coefficients which are given in the Appendix A.

The above formulae for q_1 and $t_i,\ i = 0(1)3$ are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use the series expansions for the coefficients q_1 and $t_i,\ i = 0(1)3$ of the method given in the Appendix B.

We now seek computable approximations to $y_{n\pm s}$ and $y_{n\pm q}$. For these approximations we still require to be exact to any linear combination of the functions of the form

$$\bigl\{\exp(\pm vx), x\exp(\pm vx), \ldots, x^m \exp(\pm vx)\bigr\}. \tag{15}$$

Following [19] we look for approximations of the form

$$y_{n+s} + y_{n-s} = a_0(y_{n+1} + y_{n-1}) + a_1 y_n + h^2\bigl[a_2(f_{n+1} + f_{n-1}) + a_3 f_n\bigr], \tag{16}$$

$$y_{n+s} - y_{n-s} = b_0(y_{n+1} - y_{n-1}) + h^2 b_1(f_{n+1} - f_{n-1}) \tag{17}$$

and of the form

$$y_{n+q} + y_{n-q} = c_0(y_{n+1} + y_{n-1}) + c_1 y_n + h^2\bigl[c_2(f_{n+1} + f_{n-1}) + c_3 f_n + c_4(f_{n+s} + f_{n-s})\bigr], \tag{18}$$

$$y_{n+q} - y_{n-q} = d_0(y_{n+1} - y_{n-1}) + h^2\bigl[d_1(f_{n+1} - f_{n-1}) + d_2(f_{n+s} - f_{n-s})\bigr]. \tag{19}$$

We require that the method (16) should integrate exactly any linear combination of the functions (15) (for $m = 3$). We also require that the method (17) should integrate exactly any linear combination of the functions (15) (for $m = 1$).

To construct a method of the form (16) which integrates exactly the functions (15) (with $m = 3$), we require (see [22] and [23]) that the method (16) integrates exactly

$$\bigl\{\exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x), \exp(\pm v_3 x)\bigr\} \tag{20}$$

and then put

$$v_0 = v_1 = v_2 = v_3 = v. \tag{21}$$

To construct a method of the form (17) which integrates exactly the functions (15) (with $m = 1$), we require that the method (17) integrates exactly (see [22] and [23]):

$$\bigl\{\exp(\pm v_0 x), \exp(\pm v_1 x)\bigr\} \tag{22}$$

and then put:

$$v_0 = v_1 = v. \tag{23}$$

Demanding that (16) integrates (20) exactly, we obtain the following system of equations for $a_i,\ i = 0(1)3$. Demanding, also, that (17) integrates (22) exactly, we obtain the following system of equations for $b_i,\ i = 0, 1$.

$$2a_0 \cosh(w_j) + 2a_2 w_j^2 \cosh(w_j) + a_1 + a_3 w_j^2 = 2\cosh(w_j s), \tag{24}$$

$$2b_0 \sinh(w_j) + 2b_1 w_j^2 \sinh(w_j) = 2\sinh(w_j s) \tag{25}$$

where $w_j = v_j h$, $j = 0, 1, 2, 3$ for (24) and $j = 0, 1$ for (25).

Solving for $a_i,\ i = 0(1)3$ and for $b_i,\ i = 0, 1$ and putting $s = \sqrt{21}/3$ and $q = \frac{1}{2}$, we obtain the coefficients which are given in the Appendix C.

The above formulae for a_1 and b_1 are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use the series expansions for the coefficient $a_i,\ i = 0(1)3$ and $b_i,\ i = 0, 1$ of the method given in the Appendix D.

Following the same procedure as above, we require that the method (18) should integrate exactly any linear combination of the functions (15) (for $m = 4$). We also require that the method (19) should integrate exactly any linear combination of the functions (15) (for $m = 2$).

To construct a method of the form (18) which integrates exactly the functions (15) (with $m = 4$), we require that the method (17) integrates exactly (12) (see [22] and [23]) and then put (13).

To construct a method of the form (19) which integrates exactly the functions (15) (with $m = 2$), we require that the method (19) integrates exactly (see [22] and [23]):

$$\{\exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x)\} \tag{26}$$

and then put:

$$v_0 = v_1 = v_2 = v. \tag{27}$$

Demanding that (18) integrates (12) exactly, we obtain the following system of equations for $c_i,\ i = 0(1)4$. Demanding, also, that (19) integrates (26) exactly, we obtain the following system of equations for $d_i,\ i = 0(1)2$.

$$2c_4 w^2 \cosh(w\,s) + 2c_2\, w^2 \cosh(w) + 2c_0 \cosh(w) + c_3 w^2 + c_1 = 2\cosh(w\,q), \tag{28}$$

$$2d_2 w^2 \sinh(w\,s) + 2d_0 \sinh(w) + 2d_1 w^2 \sinh(w) = 2\sinh(w\,q). \tag{29}$$

Solving for $c_i,\ i = 0(1)4$ and for $d_i,\ i = 0(1)2$ and putting $s = \sqrt{21}/3$ and $q = \frac{1}{2}$, we obtain the coefficients which are given in the Appendix E.

The above formulae for $c_i,\ i = 0(1)4$ and $d_i,\ i = 0(1)2$ are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use the series expansions for these coefficients of the method which are given in the Appendix F. Since the Taylor series expansions are very accurate (we have given series expansions of 14th order), one can use them in all cases. Finally, in the Appendix G a description of the computer algebra program, which is used for the derivation of the coefficients presented in Appendices A–F, is presented.

It is easy for one to see that the approximations of $y_{n\pm s}$ and $y_{n\pm q}$ are given by

$$\begin{aligned}
\overline{y}_{n+s} &= \tfrac{1}{2}(a_0 + b_0) y_{n+1} + \tfrac{1}{2} a_1 y_n + \tfrac{1}{2}(a_0 - b_0) y_{n-1} \\
&\quad + h^2\big(\tfrac{1}{2}(a_2 + b_1) y''_{n+1} + \tfrac{1}{2} a_3 y''_n + \tfrac{1}{2}(a_2 - b_1) y''_{n-1}\big), \\
\overline{y}_{n-s} &= \tfrac{1}{2}(a_0 - b_0) y_{n+1} + \tfrac{1}{2} a_1 y_n + \tfrac{1}{2}(a_0 + b_0) y_{n-1} \\
&\quad + h^2\big(\tfrac{1}{2}(a_2 - b_1) y''_{n+1} + \tfrac{1}{2} a_3 y''_n + \tfrac{1}{2}(a_2 + b_1) y''_{n-1}\big), \\
\overline{y}_{n+q} &= \tfrac{1}{2}(c_0 + d_0) y_{n+1} + \tfrac{1}{2} c_1 y_n + \tfrac{1}{2}(c_0 - d_0) y_{n-1} \\
&\quad + h^2\big(\tfrac{1}{2}(c_2 + d_1) y''_{n+1} + \tfrac{1}{2} c_3 y''_n + \tfrac{1}{2}(c_2 - d_1) y''_{n-1}\big), \\
&\quad + h^2\big(\tfrac{1}{2}(c_4 + d_2) \overline{y}''_{n+s} + \tfrac{1}{2}(c_4 - d_2) \overline{y}''_{n-s}\big), \\
\overline{y}_{n-q} &= \tfrac{1}{2}(c_0 - d_0) y_{n+1} + \tfrac{1}{2} c_1 y_n + \tfrac{1}{2}(c_0 + d_0) y_{n-1} \\
&\quad + h^2\big(\tfrac{1}{2}(c_2 - d_1) y''_{n+1} + \tfrac{1}{2} c_3 y''_n + \tfrac{1}{2}(c_2 + d_1) y''_{n-1}\big), \\
&\quad + h^2\big(\tfrac{1}{2}(c_4 - d_2) \overline{y}''_{n+s} + \tfrac{1}{2}(c_4 + d_2) \overline{y}''_{n-s}\big).
\end{aligned} \tag{30}$$

If $w = i\phi$, then the method (10), (30) with coefficients given by (58), (61) and (63) is exact for any linear combination of the functions:

$$\begin{aligned}
&\{\sin(\phi x), \cos(\phi x), x\sin(\phi x), x\cos(\phi x), x^2\sin(\phi x), x^2\cos(\phi x), \\
&\quad x^3\sin(\phi x), x^3\cos(\phi x), x^4\sin(\phi x), x^4\cos(\phi x)\}.
\end{aligned} \tag{31}$$

4. Error analysis

In this section we will examine theoretically the method developed in [19], the exponentially-fitted method developed in [24] and the new exponentially-fitted method. We will also find a quantitative estimation for the extend of the accuracy gain to be expected from the exponentially-fitted versions.

Definition 2. A method is called classical if it has constant coefficients.

Remark 3. An exponentially-fitted method is not a classical one because it has coefficients which are depended from the quantity vh, where v is the frequency of the problem and h is the step length.

We first write $f(x)$ of (1) in the form

$$f(x)=g(x)+d, \tag{32}$$

where $g(x)=U(x)-U_{\mathrm{c}}=g$, where U_{c} is the constant approximation of the potential and $d=w^2=U_{\mathrm{c}}-k^2$. So, $g(x)$ depends on the potential and its constant approximation and d shows the energy dependence.

The local truncation error of the method developed in [19] (with $s=\sqrt{21}/3$ and arbitrary q) is given by

$$L.T.E._{\text{clas.}}=\frac{h^{10}}{152409600(7-3q^2)}\left[3y_n^{(10)}T_1+56y_n^{(8)}F_n(13-42q^2)\right]+O(h^{12}), \tag{33}$$

where $T_1=765q^4-2007q^2+518$.

The local truncation error of the exponentially-fitted method developed in [24] is given by (with $s=\sqrt{21}/3$ and arbitrary q)

$$\begin{aligned}L.T.E._{\text{exp.[24]}}={}&\frac{h^{10}}{152409600(7-3q^2)}\\&\times\left[3(y_n^{(10)}-dy_n^{(8)})T_1+56(y_n^{(8)}-dy_n^{(6)})F_n(13-42q^2)\right]+O(h^{12}).\end{aligned} \tag{34}$$

The local truncation error of the exponentially- fitted method developed in this paper is given by (with $s=\sqrt{21}/3$ and arbitrary q)

$$\begin{aligned}L.T.E._{\text{new}}={}&h^{10}\biggl(\frac{41}{203212800}y_n^{(10)}-\frac{41}{40642560}dy_n^{(8)}-\frac{41}{203212800}y_nd^5\\&-\frac{41}{20321280}d^3y_n^{(4)}+\frac{41}{20321280}d^2y_n^{(6)}+\frac{41}{40642560}d^4y_n^{(2)}\biggr)+O(h^{12}).\end{aligned} \tag{35}$$

We express, now, the derivatives $y''(x)$, $y^{(4)}$, $y^{(6)}$, $y^{(8)}$ and $y^{(10)}$ in terms of Eq. (1), i.e.

$$\begin{aligned}y''={}&f(x)y(x),\\y^{(4)}={}&\left(\frac{\partial^2}{\partial x^2}U(x)\right)y(x)+2\left(\frac{\partial}{\partial x}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)+y(x)U(x)^2-2y(x)U(x)U_{\mathrm{c}}\\&+2y(x)U(x)d+y(x)U_{\mathrm{c}}^2-2y(x)U_{\mathrm{c}}d+y(x)d^2,\end{aligned} \tag{36}$$

etc. We note that $g^{(n)}(x)=U^{(n)}(x)$ for nth order derivative with respect to x. We also express the terms as polynomials of d.

If we introduce, now, these expressions to the local truncation error formulae (33) and (34), then we obtain the following expressions (as polynomials of d) for the local truncation error. We note that in the following expressions $q=\frac{1}{2}$.

Classical method [19].

$$L.T.E._{\text{clas.}} = h^{10}\left(d^5 \frac{41}{203212800}\,\mathrm{y}(x) + d^4 T_2 + \cdots\right) + O(h^{12}), \tag{37}$$

where

$$T_2 = -\frac{1}{3048192000}\bigl(-448y(x) - 3075y(x)U(x) + 3075y(x)U_{\mathrm{c}}\bigr).$$

Exponentially-fitted method [24].

$$L.T.E._{\text{exp.[24]}} = h^{10}\left(d^4\left(-\frac{1}{3048192000}(-615y(x)U(x) + 615y(x)U_{\mathrm{c}})\right) + \cdots\right) + O(h^{12}). \tag{38}$$

New exponentially-fitted method.

$$\begin{aligned}
L.T.E._{\text{new}} = h^{10}\Biggl[d\Biggl(&\frac{41}{5080320}\left(\frac{\partial^3}{\partial x^3}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)U(x) - \frac{41}{5080320}\left(\frac{\partial^3}{\partial x^3}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)Uc \\
&+ \frac{41}{5080320}X_1 y(x)U(x)^2 - \frac{41}{2540160}X_1 U(x)y(x)Uc + \frac{41}{5080320}X_1 y(x)Uc^2 \\
&+ \frac{41}{2540160}\left(\frac{\partial}{\partial x}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)X_1 + \frac{41}{3386880}\left(\frac{\partial}{\partial x}U(x)\right)^2 y(x)U(x) \\
&- \frac{41}{3386880}\left(\frac{\partial}{\partial x}U(x)\right)^2 y(x)Uc + \frac{533}{12700800}\left(\frac{\partial}{\partial x}U(x)\right)y(x)\left(\frac{\partial^3}{\partial x^3}U(x)\right) \\
&+ \frac{943}{50803200}\left(\frac{\partial^4}{\partial x^4}U(x)\right)y(x)U(x) \\
&- \frac{943}{50803200}\left(\frac{\partial^4}{\partial x^4}U(x)\right)y(x)Uc + \frac{697}{25401600}X_1^2 y(x) \\
&+ \frac{41}{8467200}\left(\frac{\partial^6}{\partial x^6}U(x)\right)y(x) + \frac{41}{6350400}\left(\frac{\partial^5}{\partial x^5}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)\Biggr) + \cdots\Biggr],
\end{aligned} \tag{39}$$

$$X_1 = \frac{\partial^2}{\partial x^2}U(x).$$

From the relations (37) and (38) we obtain the asymptotic expansions of the errors (in the case where $d \gg 0$ or $d \ll 0$).

Classical method [19].

$$L.T.E._{\text{clas.}} = h^{10} d^5 \frac{41}{203212800}y(x). \tag{40}$$

Exponentially-fitted method [24].

$$L.T.E._{\text{exp.[24]}} = h^{10}\left(d^4\left(-\frac{1}{3048192000}\bigl(-615y(x)U(x) + 615y(x)U_{\mathrm{c}}\bigr)\right)\right). \tag{41}$$

New exponentially-fitted method.

$$L.T.E._{\text{new}} = h^{10}\Biggl[d\Biggl(\frac{41}{5080320}\left(\frac{\partial^3}{\partial x^3}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)U(x) - \frac{41}{5080320}\left(\frac{\partial^3}{\partial x^3}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)Uc$$

$$
\begin{aligned}
&+\frac{41}{5080320}X_1 y(x)U(x)^2-\frac{41}{2540160}X_1 U(x)y(x)Uc+\frac{41}{5080320}X_1 y(x)Uc^2\\
&+\frac{41}{2540160}\left(\frac{\partial}{\partial x}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)X_1+\frac{41}{3386880}\left(\frac{\partial}{\partial x}U(x)\right)^2 y(x)U(x)\\
&-\frac{41}{3386880}\left(\frac{\partial}{\partial x}U(x)\right)^2 y(x)Uc+\frac{533}{12700800}\left(\frac{\partial}{\partial x}U(x)\right)y(x)\left(\frac{\partial^3}{\partial x^3}U(x)\right)\\
&+\frac{943}{50803200}\left(\frac{\partial^4}{\partial x^4}U(x)\right)y(x)U(x)\\
&-\frac{943}{50803200}\left(\frac{\partial^4}{\partial x^4}U(x)\right)y(x)Uc+\frac{697}{25401600}X_1^2 y(x)\\
&+\frac{41}{8467200}\left(\frac{\partial^6}{\partial x^6}U(x)\right)y(x)+\frac{41}{6350400}\left(\frac{\partial^5}{\partial x^5}U(x)\right)\left(\frac{\partial}{\partial x}y(x)\right)\Bigg)\Bigg], \qquad (42)
\end{aligned}
$$

$$X_1=\frac{\partial^2}{\partial x^2}U(x).$$

From the above equations we have that in the classical eighth-order method developed in [19] the error increases as a fifth power of d. In the exponentially-fitted eighth-order method developed in [24] the error increases as a fourth power of d. In the exponentially-fitted eighth-order method developed in this paper the error increases as a first power of d. Based on the above analysis we have the following theorem

Theorem 1. *For the exponentially-fitted method developed in this paper and for problems of the form* (1) *with* $f(x)$ *given by* (32), *the error increases as a first power of* d, *while for the exponentially-fitted method developed in* [24] *the error increases as a fourth power of* d *and for the the eighth algebraic order method developed in* [19] *the error increases as a fifth power of* d. *So the new exponentially-fitted method is more accurate than the eighth-order exponentially-fitted method of* [24] *and the eighth-order method developed in* [19] *for the problems mentioned above especially for large values of* $|d|=|U_{\mathrm{c}}-E|$.

5. Numerical illustration

5.1. Error estimation

It is known from the literature (see, for example, [25] and references therein) that there are many methods for the estimation of the local truncation error (LTE) in the integration of systems of initial-value problems. We note that the LTE is based on the algebraic order of the method.

The local error estimation algorithm used in this paper is based on the fact that when we have a method with local error of higher order then the approximation of the solution for the problems which have a periodic or oscillating solution is better.

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

Definition 3. We define the *local error* estimate in the lower order solution y_{n+1}^{L} by the quantity

$$L.T.E.=\left|y_{n+1}^{\mathrm{H}}-y_{n+1}^{\mathrm{L}}\right|. \qquad (43)$$

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

We assume that the solution y_{n+1}^{H} is obtained using the exponentially-fitted method developed in this paper and the solution y_{n+1}^{L} is obtained using the exponentially-fitted method of Simos [17].

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

$$h_{n+1} = h_n \left(\frac{acc}{L.T.E.} \right)^{1/q}, \tag{44}$$

where q is the order of the local error.

Following [14], we have considered all step changes to halving and doubling. Thus, based on the procedure developed in [14], for the Local Truncation Error, the step control procedure which we use for the Local Error is

$$\begin{aligned}
&\text{If } L.T.E. < acc, && h_{n+1} = 2h_n,\\
&\text{If } 100\,acc > L.T.E. \geqslant acc, && h_{n+1} = h_n,\\
&\text{If } L.T.E. \geqslant 100\,acc, && h_{n+1} = \frac{h_n}{2} \text{ and repeat the step.}
\end{aligned} \tag{45}$$

It is known that the local error estimate is obtained to the lower order solution. This is applied, also, in our case of the local error estimate, i.e. the local error estimate is obtained for y_{n+1}^{L}. However, if this error estimate is acceptable, i.e. less than the bound acc, we consider the widely used local extrapolation technique. Thus, although we are controlling an estimation of the local error in the lower order solution y_{n+1}^{L}, we use the higher order solution y_{n+1}^{H} at each accepted step.

5.2. Coupled differential equations

There are many problems in theoretical physics, atomic physics, physical chemistry, quantum chemistry and chemical physics which can be transformed to the solution of coupled differential equations of the Schrödinger type.

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

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{46}$$

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

We have investigated the case in which all channels are open. So we have the following boundary conditions (see for details [18]):

$$y_{ij} = 0 \quad \text{at } x = 0, \tag{47}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x), \tag{48}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. We note here that since the method presented in this paper have much larger intervals of periodicity (the property which must have a method to avoid instabilities) than the Numerov's method, the method of Cash and Raptis [15] and other finite difference methods, we can use the present methods to problems involve close channels.

Based on the detailed analysis developed in [18] and defining a matrix K' and diagonal matrices M, N by:

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

we find that the asymptotic condition (48) may be written as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}'. \tag{49}$$

One of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation is the Iterative Numerov method of Allison [18].

A real problem in theoretical physics, atomic physics, quantum chemistry and molecular physics which can be transformed to close-coupling differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [18], the entrance channel by the quantum numbers (j, l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we find that

$$\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right] y_{j'l'}^{Jjl}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l';\ J|V|j''l'';\ J\rangle y_{j''l''}^{Jjl}(x), \tag{50}$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}\right], \tag{51}$$

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 [18], the potential V may be written as

$$V(x, \hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \tag{52}$$

and the coupling matrix element is given by

$$\langle j'l';\ J|V|j''l'';\ J\rangle = \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x), \tag{53}$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [26] and $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i, $i = 0, 2$ are Legendre polynomials (see for details [26]). The boundary conditions may then be written as (see [18])

$$y_{j'l'}^{Jjl}(x) = 0 \quad \text{at } x = 0, \tag{54}$$

$$y_{j'l'}^{Jjl}(x) \sim \delta_{jj'}\delta_{ll'} \exp\left[-i\left(k_{jj}x - \tfrac{1}{2}l\pi\right)\right] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp\left[i\left(k_{j'j}x - \tfrac{1}{2}l'\pi\right)\right], \tag{55}$$

where the scattering S matrix is related to the K matrix of (48) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1}. \tag{56}$$

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

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

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

As is described in [18], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of **four, nine and sixteen coupled differential equations**, respectively. Following Bernstein [27] and Allison [18] the reduction of the interval $[0, \infty)$ to $[0, x_0]$ is obtained. The wavefunctions are then vanished in this region and consequently the boundary condition (54) may be written as

$$y_{j'l'}^{Jjl}(x_0) = 0. \tag{57}$$

Table 1
RTC (real time of computation (in seconds)) to calculate $|S|^2$ for the variable-step methods (1)–(4). $acc = 10^{-6}$. hmax is the maximum stepsize

Method	N	hmax	RTC
Iterative Numerov [18]	4	0.014	3.25
	9	0.014	23.51
	16	0.014	99.15
Variable-step method of Raptis and Cash [14]	4	0.056	1.55
	9	0.056	8.43
	16	0.056	43.32
Variable-step method of Simos [19]	4	0.056	1.05
	9	0.056	5.25
	16	0.056	27.15
Variable-step method of Simos [24]	4	0.448	0.37
	9	0.448	3.22
	16	0.448	14.22
Variable-step method of Simos [28]	4	0.448	0.35
	9	0.448	1.38
	16	0.448	6.51
New variable-step method	4	0.896	0.08
	9	0.896	0.54
	16	0.896	3.11

For the numerical solution of this problem we have used
(1) the well-known Iterative Numerov method of Allison [18],
(2) the variable-step method of Raptis and Cash [14],
(3) the variable-step method of Simos [19] and
(4) the variable-step exponentially-fitted method of Simos [24],
(5) the embedded variable-step method of Simos [28] and
(6) the new embedded variable-step exponentially-fitted method.

In Table 1 we present the real time of computation required by the methods mentioned above to calculate the square of the modulus of the **S** matrix for sets of 4, 9 and 16 coupled differential equations. In Table 1 N indicates the number of equations of the set of coupled differential equations.

All computations were carried out on an Pentium PC using double precision arithmetic of 16 digits accuracy.

6. Conclusions

In this paper an eighth algebraic order exponentially-fitted method is developed. Based on this method and on the sixth algebraic order exponentially-fitted method of Simos [17] a new variable-step method is obtained. The application of the new variable-step algorithm to the systems of 4, 9 and 16 coupled differential equations arising from the Schrödinger equation indicate that this new algorithm is much more computationally efficient than other known and efficient methods.

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References

[1] G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation, Comput. Math. Appl. 31 (1996) 85–102.
[2] L.D. Landau, F.M. Lifshitz, Quantum Mechanics, Pergamon, New York, 1965.
[3] T.E. Simos, Eighth-order method for accurate computations for the elastic scattering phase-shift problem, Int. J. Quant. Chem. 68 (1998) 191–200.
[4] V. Fack, G. Vanden Berghe, (Extended) Numerov method for computing eigenvalues of specific Schrödinger equations, J. Phys. A: Math. Gen. 20 (1987) 4153.
[5] V. Fack, G. Vanden Berghe, A finite difference approach for the calculation of perturbed oscillator energies, J. Phys. A: Math. Gen. 18 (1987) 3355.
[6] J.R. Cash, A.D. Raptis, A high order method for the numerical solution of the one-dimensional Schrödinger equation. Comput. Phys. Comm. 33 (1984) 299–304.
[7] R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor – corrector methods for the numerical integration of the radial Schrödinger equation, J. Comput. Appl. Math. 87 (1997) 215–226.
[8] A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation, Comput. Phys. Comm. 14 (1978) 1–5.
[9] A.D. Raptis, Two-step methods for the numerical solution of the Schrödinger equation, Computing 28 (1982) 373–378.
[10] T.E. Simos, A four-step method for the numerical solution of the Schrödinger equation, J. Comput. Appl. Math. 30 (1990) 251–255.
[11] A.D. Raptis, On the numerical solution of the Schrödinger equation, Comput. Phys. Commun. 24 (1981) 1–4.
[12] A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Schrödinger equation with automatic error control, Comput. Phys. Comm. 28 (1983) 427–431.
[13] T.E. Simos: Some new four-step exponential fitting methods for the numerical solution of the radial Schrödinger equation, IMA J. Numerical Anal. 11 (1991) 347–356.
[14] A.D. Raptis, J.R. Cash, Exponential and Bessel fitting methods for the numerical solution of the Schrödinger equation, Comput. Phys. Comm. 44 (1987) 95–103.
[15] J.R. Cash, A.D. Raptis, A high order method for the numerical solution of the one-dimensional Schrödinger equation, Comput. Phys. Comm. 33 (1984) 299–304.
[16] J.R. Cash, A.D. Raptis, T.E. Simos, A sixth order exponentially-fitted method for the numerical solution of the radial Schrödinger equation, J. Comput. Phys. 91 (1990) 413–423.
[17] T.E. Simos, Exponential fitted methods for the numerical solution of the Schrödinger equation, J. Comput. Math. 14 (1996) 120–134.
[18] A.C. Allison, The numerical solution of coupled differential equations arising from the Schrödinger equation, J. Comput. Phys. 6 (1970) 378–391.
[19] T.E. Simos, An eighth order method with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem, Internat. J. Modern Phys. C 7 (1996) 825–835.
[20] T. Lyche, Chebyshevian multistep methods for ordinary differential equations, Numer. Math. 10 (1972) 65–75.
[21] P. Henrici, Discrete Variable Methods in Ordinary Differential Equations, John Wiley and Sons, New York, 1962.
[22] A.D. Raptis, Exponential multistep methods for ordinary differential equations, Bull. Greek Math. Soc. 25 (1984) 113–126.
[23] T.E. Simos, Numerical solution of ordinary differential equations with periodical solution, Doctoral Dissertation, National Technical University of Athens, 1990.
[24] T.E. Simos, An eighth order exponentially-fitted method for the numerical solution of the Schrödinger equation, Internat. J. Modern Phys. C 9 (1998) 271–288.
[25] L.F. Shampine, H.A. Watts, S.M. Davenport, Solving non-stiff ordinary differential equations-the state of the art, SIAM Rev. 18 (1975) 376–411.
[26] R.B. Bernstein, A. Dalgarno, H. Massey, I.C. Percival, Thermal scattering of atoms by homonuclear diatomic molecules, Proc. Royal Soc. London Ser. A 274 (1963) 427–442.
[27] R.B. Bernstrein, Quantum mechanical (phase shift) analysis of differential elastic scattering of molecular beams, J. Chemical Phys. 33 (1960) 795–804.
[28] T.E. Simos, Eighth order methods for accurate computations for the Schrödinger equation, Comput. Phys. Comm. 105 (1997) 127–138.

Appendix A

$$
\begin{aligned}
q_1 = \big(&-486\, w^3 \sinh(\mathrm{T}_1) + 18000 \cosh(\mathrm{T}_3) + 1179\, w^2 \cosh(\mathrm{T}_6) + 3960\, w \sinh(\mathrm{T}_3) \\
&- 18000 \cosh(\mathrm{T}_4) - 6120 \cosh(\mathrm{T}_5) + 4572\, w \sinh(\mathrm{T}_5) - 1080 \sqrt{21} \cosh(\mathrm{T}_2) \\
&- 3321\, w^2 \cosh(\mathrm{T}_2) + 114\, w^3 \sinh(\mathrm{T}_6) - 11880 \cosh(\mathrm{T}_2) - 1179\, w^2 \cosh(\mathrm{T}_5) \\
&+ 3321\, w^2 \cosh(\mathrm{T}_1) + 1080 \sqrt{21} \cosh(\mathrm{T}_6) - 9828\, w \sinh(\mathrm{T}_1) + 4572\, w \sinh(\mathrm{T}_6) \\
&- 9828\, w \sinh(\mathrm{T}_2) + 300\, w^3 \sinh(\mathrm{T}_3) + 300\, w^3 \sinh(\mathrm{T}_4) + 1080 \sqrt{21} \cosh(\mathrm{T}_5) \\
&+ 114\, w^3 \sinh(\mathrm{T}_5) - 486\, w^3 \sinh(\mathrm{T}_2) + 4500\, w^2 \cosh(\mathrm{T}_3) - 4500\, w^2 \cosh(\mathrm{T}_4) \\
&+ 3960\, w \sinh(\mathrm{T}_4) - 1080 \sqrt{21} \cosh(\mathrm{T}_1) + 6120 \cosh(\mathrm{T}_6) + 11880 \cosh(\mathrm{T}_1) \\
&- 1548\, w \sqrt{21} \sinh(\mathrm{T}_2) - 960\, w \sqrt{21} \sinh(\mathrm{T}_3) - 711\, w^2 \sqrt{21} \cosh(\mathrm{T}_2) \\
&+ 450\, w^2 \sqrt{21} \cosh(\mathrm{T}_4) + 450\, w^2 \sqrt{21} \cosh(\mathrm{T}_3) + 1548\, w \sqrt{21} \sinh(\mathrm{T}_1) \\
&- 948\, w \sqrt{21} \sinh(\mathrm{T}_5) + 948\, w \sqrt{21} \sinh(\mathrm{T}_6) + 960\, w \sqrt{21} \sinh(\mathrm{T}_4) \\
&- 200\, w^3 \sqrt{21} \sinh(\mathrm{T}_4) + 200\, w^3 \sqrt{21} \sinh(\mathrm{T}_3) + 26\, w^3 \sqrt{21} \sinh(\mathrm{T}_6) \\
&- 126\, w^3 \sqrt{21} \sinh(\mathrm{T}_2) + 261\, w^2 \sqrt{21} \cosh(\mathrm{T}_5) + 126\, w^3 \sqrt{21} \sinh(\mathrm{T}_1) \\
&- 711\, w^2 \sqrt{21} \cosh(\mathrm{T}_1) + 261\, w^2 \sqrt{21} \cosh(\mathrm{T}_6) - 26\, w^3 \sqrt{21} \sinh(\mathrm{T}_5)\big) / \\
\big(&-63\, w^3 \sinh(\mathrm{T}_1) + 11880 \cosh(\mathrm{T}_3) + 324\, w \sinh(\mathrm{T}_3) - 11880 \cosh(\mathrm{T}_4) \\
&- 1080 \sqrt{21} \cosh(\mathrm{T}_2) + 1080 \sqrt{21} \cosh(\mathrm{T}_3) + 1080 \sqrt{21} \cosh(\mathrm{T}_4) + 414\, w^2 \cosh(\mathrm{T}_2) \\
&- 6120 \cosh(\mathrm{T}_2) - 414\, w^2 \cosh(\mathrm{T}_1) + 324\, w \sinh(\mathrm{T}_1) + 324\, w \sinh(\mathrm{T}_2) - 63\, w^3 \sinh(\mathrm{T}_3) \\
&- 63\, w^3 \sinh(\mathrm{T}_4) - 63\, w^3 \sinh(\mathrm{T}_2) - 486\, w^2 \cosh(\mathrm{T}_3) + 486\, w^2 \cosh(\mathrm{T}_4) \\
&+ 324\, w \sinh(\mathrm{T}_4) - 1080 \sqrt{21} \cosh(\mathrm{T}_1) + 6120 \cosh(\mathrm{T}_1) - 84\, w \sqrt{21} \sinh(\mathrm{T}_2) \\
&+ 684\, w \sqrt{21} \sinh(\mathrm{T}_3) + 126\, w^2 \sqrt{21} \cosh(\mathrm{T}_2) - 126\, w^2 \sqrt{21} \cosh(\mathrm{T}_4) \\
&- 126\, w^2 \sqrt{21} \cosh(\mathrm{T}_3) + 84\, w \sqrt{21} \sinh(\mathrm{T}_1) - 684\, w \sqrt{21} \sinh(\mathrm{T}_4) \\
&+ 33\, w^3 \sqrt{21} \sinh(\mathrm{T}_4) - 33\, w^3 \sqrt{21} \sinh(\mathrm{T}_3) - 17\, w^3 \sqrt{21} \sinh(\mathrm{T}_2) + 17\, w^3 \sqrt{21} \sinh(\mathrm{T}_1) \\
&+ 126\, w^2 \sqrt{21} \cosh(\mathrm{T}_1)\big), \\
\mathrm{T}_1 &= \tfrac{1}{6}\, w\, (9 + 2\sqrt{21}), \\
\mathrm{T}_2 &= \tfrac{1}{6}\, w\, (-9 + 2\sqrt{21}), \\
\mathrm{T}_3 &= \tfrac{1}{6}\, w\, (2\sqrt{21} - 3), \\
\mathrm{T}_4 &= \tfrac{1}{6}\, w\, (2\sqrt{21} + 3), \\
\mathrm{T}_5 &= \tfrac{1}{6}\, w\, (15 + 2\sqrt{21}), \\
\mathrm{T}_6 &= \tfrac{1}{6}\, w\, (-15 + 2\sqrt{21}), \\
t_0 = \big(&1062\, w^3 \sinh(\mathrm{T}_7) + 2592 \cosh(\mathrm{T}_9) - 4608\, w \sinh(\mathrm{T}_9) - 2592 \cosh(\mathrm{T}_{10}) \\
&+ 1728 \sqrt{21} \cosh(\mathrm{T}_8) - 1728 \sqrt{21} \cosh(\mathrm{T}_9) - 1728 \sqrt{21} \cosh(\mathrm{T}_{10}) + 5526\, w^2 \cosh(\mathrm{T}_8) \\
&+ 2592 \cosh(\mathrm{T}_8) - 5526\, w^2 \cosh(\mathrm{T}_7) + 9792\, w \sinh(\mathrm{T}_7) + 9792\, w \sinh(\mathrm{T}_8) \\
&- 6138\, w^3 \sinh(\mathrm{T}_9) - 6138\, w^3 \sinh(\mathrm{T}_{10}) + 1062\, w^3 \sinh(\mathrm{T}_8) - 8874\, w^2 \cosh(\mathrm{T}_9) \\
&+ 8874\, w^2 \cosh(\mathrm{T}_{10}) - 4608\, w \sinh(\mathrm{T}_{10}) + 1728 \sqrt{21} \cosh(\mathrm{T}_7) - 2592 \cosh(\mathrm{T}_7)
\end{aligned}
$$

$$
\begin{aligned}
&- 33\,w^5\sqrt{21}\sinh(\mathrm{T}_9) + 17\,w^5\sqrt{21}\sinh(\mathrm{T}_7) + 33\,w^5\sqrt{21}\sinh(\mathrm{T}_{10})\\
&- 284\,w^4\sqrt{21}\cosh(\mathrm{T}_{10}) - 284\,w^4\sqrt{21}\cosh(\mathrm{T}_9) - 16\,w^4\sqrt{21}\cosh(\mathrm{T}_8)\\
&- 16\,w^4\sqrt{21}\cosh(\mathrm{T}_7) - 17\,w^5\sqrt{21}\sinh(\mathrm{T}_8) - 1074\,w^4\cosh(\mathrm{T}_9) + 1074\,w^4\cosh(\mathrm{T}_{10})\\
&- 63\,w^5\sinh(\mathrm{T}_7) - 63\,w^5\sinh(\mathrm{T}_8) + 174\,w^4\cosh(\mathrm{T}_7) - 63\,w^5\sinh(\mathrm{T}_9) - 63\,w^5\sinh(\mathrm{T}_{10})\\
&- 174\,w^4\cosh(\mathrm{T}_8) + 1728\,w\sqrt{21}\sinh(\mathrm{T}_8) - 1728\,w\sqrt{21}\sinh(\mathrm{T}_9)\\
&+ 984\,w^2\sqrt{21}\cosh(\mathrm{T}_8) - 984\,w^2\sqrt{21}\cosh(\mathrm{T}_{10}) - 984\,w^2\sqrt{21}\cosh(\mathrm{T}_9)\\
&- 1728\,w\sqrt{21}\sinh(\mathrm{T}_7) + 1728\,w\sqrt{21}\sinh(\mathrm{T}_{10}) + 558\,w^3\sqrt{21}\sinh(\mathrm{T}_{10})\\
&- 558\,w^3\sqrt{21}\sinh(\mathrm{T}_9) + 258\,w^3\sqrt{21}\sinh(\mathrm{T}_8) - 258\,w^3\sqrt{21}\sinh(\mathrm{T}_7)\\
&+ 984\,w^2\sqrt{21}\cosh(\mathrm{T}_7)\big)/\big(w^4(-63\,w^3\sinh(\mathrm{T}_7) + 11880\cosh(\mathrm{T}_9) + 324\,w\sinh(\mathrm{T}_9)\\
&- 11880\cosh(\mathrm{T}_{10}) - 1080\sqrt{21}\cosh(\mathrm{T}_8) + 1080\sqrt{21}\cosh(\mathrm{T}_9) + 1080\sqrt{21}\cosh(\mathrm{T}_{10})\\
&+ 414\,w^2\cosh(\mathrm{T}_8) - 6120\cosh(\mathrm{T}_8) - 414\,w^2\cosh(\mathrm{T}_7) + 324\,w\sinh(\mathrm{T}_7)\\
&+ 324\,w\sinh(\mathrm{T}_8) - 63\,w^3\sinh(\mathrm{T}_9) - 63\,w^3\sinh(\mathrm{T}_{10}) - 63\,w^3\sinh(\mathrm{T}_8) - 486\,w^2\cosh(\mathrm{T}_9)\\
&+ 486\,w^2\cosh(\mathrm{T}_{10}) + 324\,w\sinh(\mathrm{T}_{10}) - 1080\sqrt{21}\cosh(\mathrm{T}_7) + 6120\cosh(\mathrm{T}_7)\\
&- 84\,w\sqrt{21}\sinh(\mathrm{T}_8) + 684\,w\sqrt{21}\sinh(\mathrm{T}_9) + 126\,w^2\sqrt{21}\cosh(\mathrm{T}_8)\\
&- 126\,w^2\sqrt{21}\cosh(\mathrm{T}_{10}) - 126\,w^2\sqrt{21}\cosh(\mathrm{T}_9) + 84\,w\sqrt{21}\sinh(\mathrm{T}_7)\\
&- 684\,w\sqrt{21}\sinh(\mathrm{T}_{10}) + 33\,w^3\sqrt{21}\sinh(\mathrm{T}_{10}) - 33\,w^3\sqrt{21}\sinh(\mathrm{T}_9) - 17\,w^3\sqrt{21}\sinh(\mathrm{T}_8)\\
&+ 17\,w^3\sqrt{21}\sinh(\mathrm{T}_7) + 126\,w^2\sqrt{21}\cosh(\mathrm{T}_7))\big),
\end{aligned}
$$

$$\mathrm{T}_7 = \tfrac{1}{6}\,w\,(9 + 2\sqrt{21}),$$

$$\mathrm{T}_8 = \tfrac{1}{6}\,w\,(-9 + 2\sqrt{21}),$$

$$\mathrm{T}_9 = \tfrac{1}{6}\,w\,(2\sqrt{21} - 3),$$

$$\mathrm{T}_{10} = \tfrac{1}{6}\,w\,(2\sqrt{21} + 3),$$

$$
\begin{aligned}
t_1 = -\big(&6894\,w^3\sinh(\mathrm{T}_{11}) - 43200\cosh(\mathrm{T}_{13}) + 38\,w^5\sqrt{21}\sinh(\mathrm{T}_{15})\\
&- 141\,w^4\sqrt{21}\cosh(\mathrm{T}_{15}) + 141\,w^4\sqrt{21}\cosh(\mathrm{T}_{16}) + 182\,w^5\sinh(\mathrm{T}_{16}) + 599\,w^4\cosh(\mathrm{T}_{16})\\
&+ 599\,w^4\cosh(\mathrm{T}_{15}) + 38\,w^5\sqrt{21}\sinh(\mathrm{T}_{16}) - 182\,w^5\sinh(\mathrm{T}_{15}) - 2454\,w^2\cosh(\mathrm{T}_{16})\\
&-8640\,w\sinh(\mathrm{T}_{13}) - 43200\cosh(\mathrm{T}_{14}) + 14688\cosh(\mathrm{T}_{15}) - 12096\,w\sinh(\mathrm{T}_{15})\\
&+ 2592\sqrt{21}\cosh(\mathrm{T}_{12}) + 11754\,w^2\cosh(\mathrm{T}_{12}) - 1806\,w^3\sinh(\mathrm{T}_{16}) + 28512\cosh(\mathrm{T}_{12})\\
&- 2454\,w^2\cosh(\mathrm{T}_{15}) + 11754\,w^2\cosh(\mathrm{T}_{11}) + 2592\sqrt{21}\cosh(\mathrm{T}_{16}) - 31104\,w\sinh(\mathrm{T}_{11})\\
&+ 12096\,w\sinh(\mathrm{T}_{16}) + 31104\,w\sinh(\mathrm{T}_{12}) - 13920\,w^3\sinh(\mathrm{T}_{13}) + 13920\,w^3\sinh(\mathrm{T}_{14})\\
&- 2592\sqrt{21}\cosh(\mathrm{T}_{15}) + 1806\,w^3\sinh(\mathrm{T}_{15}) - 6894\,w^3\sinh(\mathrm{T}_{12}) - 9300\,w^2\cosh(\mathrm{T}_{13})\\
&- 9300\,w^2\cosh(\mathrm{T}_{14}) + 8640\,w\sinh(\mathrm{T}_{14}) - 2592\sqrt{21}\cosh(\mathrm{T}_{11}) + 14688\cosh(\mathrm{T}_{16})\\
&+ 28512\cosh(\mathrm{T}_{11}) + 100\,w^5\sqrt{21}\sinh(\mathrm{T}_{13}) - 162\,w^5\sqrt{21}\sinh(\mathrm{T}_{11}) + 100\,w^5\sqrt{21}\sinh(\mathrm{T}_{14})\\
&- 1500\,w^4\sqrt{21}\cosh(\mathrm{T}_{14}) + 1500\,w^4\sqrt{21}\cosh(\mathrm{T}_{13}) - 1359\,w^4\sqrt{21}\cosh(\mathrm{T}_{12})\\
&+ 1359\,w^4\sqrt{21}\cosh(\mathrm{T}_{11}) - 162\,w^5\sqrt{21}\sinh(\mathrm{T}_{12}) - 1850\,w^4\cosh(\mathrm{T}_{13}) - 1850\,w^4\cosh(\mathrm{T}_{14})\\
&+ 882\,w^5\sinh(\mathrm{T}_{11}) - 882\,w^5\sinh(\mathrm{T}_{12}) - 5949\,w^4\cosh(\mathrm{T}_{11}) + 1400\,w^5\sinh(\mathrm{T}_{13})\\
&- 1400\,w^5\sinh(\mathrm{T}_{14}) - 5949\,w^4\cosh(\mathrm{T}_{12}) + 8064\,w\sqrt{21}\sinh(\mathrm{T}_{12}) - 960\,w\sqrt{21}\sinh(\mathrm{T}_{13})
\end{aligned}
$$

$$
\begin{aligned}
&+4014\,w^2\sqrt{21}\cosh(\mathrm{T}_{12})+4800\,w^2\sqrt{21}\cosh(\mathrm{T}_{14})-4800\,w^2\sqrt{21}\cosh(\mathrm{T}_{13})\\
&+8064\,w\sqrt{21}\sinh(\mathrm{T}_{11})+3264\,w\sqrt{21}\sinh(\mathrm{T}_{15})+3264\,w\sqrt{21}\sinh(\mathrm{T}_{16})\\
&-960\,w\sqrt{21}\sinh(\mathrm{T}_{14})-6180\,w^3\sqrt{21}\sinh(\mathrm{T}_{14})-6180\,w^3\sqrt{21}\sinh(\mathrm{T}_{13})\\
&-354\,w^3\sqrt{21}\sinh(\mathrm{T}_{16})-2754\,w^3\sqrt{21}\sinh(\mathrm{T}_{12})+786\,w^2\sqrt{21}\cosh(\mathrm{T}_{15})\\
&-2754\,w^3\sqrt{21}\sinh(\mathrm{T}_{11})-4014\,w^2\sqrt{21}\cosh(\mathrm{T}_{11})-786\,w^2\sqrt{21}\cosh(\mathrm{T}_{16})\\
&-354\,w^3\sqrt{21}\sinh(\mathrm{T}_{15})\big)/\big(w^4(-119\,w^3\sinh(\mathrm{T}_{11})-7560\cosh(\mathrm{T}_{13})-4788\,w\sinh(\mathrm{T}_{13})\\
&-7560\cosh(\mathrm{T}_{14})+2040\sqrt{21}\cosh(\mathrm{T}_{12})-3960\sqrt{21}\cosh(\mathrm{T}_{13})+3960\sqrt{21}\cosh(\mathrm{T}_{14})\\
&-882\,w^2\cosh(\mathrm{T}_{12})+7560\cosh(\mathrm{T}_{12})-882\,w^2\cosh(\mathrm{T}_{11})-588\,w\sinh(\mathrm{T}_{11})\\
&+588\,w\sinh(\mathrm{T}_{12})+231\,w^3\sinh(\mathrm{T}_{13})-231\,w^3\sinh(\mathrm{T}_{14})+119\,w^3\sinh(\mathrm{T}_{12})\\
&+882\,w^2\cosh(\mathrm{T}_{13})+882\,w^2\cosh(\mathrm{T}_{14})+4788\,w\sinh(\mathrm{T}_{14})-2040\sqrt{21}\cosh(\mathrm{T}_{11})\\
&+7560\cosh(\mathrm{T}_{11})-108\,w\sqrt{21}\sinh(\mathrm{T}_{12})-108\,w\sqrt{21}\sinh(\mathrm{T}_{13})-138\,w^2\sqrt{21}\cosh(\mathrm{T}_{12})\\
&-162\,w^2\sqrt{21}\cosh(\mathrm{T}_{14})+162\,w^2\sqrt{21}\cosh(\mathrm{T}_{13})-108\,w\sqrt{21}\sinh(\mathrm{T}_{11})\\
&-108\,w\sqrt{21}\sinh(\mathrm{T}_{14})+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{14})+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{13})+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{12})\\
&+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{11})+138\,w^2\sqrt{21}\cosh(\mathrm{T}_{11}))\big),\\
&\mathrm{T}_{11}=\tfrac{1}{6}\,w\,(9+2\sqrt{21}),\\
&\mathrm{T}_{12}=\tfrac{1}{6}\,w\,(-9+2\sqrt{21}),\\
&\mathrm{T}_{13}=\tfrac{1}{6}\,w\,(2\sqrt{21}-3),\\
&\mathrm{T}_{14}=\tfrac{1}{6}\,w\,(2\sqrt{21}+3),\\
&\mathrm{T}_{15}=\tfrac{1}{6}\,w\,(15+2\sqrt{21}),\\
&\mathrm{T}_{16}=\tfrac{1}{6}\,w\,(-15+2\sqrt{21}),\\
&t_2=-18\big(432\cosh(\tfrac{3}{2}\,w)-144\cosh(\tfrac{5}{2}\,w)+216\,w^3\sinh(\tfrac{1}{2}\,w)-288\cosh(\tfrac{1}{2}\,w)\\
&-288\,w\sinh(\tfrac{3}{2}\,w)-w^4\cosh(\tfrac{5}{2}\,w)+72\,w^3\sinh(\tfrac{3}{2}\,w)+15\,w^2\cosh(\tfrac{5}{2}\,w)-9\,w^2\cosh(\tfrac{3}{2}\,w)\\
&-9\,w^4\cosh(\tfrac{3}{2}\,w)-6\cosh(\tfrac{1}{2}\,w)\,w^2+864\sinh(\tfrac{1}{2}\,w)\,w+46\,w^4\cosh(\tfrac{1}{2}\,w)\big)/\\
&\big(w^4(-119\,w^3\sinh(\mathrm{T}_{17})-7560\cosh(\mathrm{T}_{19})-4788\,w\sinh(\mathrm{T}_{19})-7560\cosh(\mathrm{T}_{20})\\
&+2040\sqrt{21}\cosh(\mathrm{T}_{18})-3960\sqrt{21}\cosh(\mathrm{T}_{19})+3960\sqrt{21}\cosh(\mathrm{T}_{20})-882\,w^2\cosh(\mathrm{T}_{18})\\
&+7560\cosh(\mathrm{T}_{18})-882\,w^2\cosh(\mathrm{T}_{17})-588\,w\sinh(\mathrm{T}_{17})+588\,w\sinh(\mathrm{T}_{18})\\
&+231\,w^3\sinh(\mathrm{T}_{19})-231\,w^3\sinh(\mathrm{T}_{20})+119\,w^3\sinh(\mathrm{T}_{18})+882\,w^2\cosh(\mathrm{T}_{19})\\
&+882\,w^2\cosh(\mathrm{T}_{20})+4788\,w\sinh(\mathrm{T}_{20})-2040\sqrt{21}\cosh(\mathrm{T}_{17})+7560\cosh(\mathrm{T}_{17})\\
&-108\,w\sqrt{21}\sinh(\mathrm{T}_{18})-108\,w\sqrt{21}\sinh(\mathrm{T}_{19})-138\,w^2\sqrt{21}\cosh(\mathrm{T}_{18})\\
&-162\,w^2\sqrt{21}\cosh(\mathrm{T}_{20})+162\,w^2\sqrt{21}\cosh(\mathrm{T}_{19})-108\,w\sqrt{21}\sinh(\mathrm{T}_{17})\\
&-108\,w\sqrt{21}\sinh(\mathrm{T}_{20})+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{20})+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{19})+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{18})\\
&+21\,w^3\sqrt{21}\sinh(\mathrm{T}_{17})+138\,w^2\sqrt{21}\cosh(\mathrm{T}_{17}))\big),\\
&\mathrm{T}_{17}=\tfrac{1}{6}\,w\,(9+2\sqrt{21}),\\
&\mathrm{T}_{18}=\tfrac{1}{6}\,w\,(-9+2\sqrt{21}),\\
&\mathrm{T}_{19}=\tfrac{1}{6}\,w\,(2\sqrt{21}-3),
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{T}_{20} &= \tfrac{1}{6}\, w\, (2\sqrt{21}+3),\\
t_3 &= 32\big(324\cosh(\mathrm{T}_{26}) + 216\cosh(\tfrac{1}{3}\, w\sqrt{21})\sqrt{21} + 28\, w^4\cosh(\tfrac{1}{3}\, w\sqrt{21})\sqrt{21}\\
&\quad + 42\cosh(\tfrac{1}{3}\, w\sqrt{21})\sqrt{21}\, w^2 + 882\, w^3\sinh(\tfrac{1}{3}\, w\sqrt{21}) - 72\sinh(\tfrac{1}{3}\, w\sqrt{21})\, w\\
&\quad - 21\sqrt{21}\, w^2\cosh(\mathrm{T}_{26}) - 21\sqrt{21}\, w^2\cosh(\mathrm{T}_{25}) + 108\, w\sqrt{21}\sinh(\mathrm{T}_{26})\\
&\quad - 108\, w\sqrt{21}\sinh(\mathrm{T}_{25}) + 10\, w^4\sqrt{21}\cosh(\mathrm{T}_{26}) + 10\, w^4\sqrt{21}\cosh(\mathrm{T}_{25})\\
&\quad - 27\, w^3\sqrt{21}\sinh(\mathrm{T}_{26}) + 27\, w^3\sqrt{21}\sinh(\mathrm{T}_{25}) + 99\, w^2\cosh(\mathrm{T}_{26}) - 99\, w^2\cosh(\mathrm{T}_{25})\\
&\quad - 108\sqrt{21}\cosh(\mathrm{T}_{26}) - 108\sqrt{21}\cosh(\mathrm{T}_{25}) + 153\, w^3\sinh(\mathrm{T}_{26}) - 42\, w^4\cosh(\mathrm{T}_{26})\\
&\quad + 42\, w^4\cosh(\mathrm{T}_{25}) + 153\, w^3\sinh(\mathrm{T}_{25}) - 612\, w\sinh(\mathrm{T}_{26}) - 612\, w\sinh(\mathrm{T}_{25}) - 324\cosh(\mathrm{T}_{25})\big)/\\
&\quad \big(w^4(-63\, w^3\sinh(\mathrm{T}_{21}) + 11880\cosh(\mathrm{T}_{23}) + 324\, w\sinh(\mathrm{T}_{23}) - 11880\cosh(\mathrm{T}_{24})\\
&\quad - 1080\sqrt{21}\cosh(\mathrm{T}_{22}) + 1080\sqrt{21}\cosh(\mathrm{T}_{23}) + 1080\sqrt{21}\cosh(\mathrm{T}_{24}) + 414\, w^2\cosh(\mathrm{T}_{22})\\
&\quad - 6120\cosh(\mathrm{T}_{22}) - 414\, w^2\cosh(\mathrm{T}_{21}) + 324\, w\sinh(\mathrm{T}_{21}) + 324\, w\sinh(\mathrm{T}_{22}) - 63\, w^3\sinh(\mathrm{T}_{23})\\
&\quad - 63\, w^3\sinh(\mathrm{T}_{24}) - 63\, w^3\sinh(\mathrm{T}_{22}) - 486\, w^2\cosh(\mathrm{T}_{23}) + 486\, w^2\cosh(\mathrm{T}_{24})\\
&\quad + 324\, w\sinh(\mathrm{T}_{24}) - 1080\sqrt{21}\cosh(\mathrm{T}_{21}) + 6120\cosh(\mathrm{T}_{21}) - 84\, w\sqrt{21}\sinh(\mathrm{T}_{22})\\
&\quad + 684\, w\sqrt{21}\sinh(\mathrm{T}_{23}) + 126\, w^2\sqrt{21}\cosh(\mathrm{T}_{22}) - 126\, w^2\sqrt{21}\cosh(\mathrm{T}_{24})\\
&\quad - 126\, w^2\sqrt{21}\cosh(\mathrm{T}_{23}) + 84\, w\sqrt{21}\sinh(\mathrm{T}_{21}) - 684\, w\sqrt{21}\sinh(\mathrm{T}_{24})\\
&\quad + 33\, w^3\sqrt{21}\sinh(\mathrm{T}_{24}) - 33\, w^3\sqrt{21}\sinh(\mathrm{T}_{23}) - 17\, w^3\sqrt{21}\sinh(\mathrm{T}_{22}) + 17\, w^3\sqrt{21}\sinh(\mathrm{T}_{21})\\
&\quad + 126\, w^2\sqrt{21}\cosh(\mathrm{T}_{21}))\big),\\
\mathrm{T}_{21} &= \tfrac{1}{6}\, w\, (9+2\sqrt{21}),\\
\mathrm{T}_{22} &= \tfrac{1}{6}\, w\, (-9+2\sqrt{21}),\\
\mathrm{T}_{23} &= \tfrac{1}{6}\, w\, (2\sqrt{21}-3),\\
\mathrm{T}_{24} &= \tfrac{1}{6}\, w\, (2\sqrt{21}+3),\\
\mathrm{T}_{25} &= \tfrac{1}{3}\, w\, (-6+\sqrt{21}),\\
\mathrm{T}_{26} &= \tfrac{1}{3}\, w\, (6+\sqrt{21}).
\end{aligned} \tag{58}
$$

Appendix B

$$
\begin{aligned}
q_1 &= -2 - \frac{41}{203212800}\, w^{10} + \frac{29693}{2703868231680}\, w^{12} - \frac{25036829}{39368321453260800}\, w^{14} + \cdots,\\
t_0 &= \frac{11}{560} - \frac{41}{112896}\, w^2 - \frac{52681}{12517908480}\, w^4 + \frac{1018207991}{984208036331520}\, w^6 - \frac{9589567003}{122479222299033600}\, w^8\\
&\quad + \frac{39035969395583}{85506827727698657 28000}\, w^{10} - \frac{16890318085539089 6711}{7162979468539229608806973 44000}\, w^{12}\\
&\quad + \frac{48320189274881141 20127}{41717192424772473241691813 3145600}\, w^{14} + \cdots,\\
t_1 &= \frac{326}{735} - \frac{41}{32928}\, w^2 - \frac{355753}{3651056640}\, w^4 - \frac{1549241257}{287060677263360}\, w^6 - \frac{136765543891}{3215079585349632 00}\, w^8\\
&\quad + \frac{15775682947969709}{6060296415200642334 72000}\, w^{10} - \frac{3430040471444539 60103}{208920234499060863590203392000}\, w^{12}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{16001532342808379558999}{18435627965492885902262796288000}\,w^{14}+\cdots,\\
t_2 &= -\frac{9}{19600}+\frac{123}{2195200}\,w^2-\frac{70283}{16226918400}\,w^4+\frac{1736345993}{6379126161408000}\,w^6\\
&\quad-\frac{65306657723}{4286772780466176000}\,w^8+\frac{32313479393985497}{40401976101337615564800000}\,w^{10}\\
&\quad-\frac{2240625777206516309}{5461966915008127152685056 0000}\,w^{12}+\frac{863062913957596651103 51}{4055838152408434898497815183360 0000}\,w^{14}+\cdots,\\
t_3 &= \frac{136}{525}+\frac{41}{44100}\,w^2+\frac{55997}{977961600}\,w^4+\frac{48641363}{34950569472000}\,w^6-\frac{5688784027}{28706067726336000}\,w^8\\
&\quad+\frac{3904144288624633}{2705489471071715328000000}\,w^{10}-\frac{4673420922737697137 3}{5596077709796273131880448 0000}\,w^{12}\\
&\quad+\frac{3515534995607943334951 7}{8147889145463373680017932288 00000}\,w^{14}+\cdots. \qquad (59)
\end{aligned}
$$

Appendix C

$$
\begin{aligned}
a_0 = &-\tfrac{1}{18}\big(24\sqrt{21}\,w^2\cosh(\mathrm{T}_2)-24\sqrt{21}\,w^2\cosh(\mathrm{T}_1)+18\,w\sqrt{21}\sinh(\mathrm{T}_2)\\
&+18\,w\sqrt{21}\sinh(\mathrm{T}_1)-21\,w^3\sinh(\mathrm{T}_2)+21\,w^3\sinh(\mathrm{T}_1)-126\,w^2\cosh(\mathrm{T}_2)\\
&-126\,w^2\cosh(\mathrm{T}_1)+7\sqrt{21}\,w^3\sinh(\mathrm{T}_2)+7\sqrt{21}\,w^3\sinh(\mathrm{T}_1)-126\,w\sinh(\mathrm{T}_2)\\
&+126\,w\sinh(\mathrm{T}_1)+18\sqrt{21}\cosh(\mathrm{T}_2)-18\sqrt{21}\cosh(\mathrm{T}_1)\big)/\\
&\big(5\,w^2+w^2\cosh(2\,w)+3-3\cosh(2\,w)\big),\\
\mathrm{T}_1 = &\tfrac{1}{3}\,w\,(-3+\sqrt{21}),\\
\mathrm{T}_2 = &\tfrac{1}{3}\,w\,(3+\sqrt{21}),\\
a_1 = &\tfrac{1}{18}\big(-18\sqrt{21}\cosh(\mathrm{T}_4)+36\,w\sinh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}-15\sqrt{21}\,w^2\cosh(\mathrm{T}_4)\\
&+18\,w\sqrt{21}\sinh(\mathrm{T}_4)+18\,w\sqrt{21}\sinh(\mathrm{T}_3)-10\,w^3\sqrt{21}\sinh(\mathrm{T}_3)-10\,w^3\sqrt{21}\sinh(\mathrm{T}_4)\\
&+15\sqrt{21}\,w^2\cosh(\mathrm{T}_3)+42\,w^3\sinh(\mathrm{T}_3)+12\,w^3\sinh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}-42\,w^3\sinh(\mathrm{T}_4)\\
&-126\,w\sinh(\mathrm{T}_3)+126\,w\sinh(\mathrm{T}_4)+18\sqrt{21}\cosh(\mathrm{T}_3)+108\cosh(\tfrac{1}{3}\,w\sqrt{21})\\
&-54\cosh(\mathrm{T}_3)-54\cosh(\mathrm{T}_4)-198\cosh(\tfrac{1}{3}\,w\sqrt{21})\,w^2-45\,w^2\cosh(\mathrm{T}_4)-45\,w^2\cosh(\mathrm{T}_3)\big)/\\
&\big(5\,w^2+w^2\cosh(2\,w)+3-3\cosh(2\,w)\big),\\
\mathrm{T}_3 = &\tfrac{1}{3}\,w\,(6+\sqrt{21}),\\
\mathrm{T}_4 = &\tfrac{1}{3}\,w\,(-6+\sqrt{21}),\\
a_2 = &\tfrac{1}{18}\big(-21\,w\sinh(\tfrac{1}{3}\,w\,(3+\sqrt{21}))+21\,w\sinh(\tfrac{1}{3}\,w\,(-3+\sqrt{21}))\\
&-4\sqrt{21}\cosh(\tfrac{1}{3}\,w\,(3+\sqrt{21}))+4\sqrt{21}\cosh(\tfrac{1}{3}\,w\,(-3+\sqrt{21}))+7\,w\sqrt{21}\sinh(\tfrac{1}{3}\,w\,(3+\sqrt{21}))\\
&+7\,w\sqrt{21}\sinh(\tfrac{1}{3}\,w\,(-3+\sqrt{21}))\big)/\big(5\,w^2+w^2\cosh(2\,w)+3-3\cosh(2\,w)\big),\\
a_3 = &-\tfrac{1}{18}\big(-10\,w\sqrt{21}\sinh(\mathrm{T}_6)-10\,w\sqrt{21}\sinh(\mathrm{T}_5)+12\,w\sinh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}\\
&-13\sqrt{21}\cosh(\mathrm{T}_6)+13\sqrt{21}\cosh(\mathrm{T}_5)+42\,w\sinh(\mathrm{T}_6)-42\,w\sinh(\mathrm{T}_5)\\
&-126\cosh(\tfrac{1}{3}\,w\sqrt{21})+63\cosh(\mathrm{T}_6)+63\cosh(\mathrm{T}_5)\big)/\big(5\,w^2+w^2\cosh(2\,w)+3-3\cosh(2\,w)\big),
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{T}_5 &= \tfrac{1}{3}\, w\,(-6+\sqrt{21}),\\
\mathrm{T}_6 &= \tfrac{1}{3}\, w\,(6+\sqrt{21}),
\end{aligned}
\tag{60}
$$

$$
\begin{aligned}
b_0 &= \tfrac{1}{6}\Big(3\,w\sinh(\tfrac{1}{3}\,w\,(3+\sqrt{21})) + 3\,w\sinh(\tfrac{1}{3}\,w\,(-3+\sqrt{21})) + 6\cosh(\tfrac{1}{3}\,w\,(3+\sqrt{21}))\\
&\quad - 6\cosh(\tfrac{1}{3}\,w\,(-3+\sqrt{21})) - w\sqrt{21}\sinh(\tfrac{1}{3}\,w\,(3+\sqrt{21})) + w\sqrt{21}\sinh(\tfrac{1}{3}\,w\,(-3+\sqrt{21}))\Big)/\\
&\quad \big(-1+\cosh(2\,w)\big),\\
b_1 &= -\tfrac{1}{6}\Big(3\sinh(\tfrac{1}{3}\,w\,(3+\sqrt{21})) + 3\sinh(\tfrac{1}{3}\,w\,(-3+\sqrt{21})) - \sqrt{21}\sinh(\tfrac{1}{3}\,w\,(3+\sqrt{21}))\\
&\quad + \sqrt{21}\sinh(\tfrac{1}{3}\,w\,(-3+\sqrt{21}))\Big)/\big(w\,(-1+\cosh(2\,w))\big).
\end{aligned}
\tag{61}
$$

Appendix D

$$
\begin{aligned}
a_0 &= \frac{49}{81} - \frac{224}{729}\,w^2 - \frac{20}{729}\,w^4 - \frac{5704}{22733865}\,w^6 - \frac{93838}{18619035435}\,w^8 - \frac{10784}{451153550925}\,w^{10}\\
&\quad + \frac{403496356}{69095519784816525}\,w^{12} - \frac{178405115344}{413536685912126902125}\,w^{14} + \cdots,\\
a_1 &= \frac{64}{81} + \frac{448}{729}\,w^2 + \frac{40}{729}\,w^4 + \frac{11408}{22733865}\,w^6 - \frac{2308711}{7447614174}\,w^8 - \frac{13709449}{902307101850}\,w^{10}\\
&\quad - \frac{19619622719}{44221132662282576}\,w^{12} - \frac{6934169136149}{827073371824253804250}\,w^{14} + \cdots,\\
a_2 &= \frac{98}{243} + \frac{56}{2187}\,w^2 + \frac{4}{10935}\,w^4 + \frac{8}{13640319}\,w^6 + \frac{44816}{279285531525}\,w^8\\
&\quad - \frac{143368}{17594988486075}\,w^{10} + \frac{368000824}{1036432796772247875}\,w^{12} - \frac{15304688096}{1240610057736380706375}\,w^{14} + \cdots,\\
a_3 &= \frac{224}{243} + \frac{560}{2187}\,w^2 + \frac{292}{10935}\,w^4 + \frac{20870}{13640319}\,w^6 + \frac{53514947}{1117142126100}\,w^8\\
&\quad + \frac{30201449}{28151981577720}\,w^{10} + \frac{39208407053}{2551219192054764000}\,w^{12} + \frac{36142895623}{244304749831164200640}\,w^{14} + \cdots,\\
b_0 &= \frac{1}{3}\sqrt{21} - \frac{8}{25515}\,w^6\sqrt{21} + \frac{2}{45927}\,w^8\sqrt{21} - \frac{32}{5412825}\,w^{10}\sqrt{21}\\
&\quad + \frac{2788}{3723807087}\,w^{12}\sqrt{21} - \frac{3632}{39897933075}\,w^{14}\sqrt{21} + \cdots,\\
b_1 &= \frac{2}{27}\sqrt{21} + \frac{4}{8505}\,w^4\sqrt{21} - \frac{8}{137781}\,w^6\sqrt{21} + \frac{8}{1082565}\,w^8\sqrt{21}\\
&\quad - \frac{5576}{6206345145}\,w^{10}\sqrt{21} + \frac{1816}{17099114175}\,w^{12}\sqrt{21} - \frac{1472}{119693799225}\,w^{14}\sqrt{21} + \cdots.
\end{aligned}
\tag{62}
$$

Appendix E

$$
\begin{aligned}
c_0 &= \tfrac{1}{32}\big(2124\,w^3\sinh(\mathrm{S}_3) + 5184\cosh(\mathrm{S}_5) + 2016\,w\sinh(\mathrm{S}_5) - 5184\cosh(\mathrm{S}_6)\\
&\quad - 1728\sqrt{21}\cosh(\mathrm{S}_4) + 1728\sqrt{21}\cosh(\mathrm{S}_5) + 1728\sqrt{21}\cosh(\mathrm{S}_6) + 2664\,w^2\cosh(\mathrm{S}_4)\\
&\quad - 5184\cosh(\mathrm{S}_4) - 2664\,w^2\cosh(\mathrm{S}_3) - 7200\,w\sinh(\mathrm{S}_3) - 7200\,w\sinh(\mathrm{S}_4)\\
&\quad + 3276\,w^3\sinh(\mathrm{S}_5) + 3276\,w^3\sinh(\mathrm{S}_6) + 2124\,w^3\sinh(\mathrm{S}_4) - 7272\,w^2\cosh(\mathrm{S}_5)
\end{aligned}
$$

$$
\begin{aligned}
&+ 7272\,w^2 \cosh(S_6) + 2016\,w \sinh(S_6) - 1728\sqrt{21}\cosh(S_3) + 5184\cosh(S_3) \\
&- 33\,w^5\sqrt{21}\sinh(S_5) + 17\,w^5\sqrt{21}\sinh(S_3) + 33\,w^5\sqrt{21}\sinh(S_6) \\
&+ 146\,w^4\sqrt{21}\cosh(S_6) + 146\,w^4\sqrt{21}\cosh(S_5) + 46\,w^4\sqrt{21}\cosh(S_4) \\
&+ 46\,w^4\sqrt{21}\cosh(S_3) - 17\,w^5\sqrt{21}\sinh(S_4) - 150\,w^4\cosh(S_5) + 150\,w^4\cosh(S_6) \\
&- 63\,w^5\sinh(S_3) - 63\,w^5\sinh(S_4) - 78\,w^4\cosh(S_3) - 63\,w^5\sinh(S_5) - 63\,w^5\sinh(S_6) \\
&+ 78\,w^4\cosh(S_4) - 864\,w\sqrt{21}\sinh(S_4) - 864\,w\sqrt{21}\sinh(S_5) + 312\,w^2\sqrt{21}\cosh(S_4) \\
&- 312\,w^2\sqrt{21}\cosh(S_6) - 312\,w^2\sqrt{21}\cosh(S_5) + 864\,w\sqrt{21}\sinh(S_3) \\
&+ 864\,w\sqrt{21}\sinh(S_6) - 36\,w^3\sqrt{21}\sinh(S_6) + 36\,w^3\sqrt{21}\sinh(S_5) \\
&+ 420\,w^3\sqrt{21}\sinh(S_4) - 420\,w^3\sqrt{21}\sinh(S_3) + 312\,w^2\sqrt{21}\cosh(S_3)\big)/\big(324\cosh(S_2) \\
&+ 216\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} + 28\,w^4\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} + 42\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}\,w^2 \\
&+ 882\,w^3\sinh(\tfrac{1}{3}\,w\sqrt{21}) - 72\sinh(\tfrac{1}{3}\,w\sqrt{21})\,w - 21\sqrt{21}\,w^2\cosh(S_2) \\
&- 21\sqrt{21}\,w^2\cosh(S_1) + 108\,w\sqrt{21}\sinh(S_2) - 108\,w\sqrt{21}\sinh(S_1) \\
&+ 10\,w^4\sqrt{21}\cosh(S_2) + 10\,w^4\sqrt{21}\cosh(S_1) - 27\,w^3\sqrt{21}\sinh(S_2) + 27\,w^3\sqrt{21}\sinh(S_1) \\
&+ 99\,w^2\cosh(S_2) - 99\,w^2\cosh(S_1) - 108\sqrt{21}\cosh(S_2) - 108\sqrt{21}\cosh(S_1) \\
&+ 153\,w^3\sinh(S_2) - 42\,w^4\cosh(S_2) + 42\,w^4\cosh(S_1) + 153\,w^3\sinh(S_1) \\
&- 612\,w\sinh(S_2) - 612\,w\sinh(S_1) - 324\cosh(S_1)\big),
\end{aligned}
$$

$$
\begin{aligned}
S_1 &= \tfrac{1}{3}\,w\,(-6+\sqrt{21}), \\
S_2 &= \tfrac{1}{3}\,w\,(6+\sqrt{21}), \\
S_3 &= \tfrac{1}{6}\,w\,(9+2\sqrt{21}), \\
S_4 &= \tfrac{1}{6}\,w\,(-9+2\sqrt{21}), \\
S_5 &= \tfrac{1}{6}\,w\,(2\sqrt{21}-3), \\
S_6 &= \tfrac{1}{6}\,w\,(2\sqrt{21}+3),
\end{aligned}
$$

$$
\begin{aligned}
c_1 = -\tfrac{1}{32}\big(&-6372\,w^3\sinh(S_{11}) - 10368\cosh(S_{13}) + 26\,w^5\sqrt{21}\sinh(S_9) \\
&- 181\,w^4\sqrt{21}\cosh(S_9) - 181\,w^4\sqrt{21}\cosh(S_{10}) - 114\,w^5\sinh(S_{10}) - 843\,w^4\cosh(S_{10}) \\
&+ 843\,w^4\cosh(S_9) - 26\,w^5\sqrt{21}\sinh(S_{10}) - 114\,w^5\sinh(S_9) + 7128\,w^2\cosh(S_{10}) \\
&- 2880\,w\sinh(S_{13}) + 10368\cosh(S_{14}) - 5184\cosh(S_9) + 12384\,w\sinh(S_9) \\
&+ 5184\sqrt{21}\cosh(S_{12}) - 6912\sqrt{21}\cosh(S_{13}) - 6912\sqrt{21}\cosh(S_{14}) - 7992\,w^2\cosh(S_{12}) \\
&- 324\,w^3\sinh(S_{10}) + 15552\cosh(S_{12}) - 7128\,w^2\cosh(S_9) + 7992\,w^2\cosh(S_{11}) \\
&+ 1728\sqrt{21}\cosh(S_{10}) + 21600\,w\sinh(S_{11}) + 12384\,w\sinh(S_{10}) + 21600\,w\sinh(S_{12}) \\
&- 20520\,w^3\sinh(S_{13}) - 20520\,w^3\sinh(S_{14}) + 1728\sqrt{21}\cosh(S_9) - 324\,w^3\sinh(S_9) \\
&- 6372\,w^3\sinh(S_{12}) + 15120\,w^2\cosh(S_{13}) - 15120\,w^2\cosh(S_{14}) - 2880\,w\sinh(S_{14}) \\
&+ 5184\sqrt{21}\cosh(S_{11}) + 5184\cosh(S_{10}) - 15552\cosh(S_{11}) - 200\,w^5\sqrt{21}\sinh(S_{13}) \\
&- 126\,w^5\sqrt{21}\sinh(S_{11}) + 200\,w^5\sqrt{21}\sinh(S_{14}) - 1058\,w^4\sqrt{21}\cosh(S_{14}) \\
&- 1058\,w^4\sqrt{21}\cosh(S_{13}) + 87\,w^4\sqrt{21}\cosh(S_{12}) + 87\,w^4\sqrt{21}\cosh(S_{11}) \\
&+ 126\,w^5\sqrt{21}\sinh(S_{12}) - 6612\,w^4\cosh(S_{13}) + 6612\,w^4\cosh(S_{14}) + 486\,w^5\sinh(S_{11})
\end{aligned}
$$

$$
\begin{aligned}
&+ 486\,w^5 \sinh(S_{12}) - 1161\,w^4 \cosh(S_{11}) - 300\,w^5 \sinh(S_{13}) - 300\,w^5 \sinh(S_{14}) \\
&+ 1161\,w^4 \cosh(S_{12}) + 2592\,w\sqrt{21}\sinh(S_{12}) - 936\,w^2\sqrt{21}\cosh(S_{12}) \\
&- 480\,w^2\sqrt{21}\cosh(S_{14}) - 480\,w^2\sqrt{21}\cosh(S_{13}) - 2592\,w\sqrt{21}\sinh(S_{11}) \\
&- 2592\,w\sqrt{21}\sinh(S_9) + 2592\,w\sqrt{21}\sinh(S_{10}) + 480\,w^3\sqrt{21}\sinh(S_{14}) \\
&- 480\,w^3\sqrt{21}\sinh(S_{13}) - 12\,w^3\sqrt{21}\sinh(S_{10}) - 1260\,w^3\sqrt{21}\sinh(S_{12}) \\
&+ 1416\,w^2\sqrt{21}\cosh(S_9) + 1260\,w^3\sqrt{21}\sinh(S_{11}) - 936\,w^2\sqrt{21}\cosh(S_{11}) \\
&+ 1416\,w^2\sqrt{21}\cosh(S_{10}) + 12\,w^3\sqrt{21}\sinh(S_9)\big)/\big(324\cosh(S_8) \\
&+ 216\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} + 28\,w^4\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} + 42\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}\,w^2 \\
&+ 882\,w^3\sinh(\tfrac{1}{3}\,w\sqrt{21}) - 72\sinh(\tfrac{1}{3}\,w\sqrt{21})\,w - 21\sqrt{21}\,w^2\cosh(S_8) \\
&- 21\sqrt{21}\,w^2\cosh(S_7) + 108\,w\sqrt{21}\sinh(S_8) - 108\,w\sqrt{21}\sinh(S_7) \\
&+ 10\,w^4\sqrt{21}\cosh(S_8) + 10\,w^4\sqrt{21}\cosh(S_7) - 27\,w^3\sqrt{21}\sinh(S_8) + 27\,w^3\sqrt{21}\sinh(S_7) \\
&+ 99\,w^2\cosh(S_8) - 99\,w^2\cosh(S_7) - 108\sqrt{21}\cosh(S_8) - 108\sqrt{21}\cosh(S_7) \\
&+ 153\,w^3\sinh(S_8) - 42\,w^4\cosh(S_8) + 42\,w^4\cosh(S_7) + 153\,w^3\sinh(S_7) \\
&- 612\,w\sinh(S_8) - 612\,w\sinh(S_7) - 324\cosh(S_7)\big),
\end{aligned}
$$

$$
\begin{aligned}
S_7 &= \tfrac{1}{3}\,w\,(-6+\sqrt{21}), \\
S_8 &= \tfrac{1}{3}\,w\,(6+\sqrt{21}), \\
S_9 &= \tfrac{1}{6}\,w\,(15+2\sqrt{21}), \\
S_{10} &= \tfrac{1}{6}\,w\,(-15+2\sqrt{21}), \\
S_{11} &= \tfrac{1}{6}\,w\,(9+2\sqrt{21}), \\
S_{12} &= \tfrac{1}{6}\,w\,(-9+2\sqrt{21}), \\
S_{13} &= \tfrac{1}{6}\,w\,(2\sqrt{21}-3), \\
S_{14} &= \tfrac{1}{6}\,w\,(2\sqrt{21}+3),
\end{aligned}
$$

$$
\begin{aligned}
c_2 = -\tfrac{1}{32}\big(&-63\,w^3\sinh(S_{17}) + 486\cosh(S_{19}) + 846\,w\sinh(S_{19}) - 486\cosh(S_{20}) \\
&- 216\sqrt{21}\cosh(S_{18}) + 216\sqrt{21}\cosh(S_{19}) + 216\sqrt{21}\cosh(S_{20}) - 510\,w^2\cosh(S_{18}) \\
&- 378\cosh(S_{18}) + 510\,w^2\cosh(S_{17}) - 1170\,w\sinh(S_{17}) - 1170\,w\sinh(S_{18}) \\
&- 63\,w^3\sinh(S_{19}) - 63\,w^3\sinh(S_{20}) - 63\,w^3\sinh(S_{18}) - 738\,w^2\cosh(S_{19}) \\
&+ 738\,w^2\cosh(S_{20}) + 846\,w\sinh(S_{20}) - 216\sqrt{21}\cosh(S_{17}) + 378\cosh(S_{17}) \\
&- 198\,w\sqrt{21}\sinh(S_{18}) - 54\,w\sqrt{21}\sinh(S_{19}) - 96\,w^2\sqrt{21}\cosh(S_{18}) - 12\,w^2\sqrt{21}\cosh(S_{20}) \\
&- 12\,w^2\sqrt{21}\cosh(S_{19}) + 198\,w\sqrt{21}\sinh(S_{17}) + 54\,w\sqrt{21}\sinh(S_{20}) + 33\,w^3\sqrt{21}\sinh(S_{20}) \\
&- 33\,w^3\sqrt{21}\sinh(S_{19}) - 17\,w^3\sqrt{21}\sinh(S_{18}) + 17\,w^3\sqrt{21}\sinh(S_{17}) - 96\,w^2\sqrt{21}\cosh(S_{17})\big)/ \\
&\big(324\cosh(S_{16}) + 216\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} + 28\,w^4\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} \\
&+ 42\cosh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}\,w^2 + 882\,w^3\sinh(\tfrac{1}{3}\,w\sqrt{21}) - 72\sinh(\tfrac{1}{3}\,w\sqrt{21})\,w \\
&- 21\sqrt{21}\,w^2\cosh(S_{16}) - 21\sqrt{21}\,w^2\cosh(S_{15}) + 108\,w\sqrt{21}\sinh(S_{16}) \\
&- 108\,w\sqrt{21}\sinh(S_{15}) + 10\,w^4\sqrt{21}\cosh(S_{16}) + 10\,w^4\sqrt{21}\cosh(S_{15})
\end{aligned}
$$

$$
\begin{aligned}
&- 27\,w^3\sqrt{21}\sinh(S_{16}) + 27\,w^3\sqrt{21}\sinh(S_{15}) + 99\,w^2\cosh(S_{16}) - 99\,w^2\cosh(S_{15})\\
&- 108\sqrt{21}\cosh(S_{16}) - 108\sqrt{21}\cosh(S_{15}) + 153\,w^3\sinh(S_{16}) - 42\,w^4\cosh(S_{16})\\
&+ 42\,w^4\cosh(S_{15}) + 153\,w^3\sinh(S_{15}) - 612\,w\sinh(S_{16}) - 612\,w\sinh(S_{15}) - 324\cosh(S_{15})\big),\\
&S_{15} = \tfrac{1}{3}\,w\,(-6+\sqrt{21}),\\
&S_{16} = \tfrac{1}{3}\,w\,(6+\sqrt{21}),\\
&S_{17} = \tfrac{1}{6}\,w\,(9+2\sqrt{21}),\\
&S_{18} = \tfrac{1}{6}\,w\,(-9+2\sqrt{21}),\\
&S_{19} = \tfrac{1}{6}\,w\,(2\sqrt{21}-3),\\
&S_{20} = \tfrac{1}{6}\,w\,(2\sqrt{21}+3),\\
&c_3 = -\tfrac{1}{32}\big(882\,w^3\sinh(S_{25}) - 5940\cosh(S_{27}) + 39\,w^2\cosh(S_{24}) + 5760\,w\sinh(S_{27})\\
&- 5940\cosh(S_{28}) - 1782\cosh(S_{23}) + 1638\,w\sinh(S_{23}) + 1134\sqrt{21}\cosh(S_{26})\\
&- 1440\sqrt{21}\cosh(S_{27}) + 1440\sqrt{21}\cosh(S_{28}) - 1581\,w^2\cosh(S_{26}) + 182\,w^3\sinh(S_{24})\\
&+ 7722\cosh(S_{26}) + 39\,w^2\cosh(S_{23}) - 1581\,w^2\cosh(S_{25}) - 306\sqrt{21}\cosh(S_{24})\\
&- 2970\,w\sinh(S_{25}) - 1638\,w\sinh(S_{24}) + 2970\,w\sinh(S_{26}) + 1400\,w^3\sinh(S_{27})\\
&- 1400\,w^3\sinh(S_{28}) + 306\sqrt{21}\cosh(S_{23}) - 182\,w^3\sinh(S_{23}) - 882\,w^3\sinh(S_{26})\\
&+ 2406\,w^2\cosh(S_{27}) + 2406\,w^2\cosh(S_{28}) - 5760\,w\sinh(S_{28}) - 1134\sqrt{21}\cosh(S_{25})\\
&- 1782\cosh(S_{24}) + 7722\cosh(S_{25}) + 1302\,w\sqrt{21}\sinh(S_{26}) - 660\,w\sqrt{21}\sinh(S_{27})\\
&- 639\,w^2\sqrt{21}\cosh(S_{26}) - 2204\,w^2\sqrt{21}\cosh(S_{28}) + 2204\,w^2\sqrt{21}\cosh(S_{27})\\
&+ 1302\,w\sqrt{21}\sinh(S_{25}) - 426\,w\sqrt{21}\sinh(S_{23}) - 426\,w\sqrt{21}\sinh(S_{24})\\
&- 660\,w\sqrt{21}\sinh(S_{28}) + 100\,w^3\sqrt{21}\sinh(S_{28}) + 100\,w^3\sqrt{21}\sinh(S_{27})\\
&+ 38\,w^3\sqrt{21}\sinh(S_{24}) - 162\,w^3\sqrt{21}\sinh(S_{26}) - 29\,w^2\sqrt{21}\cosh(S_{23})\\
&- 162\,w^3\sqrt{21}\sinh(S_{25}) + 639\,w^2\sqrt{21}\cosh(S_{25}) + 29\,w^2\sqrt{21}\cosh(S_{24})\\
&+ 38\,w^3\sqrt{21}\sinh(S_{23})\big)/\big(-24\,w\sinh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21} + 294\,w^3\sinh(\tfrac{1}{3}\,w\sqrt{21})\sqrt{21}\\
&- 756\cosh(S_{22}) + 1512\cosh(\tfrac{1}{3}\,w\sqrt{21}) + 196\,w^4\cosh(\tfrac{1}{3}\,w\sqrt{21}) + 294\cosh(\tfrac{1}{3}\,w\sqrt{21})\,w^2\\
&+ 33\sqrt{21}\,w^2\cosh(S_{22}) - 33\sqrt{21}\,w^2\cosh(S_{21}) - 204\,w\sqrt{21}\sinh(S_{22})\\
&- 204\,w\sqrt{21}\sinh(S_{21}) - 14\,w^4\sqrt{21}\cosh(S_{22}) + 14\,w^4\sqrt{21}\cosh(S_{21})\\
&+ 51\,w^3\sqrt{21}\sinh(S_{22}) + 51\,w^3\sqrt{21}\sinh(S_{21}) - 147\,w^2\cosh(S_{22}) - 147\,w^2\cosh(S_{21})\\
&+ 108\sqrt{21}\cosh(S_{22}) - 108\sqrt{21}\cosh(S_{21}) - 189\,w^3\sinh(S_{22}) + 70\,w^4\cosh(S_{22})\\
&+ 70\,w^4\cosh(S_{21}) + 189\,w^3\sinh(S_{21}) + 756\,w\sinh(S_{22}) - 756\,w\sinh(S_{21}) - 756\cosh(S_{21})\big),\\
&S_{21} = \tfrac{1}{3}\,w\,(-6+\sqrt{21}),\\
&S_{22} = \tfrac{1}{3}\,w\,(6+\sqrt{21}),\\
&S_{23} = \tfrac{1}{6}\,w\,(15+2\sqrt{21}),\\
&S_{24} = \tfrac{1}{6}\,w\,(-15+2\sqrt{21}),\\
&S_{25} = \tfrac{1}{6}\,w\,(9+2\sqrt{21}),
\end{aligned}
$$

$$S_{26} = \tfrac{1}{6}\, w\, (-9 + 2\sqrt{21}),$$
$$S_{27} = \tfrac{1}{6}\, w\, (2\sqrt{21} - 3),$$
$$S_{28} = \tfrac{1}{6}\, w\, (2\sqrt{21} + 3),$$
$$\begin{aligned}
c_4 = -\tfrac{9}{16}\big(&-w^2\cosh(\tfrac{5}{2}w) - 9w^2\cosh(\tfrac{3}{2}w) - 24w\sinh(\tfrac{3}{2}w) + 15\cosh(\tfrac{5}{2}w) \\
&- 72\sinh(\tfrac{1}{2}w)\,w - 9\cosh(\tfrac{3}{2}w) - 6\cosh(\tfrac{1}{2}w) + 46\cosh(\tfrac{1}{2}w)\,w^2\big)/ \\
\big(&-24w\sinh(\tfrac{1}{3}w\sqrt{21})\sqrt{21} + 294w^3\sinh(\tfrac{1}{3}w\sqrt{21})\sqrt{21} - 756\cosh(S_{30}) \\
&+ 1512\cosh(\tfrac{1}{3}w\sqrt{21}) + 196w^4\cosh(\tfrac{1}{3}w\sqrt{21}) + 294\cosh(\tfrac{1}{3}w\sqrt{21})\,w^2 \\
&+ 33\sqrt{21}\,w^2\cosh(S_{30}) - 33\sqrt{21}\,w^2\cosh(S_{29}) - 204w\sqrt{21}\sinh(S_{30}) \\
&- 204w\sqrt{21}\sinh(S_{29}) - 14w^4\sqrt{21}\cosh(S_{30}) + 14w^4\sqrt{21}\cosh(S_{29}) \\
&+ 51w^3\sqrt{21}\sinh(S_{30}) + 51w^3\sqrt{21}\sinh(S_{29}) - 147w^2\cosh(S_{30}) - 147w^2\cosh(S_{29}) \\
&+ 108\sqrt{21}\cosh(S_{30}) - 108\sqrt{21}\cosh(S_{29}) - 189w^3\sinh(S_{30}) + 70w^4\cosh(S_{30}) \\
&+ 70w^4\cosh(S_{29}) + 189w^3\sinh(S_{29}) + 756w\sinh(S_{30}) - 756w\sinh(S_{29}) - 756\cosh(S_{29})\big),
\end{aligned}$$
$$S_{29} = \tfrac{1}{3}\, w\, (-6 + \sqrt{21}),$$
$$S_{30} = \tfrac{1}{3}\, w\, (6 + \sqrt{21}),$$
$$\begin{aligned}
d_0 = -\tfrac{1}{8}\big(&-3w^2\sqrt{21}\cosh(S_{33}) + 3w^2\sqrt{21}\cosh(S_{36}) - 3w^2\sqrt{21}\cosh(S_{35}) \\
&- 8w\sqrt{21}\sinh(S_{36}) + 8w\sqrt{21}\sinh(S_{34}) + 8w\sqrt{21}\sinh(S_{33}) - 8w\sqrt{21}\sinh(S_{35}) \\
&- 24\sqrt{21}\cosh(S_{34}) + 72\cosh(S_{34}) - 72\cosh(S_{33}) + 72\cosh(S_{35}) - 72\cosh(S_{36}) \\
&+ 3w^2\sqrt{21}\cosh(S_{34}) + 8w\sinh(S_{35}) - 56w\sinh(S_{36}) - 24\sqrt{21}\cosh(S_{36}) \\
&+ 33w^2\cosh(S_{33}) - 33w^2\cosh(S_{35}) + 17w^2\cosh(S_{36}) - 17w^2\cosh(S_{34}) \\
&+ 24\sqrt{21}\cosh(S_{33}) + 24\sqrt{21}\cosh(S_{35}) - 56w\sinh(S_{34}) + 8w\sinh(S_{33})\big)/ \\
\big(&4\sinh(\tfrac{1}{3}w\sqrt{21})\,w + 10w\sinh(S_{32}) + 10w\sinh(S_{31}) - 9\cosh(S_{32}) + 9\cosh(S_{31}) \\
&- 6\cosh(\tfrac{1}{3}w\sqrt{21})\sqrt{21} + 3\sqrt{21}\cosh(S_{32}) + 3\sqrt{21}\cosh(S_{31}) - 2w\sqrt{21}\sinh(S_{32}) \\
&+ 2w\sqrt{21}\sinh(S_{31})\big),
\end{aligned}$$
$$S_{31} = \tfrac{1}{3}\, w\, (-6 + \sqrt{21}),$$
$$S_{32} = \tfrac{1}{3}\, w\, (6 + \sqrt{21}),$$
$$S_{33} = \tfrac{1}{6}\, w\, (2\sqrt{21} + 3),$$
$$S_{34} = \tfrac{1}{6}\, w\, (9 + 2\sqrt{21}),$$
$$S_{35} = \tfrac{1}{6}\, w\, (2\sqrt{21} - 3),$$
$$S_{36} = \tfrac{1}{6}\, w\, (-9 + 2\sqrt{21}),$$
$$\begin{aligned}
d_1 = \tfrac{1}{8}\big(&-3w^2\sqrt{21}\cosh(S_{39}) + 3w^2\sqrt{21}\cosh(S_{41}) - 3w^2\sqrt{21}\cosh(S_{42}) \\
&+ 8w\sqrt{21}\sinh(S_{41}) - 8w\sqrt{21}\sinh(S_{40}) + 24w\sqrt{21}\sinh(S_{39}) - 24w\sqrt{21}\sinh(S_{42}) \\
&- 12\cosh(S_{40}) + 36\cosh(S_{39}) - 36\cosh(S_{42}) + 12\cosh(S_{41}) + 3w^2\sqrt{21}\cosh(S_{40}) \\
&- 18w\sinh(S_{42}) + 18w\sinh(S_{41}) + 33w^2\cosh(S_{39}) - 33w^2\cosh(S_{42}) + 17w^2\cosh(S_{41}) \\
&- 17w^2\cosh(S_{40}) + 18w\sinh(S_{40}) - 18w\sinh(S_{39})\big)/\big(w^2(4\sinh(\tfrac{1}{3}w\sqrt{21})\,w
\end{aligned}$$

$$
\begin{aligned}
&+ 10\,w \sinh(S_{38}) + 10\,w \sinh(S_{37}) - 9\cosh(S_{38}) + 9\cosh(S_{37}) - 6\cosh(\tfrac{1}{3}\,w\,\sqrt{21})\,\sqrt{21} \\
&+ 3\sqrt{21}\cosh(S_{38}) + 3\sqrt{21}\cosh(S_{37}) - 2\,w\,\sqrt{21}\sinh(S_{38}) + 2\,w\,\sqrt{21}\sinh(S_{37}))\big), \\
&S_{37} = \tfrac{1}{3}\,w\,(-6+\sqrt{21}), \\
&S_{38} = \tfrac{1}{3}\,w\,(6+\sqrt{21}), \\
&S_{39} = \tfrac{1}{6}\,w\,(2\sqrt{21}+3), \\
&S_{40} = \tfrac{1}{6}\,w\,(9+2\sqrt{21}), \\
&S_{41} = \tfrac{1}{6}\,w\,(-9+2\sqrt{21}), \\
&S_{42} = \tfrac{1}{6}\,w\,(2\sqrt{21}-3), \\
d_2 &= \tfrac{3}{4}\big(22\sinh(\tfrac{1}{2}\,w)\,w + w\sinh(\tfrac{5}{2}\,w) - 9\,w\sinh(\tfrac{3}{2}\,w) + 4\cosh(\tfrac{1}{2}\,w) + 2\cosh(\tfrac{5}{2}\,w) - 6\cosh(\tfrac{3}{2}\,w)\big)/ \\
&\big(w^2(4\sinh(\tfrac{1}{3}\,w\,\sqrt{21})\,w + 10\,w\sinh(S_{44}) + 10\,w\sinh(S_{43}) - 9\cosh(S_{44}) + 9\cosh(S_{43}) \\
&- 6\cosh(\tfrac{1}{3}\,w\,\sqrt{21})\,\sqrt{21} + 3\sqrt{21}\cosh(S_{44}) + 3\sqrt{21}\cosh(S_{43}) - 2\,w\,\sqrt{21}\sinh(S_{44}) \\
&+ 2\,w\,\sqrt{21}\sinh(S_{43}))\big), \\
&S_{43} = \tfrac{1}{3}\,w\,(-6+\sqrt{21}), \\
&S_{44} = \tfrac{1}{3}\,w\,(6+\sqrt{21}). \qquad (63)
\end{aligned}
$$

Appendix F

$$
\begin{aligned}
c_0 &= \frac{451}{4352} - \frac{3211}{1775616}\,w^2 - \frac{2445823}{47813787648}\,w^4 + \frac{4001907731}{6145027988520960}\,w^6 \\
&+ \frac{597166167641357}{1434102051849067560960}\,w^8 - \frac{15449745768882434917}{3071846595060702715576320000}\,w^{10} \\
&+ \frac{613771437522347047212407}{1571655017124097451775743754240000}\,w^{12} \\
&- \frac{4393658945657064254276762749}{17505722242735047056858944232226816000}\,w^{14} + \cdots, \\
c_1 &= \frac{3901}{2176} + \frac{3211}{887808}\,w^2 + \frac{2445823}{23906893824}\,w^4 - \frac{4001907731}{3072513994260480}\,w^6 \\
&- \frac{597166167641357}{717051025924533780480}\,w^8 - \frac{16474834626837596 3}{1535923297530351357788160000}\,w^{10} \\
&\frac{2453503786185763572970 33}{7858275085620487258878718771200 0}\,w^{12} \\
&- \frac{26881153596485830424293940 51}{875286112136752352842947211611340 8000}\,w^{14} + \cdots, \\
c_2 &= -\frac{3967}{1044480} + \frac{93119}{426147840}\,w^2 - \frac{238457299}{80327163248640}\,w^4 - \frac{100832529217}{210686673892147200}\,w^6 \\
&+ \frac{26473419115079029}{481858289421286700482560}\,w^8 \\
&- \frac{5950569274099655743}{150457792411136459538432 0000}\,w^{10}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{63211306505625208566244139}{264038042876848371898324950712320000}\,w^{12}\\
&-\frac{8132174607689063497190745361}{60019619117948732766373523081920512000 0}\,w^{14}+\cdots,\\
c_3 &= \frac{70211}{456960}+\frac{266513}{186439680}\,w^2+\frac{1788502847}{35143133921280}\,w^4+\frac{524971765007}{645227938794700800}\,w^6\\
&-\frac{2262875218912381}{4216260032436258629 2224}\,w^8+\frac{46528191032221262831}{3225438924813737851355136 0000}\,w^{10}\\
&+\frac{5600312588614821667047833}{115516643758621162705517165936640000}\,w^{12}\\
&-\frac{15484931228512156056520038289}{183810083548717994097018914438381568 0000}\,w^{14}+\cdots,\\
c_4 &= \frac{387}{2437120}-\frac{9633}{331448320}\,w^2+\frac{21513797}{6941853614080}\,w^4-\frac{32352872623}{127452432354508800}\,w^6\\
&+\frac{2229629828948647}{12492622318329655197696 0}\,w^8\\
&-\frac{21914159576560202597}{191137121470443724524748 80000}\,w^{10}\\
&+\frac{480133840912449733490008 9}{684543074125162445662323946291 20000}\,w^{12}\\
&-\frac{15264609809617318475594187 19}{363081646515986161179296621112852480000}\,w^{14}+\cdots,\\
d_0 &= \frac{1}{2}-\frac{61}{92160}\,w^6+\frac{283}{1769472}\,w^8-\frac{137287}{6688604160}\,w^{10}+\frac{863953}{706316599296}\,w^{12}\\
&+\frac{43731142691}{385648863215616000}\,w^{14}+\cdots,\\
d_1 &= -\frac{47}{512}+\frac{183}{20480}\,w^2+\frac{179}{327680}\,w^4-\frac{6498257}{22295347200}\,w^6+\frac{1113076207}{23543886643200}\,w^8\\
&-\frac{1033277723411}{257099242143744000}\,w^{10}-\frac{13597048809341}{3332006178182922240 00}\,w^{12}\\
&+\frac{32427119523995353}{432554983858655723520000}\,w^{14}+\cdots,\\
d_2 &= \frac{15}{3584}\sqrt{21}-\frac{183}{143360}\,w^2\sqrt{21}+\frac{283}{1376256}\,w^4\sqrt{21}-\frac{3010543}{156067430400}\,w^6\sqrt{21}\\
&+\frac{3038527}{10987147100160}\,w^8\sqrt{21}+\frac{477793048211}{17996946950062080 00}\,w^{10}\sqrt{21}\\
&-\frac{143327944745}{2665604942546337792}\,w^{12}\sqrt{21}+\frac{61509757733996239}{1110224458570549690368 0000}\,w^{14}\sqrt{21}+\cdots.
\end{aligned}
\tag{64}
$$

Appendix G

PROGRAM SUMMARY

Title of program (32 characters maximum)*:* MAPLESIM

Catalogue identifier: ADLI

Program Summary URL:
http://cpc.cs.qub.ac.uk/summaries/ADLI

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Computer for which the program is designed and others on which it has been tested: IBM Compatible Pentium

Operating systems or monitors under which the program has been tested: DOS, Windows

Programming language used: Maple Language

Memory required to execute with typical data: words: 20 MBytes

No. of bits in a word: 16

No. of processors used: 1

Has the code been vectorized or parallelized?: No

No. of bytes in distributed program, including test data, etc.: 16 462

Distribution format: default ASCII else uuencoded compressed tar file

Keywords (descriptive of problem and method of solution)*:* Maple programming, construction of exponentially-fitted methods

Please enclose a summary (300 words maximum), under the following headings:

Nature of physical problem
With the present program the derivation of the coefficients produced by Eq. (14) is obtain. The first part of the proposed program consists of the calculation of the matrix elements which form the coefficients of the system of equations. The second part of the proposed program, as this has been explained in [20,22,23], consists of the iterative application of the L'Hospital's rule (to avoid coefficients of the form $\frac{0}{0}$) for the computation of the solution of these equations that make up the coefficients of the method (14). We note that the system of equations produced by Eq. (14) is solved by an application of Cramer's rule.
The above procedure is repeated for the calculation of the coefficients of the methods (24)–(25) and for the methods (28)–(29).

Method of solution: Symbolic Computation using Maple

Restrictions on the complexity of the problem: None

Typical running time: 1800 seconds

Unusual features of the program: None

Computer Algebra Program Written in Maple for the Derivation of the Formulae of the New Method

```
%
%
% Derivation of the coefficients produced by the equation (14).
% The first part of the proposed program consists of the calculation of the
% matrix elements which form the coefficients of the system of equations.
% The second part of the proposed program, as this has been explained
% in [20], [22] and [23], consists of the iteratiove application of the
% L'Hospital's rule (to avoid coefficients of the form 0/0) for the computation
% of the solution of these equations that make up the coefficients of the
% method (14).
%
% The elements of the matrices for the solution of the system of equations
% are determined.
%
```

par1:=-1; (formula of the coefficient of q_1)
par2:=$2w^2\cosh(w)$; (formula of the coefficient of t_0)
par3:=w^2; (formula of the coefficient of t_1)
par4:=$2w^2\cosh\left(\frac{w\sqrt{21}}{3}\right)$; (formula of the coefficient of t_2)
par5:=$2w^2\cosh\left(\frac{w}{2}\right)$; (formula of the coefficient of t_3)
par6:=$2\cosh(w)$; (formula of the right hand side of the equation)
par10:=subs($w = w_0$,par1);
par11:=subs($w = w_1$,par1);
par12:=subs($w = w_2$,par1);
par13:=subs($w = w_3$,par1);
par14:=subs($w = w_4$,par1);
par20:=subs($w = w_0$,par2);
par21:=subs($w = w_1$,par2);
par22:=subs($w = w_2$,par2);
par23:=subs($w = w_3$,par2);
par24:=subs($w = w_4$,par2);
par30:=subs($w = w_0$,par3);
par31:=subs($w = w_1$,par3);
par32:=subs($w = w_2$,par3);
par33:=subs($w = w_3$,par3);
par34:=subs($w = w_4$,par3);
par40:=subs($w = w_0$,par4);
par41:=subs($w = w_1$,par4);
par42:=subs($w = w_2$,par4);
par43:=subs($w = w_3$,par4);
par44:=subs($w = w_4$,par4);

```
par50:=subs(w = w0,par5);
par51:=subs(w = w1,par5);
par52:=subs(w = w2,par5);
par53:=subs(w = w3,par5);
par54:=subs(w = w4,par5);
par60:=subs(w = w0,par6);
par61:=subs(w = w1,par6);
par62:=subs(w = w2,par6);
par63:=subs(w = w3,par6);
par64:=subs(w = w4,par6);
with(linalg);
%
% Derivation of the denominator of the coefficients
%
matd:=array(1..5,1..5,[[par10,par20,par30,par40,par50],[par11,par21,par31,par41,par5
1], [par12,par22,par32,par42,par52], [par13,par23,par33,par43,par53], [par14,par24,
par34,par44,par54]]);
den=det(matd);
%
% The equations will be solved by an application of Cramer's rule.
% From the theory of exponentially-fitted methods it has been proved
% that to avoid divisions by zero valued determinants we must apply
% the L'Hospital's rule. Hence we find the appropriate derivatives of the
% determinants of the matrices. The theory shows that in order formula
% (14) integrates exactly (11), we must find:
%
% The 4th derivative w.r.t w0, the 3th derivative w.r.t w1, the 2nd
% derivative w.r.t w2 and the 1st derivative w.r.t w3.
%
%
den:=diff(den,w0$4);
den:=diff(den,w1$3);
den:=diff(den,w2$2);
den:=diff(den,w3$1);
%
% We subsititute the values w0 = w1 = w2 = w3 = w4 = w.
%
den:=subs(w0=w,den);
den:=subs(w1=w,den);
den:=subs(w2=w,den);
den:=subs(w3=w,den);
den:=subs(w4=w,den);
den:=combine(den);
%
% For the following matrices we repeat the steps described above.
% These will determine the appropriate numerators.
%
%
```

```
% Calculation of the coefficient q1.
%
matq1:=array(1..5,1..5,[[par60,par20,par30,par40,par50],[par61,par21,par31,par41,par
51], [par62,par22,par32,par42,par52], [par63,par23,par33,par43,par53], [par64,par24,
par34,par44,par54]]);
dq1=det(matq1);
dq1:=diff(dq1,w0$4);
dq1:=diff(dq1,w1$3);
dq1:=diff(dq1,w2$2);
dq1:=diff(dq1,w3$1);
dq1:=subs(w0=w,dq1);
dq1:=subs(w1=w,dq1);
dq1:=subs(w2=w,dq1);
dq1:=subs(w3=w,dq1);
dq1:=subs(w4=w,dq1);
dq1:=combine(dq1);
q1:=combine(dq1/den);
%
% Calculation of the coefficient t0.
%
matt0:=array(1..5,1..5,[[par10,par60,par30,par40,par50],[par11,par61,par31,par41,par
51], [par12,par62,par32,par42,par52], [par13,par63,par33,par43,par53], [par14,par64,
par34,par44,par54]]);
dt0=det(matt0);
dt0:=diff(dt0,w0$4);
dt0:=diff(dt0,w1$3);
dt0:=diff(dt0,w2$2);
dt0:=diff(dt0,w3$1);
dt0:=subs(w0=w,dt0);
dt0:=subs(w1=w,dt0);
dt0:=subs(w2=w,dt0);
dt0:=subs(w3=w,dt0);
dt0:=subs(w4=w,dt0);
dt0:=combine(dt0);
t0:=combine(dt0/den);
%
% Calculation of the coefficient t1.
%
matt1:=array(1..5,1..5,[[par10,par20,par60,par40,par50],[par11,par21,par61,par41,par
51], [par12,par22,par62,par42,par52], [par13,par23,par63,par43,par53], [par14,par24,
par64,par44,par54]]);
dt1=det(matt1);
dt1:=diff(dt1,w0$4);
dt1:=diff(dt1,w1$3);
dt1:=diff(dt1,w2$2);
dt1:=diff(dt1,w3$1);
dt1:=subs(w0=w,dt1);
dt1:=subs(w1=w,dt1);
```

```
dt1:=subs(w_2=w,dt1);
dt1:=subs(w_3=w,dt1);
dt1:=subs(w_4=w,dt1);
dt1:=combine(dt1);
t1:=combine(dt1/den);
%
% Calculation of the coefficient t_2.
%
matt2:=array(1..5,1..5,[[par10,par20,par30,par60,par50],[par11,par21,par31,par61,par
51], [par12,par22,par32,par62,par52], [par13,par23,par33,par63,par53], [par14,par24,
par34,par64,par54]]);
dt2=det(matt2);
dt2:=diff(dt2,w_0$4);
dt2:=diff(dt2,w_1$3);
dt2:=diff(dt2,w_2$2);
dt2:=diff(dt2,w_3$1);
dt2:=subs(w_0=w,dt2);
dt2:=subs(w_1=w,dt2);
dt2:=subs(w_2=w,dt2);
dt2:=subs(w_3=w,dt2);
dt2:=subs(w_4=w,dt2);
dt2:=combine(dt2);
t2:=combine(dt2/den);
%
% Calculation of the coefficient t_3.
%
matt3:=array(1..5,1..5,[[par10,par20,par30,par40,par60],[par11,par21,par31,par41,par
61], [par12,par22,par32,par42,par62], [par13,par23,par33,par43,par63], [par14,par24,
par34,par44,par64]]);
dt3=det(matt3);
dt3:=diff(dt3,w_0$4);
dt3:=diff(dt3,w_1$3);
dt3:=diff(dt3,w_2$2);
dt3:=diff(dt3,w_3$1);
dt3:=subs(w_0=w,dt3);
dt3:=subs(w_1=w,dt3);
dt3:=subs(w_2=w,dt3);
dt3:=subs(w_3=w,dt3);
dt3:=subs(w_4=w,dt3);
dt3:=combine(dt3);
t3:=combine(dt3/den);


%
% Taylor series expansion of the coefficients.
%
q1t:=convert(taylor(q1,w=0,26),polynom);
```

```
t0t:=convert(taylor(t0,w=0,26),polynom);
t1t:=convert(taylor(t1,w=0,26),polynom);
t2t:=convert(taylor(t2,w=0,26),polynom);
t3t:=convert(taylor(t3,w=0,26),polynom);
%
%
% We repeat, now, the above procedure for the calculation
% of the coefficients of the methods (16)-(17)
%
%
% Calculation of the coefficients of the formula (16)
%
```

par1:= $2\cosh(w)$; (formula of the coefficient of a_0)
par2:=1; (formula of the coefficient of a_1)
par3:= $2w^2\cosh(w)$; (formula of the coefficient of a_2)
par4:= w^2; (formula of the coefficient of a_3)
par5:=$2\cosh\left(\frac{w\sqrt{21}}{3}\right)$; (formula of the right hand side of the equation)

```
par10:=subs(w = w0,par1);
par11:=subs(w = w1,par1);
par12:=subs(w = w2,par1);
par13:=subs(w = w3,par1);
par20:=subs(w = w0,par2);
par21:=subs(w = w1,par2);
par22:=subs(w = w2,par2);
par23:=subs(w = w3,par2);
par30:=subs(w = w0,par3);
par31:=subs(w = w1,par3);
par32:=subs(w = w2,par3);
par33:=subs(w = w3,par3);
par40:=subs(w = w0,par4);
par41:=subs(w = w1,par4);
par42:=subs(w = w2,par4);
par43:=subs(w = w3,par4);
par50:=subs(w = w0,par5);
par51:=subs(w = w1,par5);
par52:=subs(w = w2,par5);
par53:=subs(w = w3,par5);
with(linalg);


%
% Derivation of the denominator of the coefficients
%
matd:=array(1..4,1..4,[[par10,par20,par30,par40],[par11,par21,par31,par41],
[par12,par22,par32,par42], [par13,par23,par33,par43]]);
```

```
den=det(matd);
%
% The theory shows that in order formula (16) integrates exactly (20)-(21),
% we must find:
%
% The 3th derivative w.r.t w0, the 2nd derivative w.r.t w1
% and the 1st derivative w.r.t w2.
%
%
den:=diff(den,w0$3);
den:=diff(den,w1$2);
den:=diff(den,w2$1);
%
% We substitute the values w0 = w1 = w2 = w3 = w.
%
den:=subs(w0=w,den);
den:=subs(w1=w,den);
den:=subs(w2=w,den);
den:=subs(w3=w,den);
den:=combine(den);
%
% Calculation of the coefficient a0 .
%
mata0:=array(1..4,1..4,[[par50,par20,par30,par40],[par51,par21,par31,par41],
[par52,par22,par32,par42], [par53,par23,par33,par43]]);
da0=det(mata0);
da0:=diff(da0,w0$3);
da0:=diff(da0,w1$2);
da0:=diff(da0,w2$1);
da0:=subs(w0=w,da0);
da0:=subs(w1=w,da0);
da0:=subs(w2=w,da0);
da0:=subs(w3=w,da0);
da0:=combine(da0);
a0:=combine(da0/den);

%
% Calculation of the coefficient a1 .
%
mata1:=array(1..4,1..4,[[par10,par50,par30,par40],[par11,par51,par31,par41],
[par12,par52,par32,par42], [par13,par53,par33,par43]]);
da1=det(mata1);
da1:=diff(da1,w0$3);
da1:=diff(da1,w1$2);
da1:=diff(da1,w2$1);
da1:=subs(w0=w,da1);
da1:=subs(w1=w,da1);
da1:=subs(w2=w,da1);
```

```
da1:=subs(w3=w,da1);
da1:=combine(da1);
a1:=combine(da1/den);
%
% Calculation of the coefficient a2 .
%
mata2:=array(1..5,1..5,[[par10,par20,par50,par40],[par11,par21,par51,par41],
[par12,par22,par52,par42], [par13,par23,par53,par43]]);
da2=det(mata2);
da2:=diff(da2,w0$3);
da2:=diff(da2,w1$2);
da2:=diff(da2,w2$1);
da2:=subs(w0=w,da2);
da2:=subs(w1=w,da2);
da2:=subs(w2=w,da2);
da2:=subs(w3=w,da2);
da2:=combine(da2);
a2:=combine(da2/den);
%
% Calculation of the coefficient a3 .
%
mata3:=array(1..5,1..5,[[par10,par20,par30,par50],[par11,par21,par31,par51],
[par12,par22,par32,par52], [par13,par23,par33,par53]]);
da3=det(mata3);
da3:=diff(da3,w0$3);
da3:=diff(da3,w1$2);
da3:=diff(da3,w2$1);
da3:=subs(w0=w,da3);
da3:=subs(w1=w,da3);
da3:=subs(w2=w,da3);
da3:=subs(w3=w,da3);
da3:=combine(da3);
a3:=combine(da3/den);
%
% Taylor series expansion of the coefficients.
%
a0t:=convert(taylor(a0,w=0,26),polynom);
a1t:=convert(taylor(a1,w=0,26),polynom);
a2t:=convert(taylor(a2,w=0,26),polynom);
a3t:=convert(taylor(a3,w=0,26),polynom);
%
%
% Calculation of the coefficients of the formula (17)
%
par1:= 2sinh(w); (formula of the coefficient of b0)
par2:= 2w^2 sinh(w); (formula of the coefficient of b1)
```

```
par3:=2 sinh(w√21/3); (formula of the right hand side of the equation)
par10:=subs(w = w0,par1);
par11:=subs(w = w1,par1);
par20:=subs(w = w0,par2);
par21:=subs(w = w1,par2);
par30:=subs(w = w0,par3);
par31:=subs(w = w1,par3);
with(linalg);
%
% Derivation of the denominator of the coefficients
%
matd:=array(1..2,1..2,[[par10,par20],[par11,par21]]);
den=det(matd);
%
% The theory shows that in order formula (17) integrates exactly (22)-(23),
% we must find:
%
% The 1st derivative w.r.t w0.
%
%
den:=diff(den,w0$1);
%
% We subsititute the values w0 = w1 = w.
%
den:=subs(w0=w,den);
den:=subs(w1=w,den);
den:=combine(den);
%
% Calculation of the coefficient b0.
%
matb0:=array(1..4,1..4,[[par30,par20],[par31,par21]]);
db0=det(matb0);
db0:=diff(db0,w0$1);
db0:=subs(w0=w,db0);
db0:=subs(w1=w,db0);
db0:=combine(db0);
b0:=combine(db0/den);
%
% Calculation of the coefficient b1.
%
matb1:=array(1..4,1..4,[[par10,par30],[par11,par31]]);
db1=det(matb1);
db1:=diff(db1,w0$1);
db1:=subs(w0=w,db1);
db1:=subs(w1=w,db1);
db1:=combine(db1);
```

```
b1:=combine(db1/den);
%
% Taylor series expansion of the coefficients.
%
b0t:=convert(taylor(b0,w=0,26),polynom);
b1t:=convert(taylor(b1,w=0,26),polynom);
%
%
% We repeat, now, the above procedure for the calculation
% of the coefficients of the methods (18)-(19)
%
%
% Calculation of the coefficients of the formula (18)
%
```

par1:= $2\cosh(w)$; (formula of the coefficient of c_0)
par2:=1; (formula of the coefficient of c_1)
par3:= $2w^2\cosh(w)$; (formula of the coefficient of c_2)
par4:= w^2; (formula of the coefficient of c_3)
par5:= $2w^2\cosh\left(\frac{w\sqrt{21}}{3}\right)$; (formula of the coefficient of c_4)
par6:= $2w^2\cosh\left(\frac{w}{2}\right)$; (formula of the right hand side of the equation)
par10:=subs($w = w_0$,par1);
par11:=subs($w = w_1$,par1);
par12:=subs($w = w_2$,par1);
par13:=subs($w = w_3$,par1);
par14:=subs($w = w_4$,par1);
par20:=subs($w = w_0$,par2);
par21:=subs($w = w_1$,par2);
par22:=subs($w = w_2$,par2);
par23:=subs($w = w_3$,par2);
par24:=subs($w = w_4$,par2);
par30:=subs($w = w_0$,par3);
par31:=subs($w = w_1$,par3);
par32:=subs($w = w_2$,par3);
par33:=subs($w = w_3$,par3);
par34:=subs($w = w_4$,par3);
par40:=subs($w = w_0$,par4);
par41:=subs($w = w_1$,par4);
par42:=subs($w = w_2$,par4);
par43:=subs($w = w_3$,par4);
par44:=subs($w = w_4$,par4);
par50:=subs($w = w_0$,par5);
par51:=subs($w = w_1$,par5);
par52:=subs($w = w_2$,par5);
par53:=subs($w = w_3$,par5);
par54:=subs($w = w_4$,par5);

```
par60:=subs(w = w_0,par6);
par61:=subs(w = w_1,par6);
par62:=subs(w = w_2,par6);
par63:=subs(w = w_3,par6);
par64:=subs(w = w_4,par6);
with(linalg);
%
% Derivation of the denominator of the coefficients
%
matd:=array(1..5,1..5,[[par10,par20,par30,par40,par50],[par11,par21,par31,par41,par5
1], [par12,par22,par32,par42,par52], [par13,par23,par33,par43,par53], [par14,par24,
par34,par44,par54]]);
den=det(matd);
%
% The theory shows that in order formula (18) integrates exactly (11), we must find:
%
% The 4th derivative w.r.t w_0, the 3th derivative w.r.t w_1, the 2nd
% derivative w.r.t w_2 and the 1st derivative w.r.t w_3.
%
%
den:=diff(den,w_0$4);
den:=diff(den,w_1$3);
den:=diff(den,w_2$2);
den:=diff(den,w_3$1);
%
% We subsititute the values w_0 = w_1 = w_2 = w_3 = w_4 = w.
%
den:=subs(w_0=w,den);
den:=subs(w_1=w,den);
den:=subs(w_2=w,den);
den:=subs(w_3=w,den);
den:=subs(w_4=w,den);
den:=combine(den);
%
% Calculation of the coefficient c_0.
%
matc0:=array(1..5,1..5,[[par60,par20,par30,par40,par50],[par61,par21,par31,par41,par
51], [par62,par22,par32,par42,par52], [par63,par23,par33,par43,par53], [par64,par24,
par34,par44,par54]]);
dc0=det(matc0);
dc0:=diff(dc0,w_0$4);
dc0:=diff(dc0,w_1$3);
dc0:=diff(dc0,w_2$2);
dc0:=diff(dc0,w_3$1);
dc0:=subs(w_0=w,dc0);
dc0:=subs(w_1=w,dc0);
dc0:=subs(w_2=w,dc0);
dc0:=subs(w_3=w,dc0);
```

```
dc0:=subs(w_4=w,dc0);
dc0:=combine(dc0);
c0:=combine(dc0/den);
%
% Calculation of the coefficient c_1.
%
matc1:=array(1..5,1..5,[[par10,par60,par30,par40,par50],[par11,par61,par31,par41,par
51], [par12,par62,par32,par42,par52], [par13,par63,par33,par43,par53], [par14,par64,
par34,par44,par54]]);
dc1=det(matc1);
dc1:=diff(dc1,w_0$4);
dc1:=diff(dc1,w_1$3);
dc1:=diff(dc1,w_2$2);
dc1:=diff(dc1,w_3$1);
dc1:=subs(w_0=w,dc1);
dc1:=subs(w_1=w,dc1);
dc1:=subs(w_2=w,dc1);
dc1:=subs(w_3=w,dc1);
dc1:=subs(w_4=w,dc1);
dc1:=combine(dc1);
c1:=combine(dc1/den);
%
% Calculation of the coefficient c_2.
%
matc2:=array(1..5,1..5,[[par10,par20,par60,par40,par50],[par11,par21,par61,par41,par
51], [par12,par22,par62,par42,par52], [par13,par23,par63,par43,par53], [par14,par24,
par64,par44,par54]]);
dc2=det(matc2);
dc2:=diff(dc2,w_0$4);
dc2:=diff(dc2,w_1$3);
dc2:=diff(dc2,w_2$2);
dc2:=diff(dc2,w_3$1);
dc2:=subs(w_0=w,dc2);
dc2:=subs(w_1=w,dc2);
dc2:=subs(w_2=w,dc2);
dc2:=subs(w_3=w,dc2);
dc2:=subs(w_4=w,dc2);
dc2:=combine(dc2);
c2:=combine(dc2/den);
%
% Calculation of the coefficient c_3.
%
matc3:=array(1..5,1..5,[[par10,par20,par30,par60,par50],[par11,par21,par31,par61,par
51], [par12,par22,par32,par62,par52], [par13,par23,par33,par63,par53], [par14,par24,
par34,par64,par54]]);
dc3=det(matc3);
dc3:=diff(dc3,w_0$4);
dc3:=diff(dc3,w_1$3);
```

```
dc3:=diff(dc3,w_2$2);
dc3:=diff(dc3,w_3$1);
dc3:=subs(w_0=w,dc3);
dc3:=subs(w_1=w,dc3);
dc3:=subs(w_2=w,dc3);
dc3:=subs(w_3=w,dc3);
dc3:=subs(w_4=w,dc3);
dc3:=combine(dc3);
c3:=combine(dc3/den);
%
% Calculation of the coefficient c_4.
%
matc4:=array(1..5,1..5,[[par10,par20,par30,par40,par60],[par11,par21,par31,par41,par
61], [par12,par22,par32,par42,par62], [par13,par23,par33,par43,par63], [par14,par24,
par34,par44,par64]]);
dc4=det(matc4);
dc4:=diff(dc4,w_0$4);
dc4:=diff(dc4,w_1$3);
dc4:=diff(dc4,w_2$2);
dc4:=diff(dc4,w_3$1);
dc4:=subs(w_0=w,dc4);
dc4:=subs(w_1=w,dc4);
dc4:=subs(w_2=w,dc4);
dc4:=subs(w_3=w,dc4);
dc4:=subs(w_4=w,dc4);
dc4:=combine(dc4);
c4:=combine(dc4/den);
%
% Taylor series expansion of the coefficients.
%
c0t:=convert(taylor(c0,w=0,26),polynom);
c1t:=convert(taylor(c1,w=0,26),polynom);
c2t:=convert(taylor(c2,w=0,26),polynom);
c3t:=convert(taylor(c3,w=0,26),polynom);
c4t:=convert(taylor(c4,w=0,26),polynom);
```

```
%
% Calculation of the coefficients of the formula (19)
%
```

par1:= $2\sinh(w)$; (formula of the coefficient of d_0)

par2:= $2w^2\sinh(w)$; (formula of the coefficient of d_1)

par3:= $2w^2\sinh\left(\frac{w\sqrt{21}}{3}\right)$; (formula of the coefficient of d_2)

par4:= $2w^2\sinh\left(\frac{w}{2}\right)$; (formula of the right hand side of the equation)

```
par10:=subs(w = w0,par1);
par11:=subs(w = w1,par1);
par12:=subs(w = w2,par1);
par20:=subs(w = w0,par2);
par21:=subs(w = w1,par2);
par22:=subs(w = w2,par2);
par30:=subs(w = w0,par3);
par31:=subs(w = w1,par3);
par32:=subs(w = w2,par3);
par40:=subs(w = w0,par4);
par41:=subs(w = w1,par4);
par42:=subs(w = w2,par4);
with(linalg);
%
% Derivation of the denominator of the coefficients
%
matd:=array(1..3,1..3,[[par10,par20,par30],[par11,par21,par31], [par12,par22,
par32]]);
den=det(matd);
%
% The theory shows that in order formula (19) integrates exactly (26)-(27), we must
find:
%
% The 2nd derivative w.r.t w0 and the 1st derivative w.r.t w1.
%
%
den:=diff(den,w0$2);
den:=diff(den,w1$1);
%
% We subsititute the values w0 = w1 = w2 = w.
%
den:=subs(w0=w,den);
den:=subs(w1=w,den);
den:=subs(w2=w,den);
den:=combine(den);


%
% Calculation of the coefficient d0.
%
matd0:=array(1..3,1..3,[[par40,par20,par30],[par41,par21,par31], [par42,par22,
par32]]);
dd0=det(matd0);
dd0:=diff(dd0,w0$2);
dd0:=diff(dd0,w1$1);
dd0:=subs(w0=w,dd0);
dd0:=subs(w1=w,dd0);
dd0:=subs(w2=w,dd0);
```

```
dd0:=combine(dd0);
d0:=combine(dd0/den);
%
% Calculation of the coefficient d1.
%
matd1:=array(1..3,1..3,[[par10,par40,par30],[par11,par41,par31], [par12,par42,
par32]]);
dd1=det(matd1);
dd1:=diff(dd1,w0$2);
dd1:=diff(dd1,w1$1);
dd1:=subs(w0=w,dd1);
dd1:=subs(w1=w,dd1);
dd1:=subs(w2=w,dd1);
dd1:=combine(dd1);
d1:=combine(dd1/den);
%
% Calculation of the coefficient d2.
%
matd2:=array(1..3,1..3,[[par10,par20,par40],[par11,par21,par41], [par12,par22,
par42]]);
dd2=det(matd2);
dd2:=diff(dd2,w0$2);
dd2:=diff(dd2,w1$1);
dd2:=subs(w0=w,dd2);
dd2:=subs(w1=w,dd2);
dd2:=subs(w2=w,dd2);
dd2:=combine(dd2);
d2:=combine(dd2/den);
%
% Taylor series expansion of the coefficients.
%
d0t:=convert(taylor(d0,w=0,26),polynom);
d1t:=convert(taylor(d1,w=0,26),polynom);
d2t:=convert(taylor(d2,w=0,26),polynom);
```