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A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems

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In this paper a family of trigonometrically-fitted symmetric ten-step methods for the efficient solution of the Schrödinger equation and related problems is presented. Construction and stability analysis of the new methods is described. Numerical results obtained for the resonance problem of the one-dimensional Schrödinger equation show the efficiency of the new methods when they are compared with known methods in the literature.

KEY WORDS: numerical solution, initial-value problems (IVPs), explicit methods, symmetric methods, trigonometric-fitting, multistep methods

AMS subject classification: 65L05, 65L06

1. Introduction

The investigation of the integration of second order differential equations of the form

$$\mathbf{y}''(\mathbf{x}) = \mathbf{f}(\mathbf{x}, \mathbf{y}), \quad \mathbf{y}(\mathbf{x}_0) = \mathbf{y}_0, \quad \mathbf{y}'(\mathbf{x}_0) = \mathbf{y}'_0, \tag{1}$$

where the function **f** is independent of the first derivative of **y**, is presented in this paper. This type of equations are very important (especially when their solution has oscillatory behavior) in many areas of quantum mechanics, quantum chemistry, physical chemistry and chemical physics, celestial mechanics, astrophysics, astronomy, electronics (see [1,2]).

For the approximate solution of the above differential equations the most important properties are the following: (i) algebraic order of the method, (ii) interval of periodicity of the method, (iii) minimization of the phase-lag of the method, (iv) symmetry of the method, (v) exponential fitting and in special cases (vi) adaptive properties such as

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Bessel and Neumann fitting. For more details for one the above one can see [3–5]. The development of methods with these properties is an open problem.

In [5] Simos has divided the methods for the solution of (1) into two categories:

(1) methods with constant coefficients and

(2) methods with coefficients dependent on the frequency of the problem.

For the first category of methods important properties are the properties (i)–(iv) mentioned above while for the second category of methods important properties are (i), (ii) and (iv) and (v) or (vi) mentioned above.

In the last two decades there has been much research for the numerical solution of (1) (see [6–12] and references therein, [13–42]. For a complete reference about the methods developed for the solution of (1) see [3–5,43] and references therein. We note that the most finite difference methods developed in the literature for the numerical solution of (1) belong to the class of multistep and hybrid techniques.

As we have mentioned above a useful approach for developing powerful methods for the approximate solution of second order initial value problems with oscillating or periodic solution is to use exponential fitting, first introduced by Lyche [44], especially in cases of the Schrödinger type equations. Raptis and Allison [19] have produced a Numerov type exponentially fitted method. The numerical results obtained in [19] indicate that these fitted methods are much more efficient than Numerov's method for the solution of the Schrödinger type equations. Generally for the Schrödinger equation and related problems the methods with coefficients dependent on the frequency of the problem are much more efficient than the methods with constant coefficients.

A popular family of multistep methods for the solution of (1) is the family of Störmer–Cowell methods. These methods have been widely used for long-term integrations of planetary orbits (see Quinlan and Tremaine [45] and references therein). A characteristic of these methods is the *orbital instability* when the number of steps exceeds 2. This characteristic exists since the methods are *dissipative*, i.e., non-symmetric and as consequence they have empty interval of periodicity. In order to solve the problem of orbital instability, Lambert and Watson [46] have constructed the symmetric multistep methods and the property of the interval of periodicity. Lambert and Watson have proved that the symmetric methods have nonvanishing interval of periodicity (which is the interval of guaranteed periodic solution and is determined by the application of the symmetric multistep method to the test equation $y''(t) = -q^2 y(t)$; if $q^2h^2 \in (0, T^2)$, where h is the steplength of the integration, then this interval is called interval of periodicity). Quinlan and Tremaine [45] have constructed high order symmetric multistep methods based on the work of Lambert and Watson. We note here that the linear symmetric multistep methods developed by Lambert and Watson [46] and Quinlan and Tremaine [45] are much simpler than the hybrid (Runge–Kutta type) methods. For the above reasons of simplicity and accuracy in long-time integration of periodic initial value problems we give attention to this family of methods.

The purpose of this paper is to construct a family of trigonometrically-fitted linear symmetric ten-step methods for the efficient solution of the Schrödinger equation and related problems.

The paper is constucted as follows. In section 2 a family of trigonometrically-fitted simple *linear multistep methods* are developed. These methods are based on a linear classical (with constant coefficients) ten-step method developed by Jenkins [47]. In section 3 a stability analysis for the methods developed in section 2 is presented. In section 4 numerical illustrations are presented. Finally, in section 5 concluding remarks are presented.

2. Family of trigonometrically-fitted eighth algebraic order symmetric methods

2.1. First trigonometrically-fitted method of the family

We consider the symmetric multistep explicit method:

$$\begin{aligned} &y_{n+9/2} - y_{n+7/2} - y_{n-7/2} + y_{n-9/2} \\ &\quad = h^2\big(c_0 y''_{n+7/2} + c_1 y''_{n+5/2} + c_2 y''_{n+3/2} + c_3 y''_{n+1/2} \\ &\qquad + c_3 y''_{n-1/2} + c_2 y''_{n-3/2} + c_1 y''_{n-5/2} + c_0 y''_{n-7/2}\big). \end{aligned} \tag{2}$$

In order the above method to be exact for any linear combination of the functions

$$\big\{1, x, x^2, x^3, x^4, x^5, \cos(\pm wx), \sin(\pm wx), x\cos(\pm wx), x\sin(\pm wx)\big\}, \tag{3}$$

the following system of equations must hold:

$$\begin{aligned} &4 = c_0 + c_2 + c_3 + c_1, \\ &260 = 147c_0 + 75c_1 + 27c_2 + 3c_3, \\ &2\cos\left(\frac{9}{2}wh\right) - 2\cos\left(\frac{7}{2}wh\right) \\ &\quad = -2h^2w^2c_1\cos\left(\frac{5}{2}wh\right) - 2h^2w^2c_3\cos\left(\frac{1}{2}wh\right) - 2h^2w^2c_2\cos\left(\frac{3}{2}wh\right) \\ &\qquad - 2h^2w^2c_0\cos\left(\frac{7}{2}wh\right) - h\left(-9\sin\left(\frac{9}{2}wh\right) + 7\sin\left(\frac{7}{2}wh)\right)\right) \\ &\quad = -h^2w\left(-4c_0\cos\left(\frac{7}{2}wh\right) + 7c_0w\sin\left(\frac{7}{2}wh\right)h - 4c_1\cos\left(\frac{5}{2}wh\right)\right. \\ &\qquad + 5c_1w\sin\left(\frac{5}{2}wh\right)h - 4c_2\cos\left(\frac{3}{2}wh\right) + 3c_2w\sin\left(\frac{3}{2}wh\right)h \\ &\qquad \left. - 4c_3\cos\left(\frac{1}{2}wh\right) + c_3w\sin\left(\frac{1}{2}wh\right)h\right). \end{aligned} \tag{4}$$

The solution of the above system of equations is given in appendix A. For small values of v the given formulae are subject to heavy cancelations. In this case the Taylor series expansions given in appendix B must be used.

The local truncation error of the above method is given by:

$$LTE(h) = \frac{h^{10}}{64800}\left(8183 y_n^{(10)} + 16366 v^2 y_n^{(8)} + 8183 v^4 y_n^{(6)}\right). \tag{5}$$

2.2. Second trigonometrically-fitted method of the family

If we require the above method to be exact for any linear combination of the functions:

$$\begin{aligned}&\big\{1, x, x^2, \cos(\pm wx), \sin(\pm wx), x\cos(\pm wx), x\sin(\pm wx),\\ &x^2\cos(\pm wx), x^2\sin(\pm wx)\big\},\end{aligned} \tag{6}$$

the following system of equations must hold:

$$\begin{aligned}
&4 = c_0 + c_2 + c_3 + c_1,\\
&2\cos\left(\frac{9}{2}wh\right) - 2\cos\left(\frac{7}{2}wh\right)\\
&\quad = -2h^2w^2c_1\cos\left(\frac{5}{2}wh\right) - 2h^2w^2c_3\cos\left(\frac{1}{2}wh\right) - 2h^2w^2c_2\cos\left(\frac{3}{2}wh\right)\\
&\qquad - 2h^2w^2c_0\cos\left(\frac{7}{2}wh\right) - h\left(-9\sin\left(\frac{9}{2}wh\right) + 7\sin\left(\frac{7}{2}wh\right)\right)\\
&\quad = -h^2w\left(-4c_0\cos\left(\frac{7}{2}wh\right) + 7c_0w\sin\left(\frac{7}{2}wh\right)h - 4c_1\cos\left(\frac{5}{2}wh\right)\right.\\
&\qquad\qquad + 5c_1w\sin\left(\frac{5}{2}wh\right)h - 4c_2\cos\left(\frac{3}{2}wh\right) + 3c_2w\sin\left(\frac{3}{2}wh\right)h\\
&\qquad\qquad \left.- 4c_3\cos\left(\frac{1}{2}wh\right) + c_3w\sin\left(\frac{1}{2}wh\right)h\right),\\
&2\cos\left(\frac{9}{2}wh\right)x^2 + \frac{81}{2}\cos\left(\frac{9}{2}wh\right)h^2 - 2\cos\left(\frac{7}{2}wh\right)x^2 - \frac{49}{2}\cos\left(\frac{7}{2}wh\right)h^2\\
&\quad = -\frac{1}{2}h^2\left(h^2w^2c_3\cos\left(\frac{1}{2}wh\right) + 40c_1w\sin\left(\frac{5}{2}wh\right)h + 24c_2w\sin\left(\frac{3}{2}wh\right)h\right.\\
&\qquad + 56c_0w\sin\left(\frac{7}{2}wh\right)h + 9h^2w^2c_2\cos\left(\frac{3}{2}wh\right) + 25h^2w^2c_1\cos\left(\frac{5}{2}wh\right)\\
&\qquad + 4c_0w^2\cos\left(\frac{7}{2}wh\right)x^2 + 4c_3w^2\cos\left(\frac{1}{2}wh\right)x^2 + 4c_1w^2\cos\left(\frac{5}{2}wh\right)x^2
\end{aligned} \tag{7}$$

$$
\begin{aligned}
&+ 4c_2 w^2 \cos\left(\frac{3}{2}wh\right)x^2 + 49h^2w^2c_0\cos\left(\frac{7}{2}wh\right) - 8c_3\cos\left(\frac{1}{2}wh\right) \\
&- 8c_2\cos\left(\frac{3}{2}wh\right) - 8c_1\cos\left(\frac{5}{2}wh\right) - 8c_0\cos\left(\frac{7}{2}wh\right) + 8c_3 w\sin\left(\frac{1}{2}wh\right)h\Big), \\
&-2xh\left(-9\sin\left(\frac{9}{2}wh\right) + 7\sin\left(\frac{7}{2}wh\right)\right) \\
= {}&-2h^2wx\Big(-4c_0\cos\left(\frac{7}{2}wh\right) + 7c_0w\sin\left(\frac{7}{2}wh\right)h - 4c_1\cos\left(\frac{5}{2}wh\right) \\
&\quad + 5c_1w\sin\left(\frac{5}{2}wh\right)h - 4c_2\cos\left(\frac{3}{2}wh\right) + 3c_2w\sin\left(\frac{3}{2}wh\right)h \\
&\quad - 4c_3\cos\left(\frac{1}{2}wh\right) + c_3w\sin\left(\frac{1}{2}wh\right)h\Big).
\end{aligned}
$$

The solution of the above system of equations is given in appendix C. For small values of v the given formulae are subject to heavy cancelations. In this case the Taylor series expansions given in appendix D must be used.

The local truncation error of the above method is given by

$$
LTE(h) = \frac{h^{10}}{64800}\left(8183y_n^{(10)} + 24549v^2y_n^{(8)} + 24549v^4y_n^{(6)} + 8183v^6y_n^{(4)}\right). \tag{8}
$$

2.3. *Third trigonometrically-fitted method of the family*

If we require the above method to be exact for any linear combination of the functions:

$$
\begin{aligned}
&\{1, x, \cos(\pm wx), \sin(\pm wx), x\cos(\pm wx), x\sin(\pm wx), x^2\cos(\pm wx), \\
&x^2\sin(\pm wx), x^3\cos(\pm wx), x^3\sin(\pm wx)\},
\end{aligned} \tag{9}
$$

the following system of equations must hold:

$$
\begin{aligned}
&2\cos\left(\frac{9}{2}wh\right) - 2\cos\left(\frac{7}{2}wh\right) \\
&= -2h^2w^2c_1\cos\left(\frac{5}{2}wh\right) - 2h^2w^2c_3\cos\left(\frac{1}{2}wh\right) - 2h^2w^2c_2\cos\left(\frac{3}{2}wh\right) \\
&\quad - 2h^2w^2c_0\cos\left(\frac{7}{2}wh\right) - h\left(-9\sin\left(\frac{9}{2}wh\right) + 7\sin\left(\frac{7}{2}wh\right)\right) \\
&= -h^2w\left(-4c_0\cos\left(\frac{7}{2}wh\right) + 7c_0w\sin\left(\frac{7}{2}wh\right)h - 4c_1\cos\left(\frac{5}{2}wh\right)\right.
\end{aligned}
$$

$$
\begin{aligned}
&+ 5c_1 w \sin\left(\frac{5}{2}wh\right)h - 4c_2 \cos\left(\frac{3}{2}wh\right) + 3c_2 w \sin\left(\frac{3}{2}wh\right)h - 4c_3 \cos\left(\frac{1}{2}wh\right) \\
&+ c_3 w \sin\left(\frac{1}{2}wh\right)h\Bigg),
\end{aligned}
$$

$$
\begin{aligned}
&2\cos\left(\frac{9}{2}wh\right)x^2 + \frac{81}{2}\cos\left(\frac{9}{2}wh\right)h^2 - 2\cos\left(\frac{7}{2}wh\right)x^2 - \frac{49}{2}\cos\left(\frac{7}{2}wh\right)h^2 \\
&= -\frac{1}{2}h^2\Bigg(h^2w^2c_3\cos\left(\frac{1}{2}wh\right) + 40c_1 w\sin\left(\frac{5}{2}wh\right)h + 24c_2 w\sin\left(\frac{3}{2}wh\right)h \\
&\quad + 56c_0 w\sin\left(\frac{7}{2}wh\right)h + 9h^2w^2c_2\cos\left(\frac{3}{2}wh\right) + 25h^2w^2c_1\cos\left(\frac{5}{2}wh\right) \\
&\quad + 4c_0w^2\cos\left(\frac{7}{2}wh\right)x^2 + 4c_3w^2\cos\left(\frac{1}{2}wh\right)x^2 + 4c_1w^2\cos\left(\frac{5}{2}wh\right)x^2 \\
&\quad + 4c_2w^2\cos\left(\frac{3}{2}wh\right)x^2 + 49h^2w^2c_0\cos\left(\frac{7}{2}wh\right) - 8c_3\cos\left(\frac{1}{2}wh\right) \\
&\quad - 8c_2\cos\left(\frac{3}{2}wh\right) - 8c_1\cos\left(\frac{5}{2}wh\right) - 8c_0\cos\left(\frac{7}{2}wh\right) + 8c_3 w\sin\left(\frac{1}{2}wh\right)h\Bigg) \\
&\quad - 2xh\left(-9\sin\left(\frac{9}{2}wh\right) + 7\sin\left(\frac{7}{2}wh\right)\right) \\
&= -2h^2wx\Bigg(-4c_0\cos\left(\frac{7}{2}wh\right) + 7c_0 w\sin\left(\frac{7}{2}wh\right)h - 4c_1\cos\left(\frac{5}{2}wh\right) \\
&\qquad + 5c_1 w\sin\left(\frac{5}{2}wh\right)h - 4c_2\cos\left(\frac{3}{2}wh\right) + 3c_2 w\sin\left(\frac{3}{2}wh\right)h \qquad (10) \\
&\qquad - 4c_3\cos\left(\frac{1}{2}wh\right) + c_3 w\sin\left(\frac{1}{2}wh\right)h\Bigg),
\end{aligned}
$$

$$
\begin{aligned}
&2\cos\left(\frac{9}{2}wh\right)x^3 + \frac{243}{2}\cos\left(\frac{9}{2}wh\right)xh^2 - 2\cos\left(\frac{7}{2}wh\right)x^3 - \frac{147}{2}\cos\left(\frac{7}{2}wh\right)xh^2 \\
&= -\frac{1}{2}h^2x\Bigg(72c_2 w\sin\left(\frac{3}{2}wh\right)h + 147h^2w^2c_0\cos\left(\frac{7}{2}wh\right) + 75h^2w^2c_1\cos\left(\frac{5}{2}wh\right) \\
&\quad + 27h^2w^2c_2\cos\left(\frac{3}{2}wh\right) + 3h^2w^2c_3\cos\left(\frac{1}{2}wh\right) + 168c_0 w\sin\left(\frac{7}{2}wh\right)h \\
&\quad + 120c_1 w\sin\left(\frac{5}{2}wh\right)h + 4c_3w^2\cos\left(\frac{1}{2}wh\right)x^2 - 24c_3\cos\left(\frac{1}{2}wh\right) \\
&\quad + 4c_2w^2\cos\left(\frac{3}{2}wh\right)x^2 + 4c_0w^2\cos\left(\frac{7}{2}wh\right)x^2 - 24c_0\cos\left(\frac{7}{2}wh\right) \\
&\quad + 4c_1w^2\cos\left(\frac{5}{2}wh\right)x^2 - 24c_2\cos\left(\frac{3}{2}wh\right) - 24c_1\cos\left(\frac{5}{2}wh\right)
\end{aligned}
$$

$$
\begin{aligned}
&+ 24c_3 w \sin\left(\frac{1}{2}wh\right)h\Bigg) - \frac{1}{4}h\left(-108\sin\left(\frac{9}{2}wh\right)x^2 - 729\sin\left(\frac{9}{2}wh\right)h^2\right.\\
&\left.+ 84\sin\left(\frac{7}{2}wh\right)x^2 + 343\sin\left(\frac{7}{2}wh\right)h^2\right)\\
= &-\frac{1}{4}h^2\Bigg(-108c_2 w\cos\left(\frac{3}{2}wh\right)h^2 - 300c_1 w\cos\left(\frac{5}{2}wh\right)h^2 - 48c_1 w\cos\left(\frac{5}{2}wh\right)x^2\\
&+ 12c_3 w^2\sin\left(\frac{1}{2}wh\right)x^2 h + 36c_2 w^2\sin\left(\frac{3}{2}wh\right)x^2 h - 12c_3 w\cos\left(\frac{1}{2}wh\right)h^2\\
&- 168c_0\sin\left(\frac{7}{2}wh\right)h + 60c_1 w^2\sin\left(\frac{5}{2}wh\right)x^2 h + 27c_2 w^2\sin\left(\frac{3}{2}wh\right)h^3\\
&+ 343c_0 w^2\sin\left(\frac{7}{2}wh\right)h^3 + 125c_1 w^2\sin\left(\frac{5}{2}wh\right)h^3 + 84c_0 w^2\sin\left(\frac{7}{2}wh\right)x^2 h\\
&+ c_3 w^2\sin\left(\frac{1}{2}wh\right)h^3 - 24c_3\sin\left(\frac{1}{2}wh\right)h - 72c_2\sin\left(\frac{3}{2}wh\right)h\\
&- 120c_1\sin\left(\frac{5}{2}wh\right)h - 48c_0 w\cos\left(\frac{7}{2}wh\right)x^2 - 48c_3 w\cos\left(\frac{1}{2}wh\right)x^2\\
&- 588c_0 w\cos\left(\frac{7}{2}wh\right)h^2 - 48c_2 w\cos\left(\frac{3}{2}wh\right)x^2\Bigg).
\end{aligned}
$$

The solution of the above system of equations is given in appendix E. For small values of v the given formulae are subject to heavy cancelations. In this case the Taylor series expansions given in appendix F must be used.

The local truncation error of the above method is given by

$$
LTE(h) = \frac{h^{10}}{64800}\left(32732v^2 y_n^{(8)} + 32732v^6 y_n^{(4)} + 49098v^4 y_n^{(6)} + 8183y_n^{(10)} + 8183v^8 y_n^{(2)}\right) \tag{11}
$$

It can be seen that when $v \to 0$ the above methods become the classical symmetric eighth algebraic order explicit method developed by Jenkins [47].

We note that if we substitute w with $\mathrm{i}\phi$ in the above formulae, the coefficients of the exponentially-fitted eighth algebraic order symmetric methods are obtained.

Following similar procedures methods of the above type for multifrequency cases can be produced. This will be a subject of another paper.

3. Stability analysis

In the last decade there has been a great interest in the numerical solution of special second order periodic initial-value problems (see [3,4,48,49] and references therein)

$$
y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0. \tag{12}
$$

In order to investigate the periodic stability properties of numerical methods for solving the initial-value problem (12) Lambert and Watson [46] introduce the scalar test equation

$$y'' = -q^2 y \tag{13}$$

and the *interval of periodicity*.

Based on the theory developed in [46], when a symmetric multistep method

$$\sum_{j=0}^{k} a_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f_{n+j} \tag{14}$$

is applied to the scalar test equation (13), a difference equation of the form

$$\sum_{i=0}^{k} \left(a_i + H^2 \beta_i\right) y_{n+i} = 0 \tag{15}$$

is obtained, where $H = qh$, h is the step length and y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2, \ldots$.

The general solution of the above difference equation is given by

$$y_n = \sum_{j=1}^{k} A_j P_j^n, \tag{16}$$

where P_j, $j = 1(1)k$ are the distinct roots of the polynomial

$$P\left(P; H^2\right) = \rho(P) + H^2 \sigma(P), \tag{17}$$

where ρ and σ are polynomials given by

$$\rho(p) = \sum_{i=0}^{k} a_i p^i, \qquad \sigma(p) = \sum_{i=0}^{k} \beta_i p^i. \tag{18}$$

We note here that the roots of the polynomial (17) are perturbations of the roots of ρ. We denote as P_1 and P_2 the perturbations of the principal roots of ρ.

Based on Lambert and Watson [46] when a symmetric multistep method is applied to the scalar test equation $y'' = -q^2 y$, a difference equation (15) is obtained. The characteristic equation associated with (15) is given by (17). The roots of the characteristic polynomial (17) are denoted as P_i, $i = 1(1)k$.

We have the following definitions.

Definition 1. Following Lambert and Watson [46] we say that the numerical method (15) has an *interval of periodicity* $(0, H_0^2)$, if for all $H^2 \in (0, H_0^2)$, P_i, $i = 1(1)k$, satisfy:

$$|P_1| = |P_2| = 1, \qquad |P_j| \leqslant 1, \quad j = 3(1)k. \tag{19}$$

Definition 2 [46].The method (15) is *P-stable* if its interval of periodicity is $(0, \infty)$.

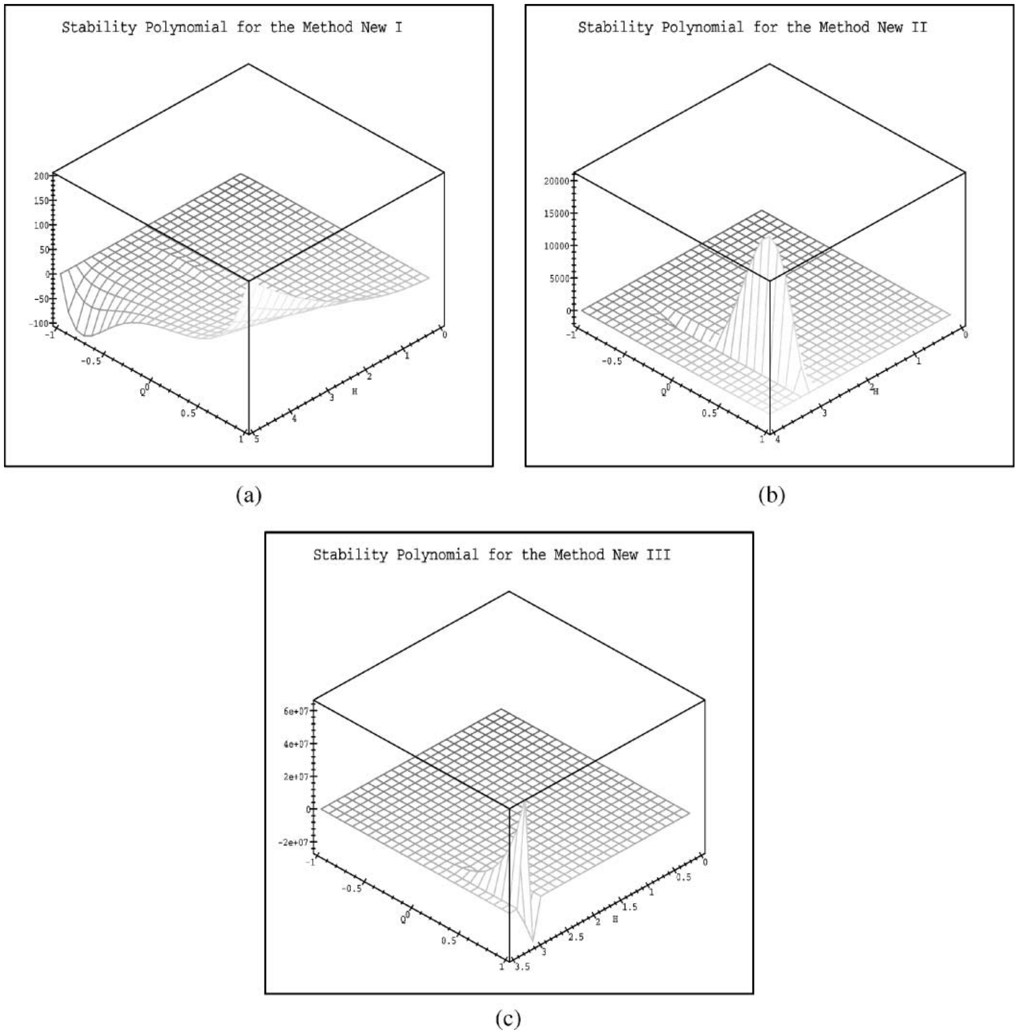

Figure 1. Stability region for the trigonometrically-fitted methods developed in the paper. (a) new method I, (b) new method II, (c) new method III.

For the method developed in this paper we have that the polynomials ρ and σ are given by (18) with $k = 7$ and

$$a_0 = a_9 = 1, \quad a_1 = a_8 = -1, \quad a_2 = a_3 = a_4 = a_5 = a_6 = a_7 = 0 \tag{20}$$

and the coefficients $\beta_0 = \beta_9 = 0$, $\beta_1 = \beta_8 = c_0$, $\beta_2 = \beta_7 = c_1$, $\beta_3 = \beta_6 = c_2$, $\beta_4 = \beta_5 = c_3$ be given by (28) for the first trigonometrically-fitted method, by (30) for the second trigonometrically-fitted method and by (32) for the third trigonometrically-fitted method.

In figure 1 we present the stability polynomials for the three new developed methods (we note here that we present the first trigonometrically-fitted method as new method I, the second trigonometrically-fitted method as new method II and the third trigonometrically-fitted method as new method III).

Based on the above theory and on the coefficients given above we find that the interval of periodicity of the new method I is equal to (0, 9.77), for the second new method II is equal to (0, 7.22) and for the third new method III is equal to (0, 3.26), i.e., is greater than the interval of periodicity of the classical method which is equal to (0, 0.74).

4. Numerical illustrations

In this section we apply the new explicit proposed methods to the resonance problem of the radial Schrödinger equation. We note here that similar results have been obtained for the coupled differential equations arising from the Schrödinger equation.

4.1. *The Schrödinger equation*

Let us consider the numerical solution of the radial Schrödinger equation

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

In (21) the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k^2 is a real number denoting *the energy*, l is a given integer, related to the angular momentum and V is a given function representing the potential. The boundary conditions are:

$$y(0) = 0 \tag{22}$$

and a second boundary condition, for large values of x, determined by physical considerations. It is known that in the asymptotic region the equation (21) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{23}$$

for x greater than some value R, where R defines the asymptotic region.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx), n_l(kx)$ are *spherical Bessel and Neumann functions*, respectively. Thus the solution of equation (21) has the asymptotic form (when $x \to \infty$)

$$y(x) \sim Akxj_l(kx) - Bn_l(kx) \sim D\left(\sin\left(kx - \frac{\pi l}{2}\right) + \tan\delta_l \cos\left(kx - \frac{\pi l}{2}\right)\right), \tag{24}$$

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

$$\tan\delta_l = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})} \tag{25}$$

for x_i and x_{i+1} distinct points on the asymptotic region (for which we have that x_{i+1} is the right-hand end point of the interval of integration and $x_i = x_{i+1} - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

We evaluate the phase shift δ_l from the above relation at x_i in the asymptotic region. For the illustration of the accuracy of the new proposed method we consider the numerical integration of the one-dimensional Schrödinger equation (21) with $l = 0$ in the case where $V(x)$ is the Woods–Saxon potential:

$$V(x) = V_W(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{a(1+z)^2} \tag{26}$$

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

For positive energies one has the so-called resonance problem. This problem consists either of finding the phase shift $\delta(E) = \delta_l$ or finding those $E \in [1, 1000]$, at which δ equals $\pi/2$. We actually solve the latter problem, using the technique fully described in [50], when *the positive eigenenergies lie under the potential barrier*.

The boundary conditions for this problem are:

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

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

For comparison purposes in our numerical illustration we use:

(1) Explicit version of Numerov's method produced by Chawla [51] (which is indicated as method [a]). We note here that this method has larger interval of periodicity (interval of periodicity equal to $(0, 12)$) than the classical Numerov's method (interval of periodicity equal to $(0, 6)$).

(2) Sixth algebraic order explicit method with phase-lag order eight of Chawla [52] (which is indicated as method [b]).

(3) The linear classical (with constant coefficients) multistep method of algebraic order eight developed by Jenkins [47](which is indicated as method [c]).

(4) Exponentially-fitted eighth algebraic order linear ten-step method produced in this paper (coefficients given by (28) (which is indicated as method [d]).

(5) Exponentially-fitted eighth algebraic order linear ten-step method produced in this paper (coefficients given by (30) (which is indicated as method [e]).

(6) Exponentially-fitted eighth algebraic order linear ten-step method produced in this paper (coefficients given by (32) (which is indicated as method [f]).

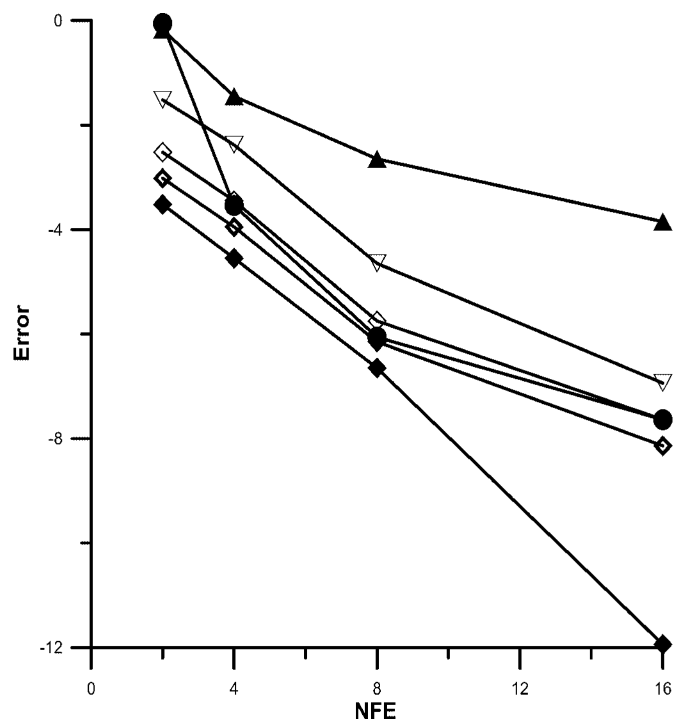

Figure 2. Error versus number of function evaluations $=$ NFE$\cdot$100 for the eigenvalue $E_0 = 53.588872$. The non-existance of a value for a method indicates that error is positive. —▲— method [a]; —▽— method [b]; —●— method [c]; —◇— method [d]; —◈— method [e]; —◆— method [f].

The numerical results obtained by these six methods, with the same number of function evaluations (which are equal to NFE $\cdot$ 100, where NFE is the number presented in the figure) were compared with the analytic solution of the Woods–Saxon potential resonance problem, rounded to six decimal places. Figure 2 shows the errors $Error = \log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$ for the lowest eigenenergy $E_0 = 53.588872$. Figure 3 shows the errors $Error = \log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$ for the highest eigenenergy $E_3 = 989.701916$.

Since the methods used are of multistep type, in order to determine the appropriate initial conditions an eighth algebraic order Runge–Kutta–Nyström method developed by Dormand et al. [53] is used.

5. Remarks and conclusion

Based on the above numerical results we present the following remarks.

For low and high energies the second and third trigonometrically-fitted methods developed above are much more efficient than all the other methods used for comparison purposes.

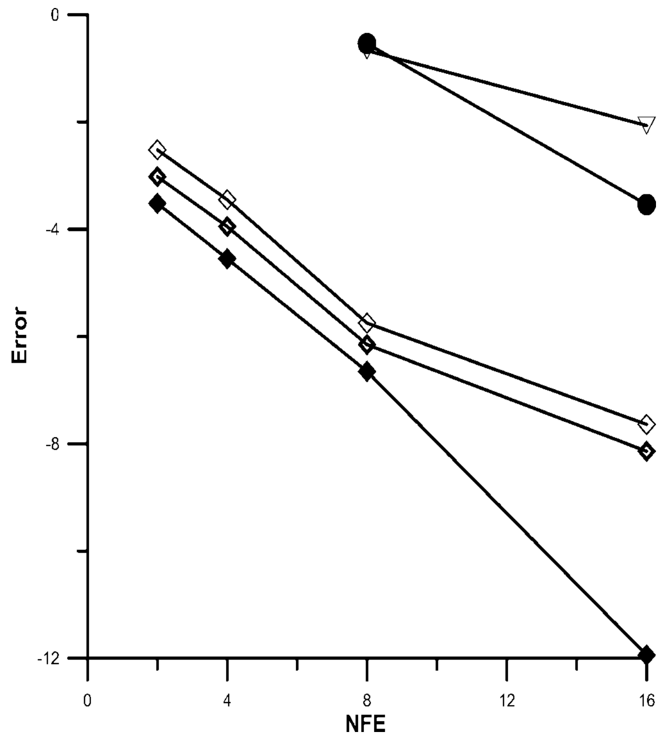

Figure 3. Error versus number of function evaluations = NFE · 100 for the eigenvalue $E_3 = 989.701916$. The non-existance of a value for a method indicates that error is positive. —▲— method [a]; —▽— method [b]; —●— method [c]; —◇— method [d]; —◈— method [e]; —◆— method [f].

For low energies the classical linear ten-step symmetric method and for number of function evaluations grater than 400, has approximately similar behavior with the first and second trigonometrically-fitted methods developed above.

For high energies the method [a] does not converge.

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

Appendix A.

$$\begin{aligned}
c_0 = {} & \big(-6v + 24v^3\cos(v) + 18v\cos(4v) - 6v\cos(3v) - 12v\cos(2v) + 12v\cos(v) \\
& + 31v^3\cos(2v) - 6v\cos(5v) - 7v^3 + 6\sin(5v) - 12\sin(4v) + 6\sin(3v)\big)\big/ \\
& \big(-15v^3 + 12v^3\cos(v) - 12v^3\cos(3v) + 12v^3\cos(2v) + 3v^3\cos(4v)\big), \\
c_1 = {} & \big(6v - 62v^3\cos(3v) - 6\sin(6v) - 58v^3\cos(v) - 42v\cos(4v) + 6v\cos(3v) \\
& + 33v\cos(2v) - 12v\cos(v) - 67v^3\cos(2v) + 6v\cos(5v) + 3v\cos(6v)
\end{aligned}$$

$$
\begin{aligned}
&- 53v^3 - 6\sin(5v) + 24\sin(4v) - 6\sin(2v) - 6\sin(3v)\big)\big/ \\
&\big(-15v^3 + 12v^3\cos(v) - 12v^3\cos(3v) + 12v^3\cos(2v) + 3v^3\cos(4v)\big), \qquad (27)\\
c_2 = {} &\big(18v + 62v^3\cos(3v) + 18\sin(6v) + 31v^3\cos(4v) + 154v^3\cos(v) \\
&+ 18v\cos(4v) + 18v\cos(3v) - 27v\cos(2v) - 36v\cos(v) + 139v^3\cos(2v) \\
&+ 18v\cos(5v) - 9v\cos(6v) + 46v^3 - 18\sin(5v) + 18\sin(2v) - 18\sin(3v)\big)\big/ \\
&\big(-15v^3 + 12v^3\cos(v) - 12v^3\cos(3v) + 12v^3\cos(2v) + 3v^3\cos(4v)\big), \\
c_3 = {} &\big(-18v - 48v^3\cos(3v) - 12\sin(6v) - 19v^3\cos(4v) - 72v^3\cos(v) + 6v\cos(4v) \\
&- 18v\cos(3v) + 6v\cos(2v) + 36v\cos(v) - 55v^3\cos(2v) - 18v\cos(5v) \\
&+ 6v\cos(6v) - 46v^3 + 18\sin(5v) - 12\sin(4v) - 12\sin(2v) + 18\sin(3v)\big)\big/ \\
&\big(-15v^3 + 12v^3\cos(v) - 12v^3\cos(3v) + 12v^3\cos(2v) + 3v^3\cos(4v)\big).
\end{aligned}
$$

where $v = wh$.

Appendix B.

$$
\begin{aligned}
c_0 &= \frac{22081}{15120} - \frac{8183}{64800}v^2 + \frac{602003}{119750400}v^4 - \frac{2612693}{29719872000}v^6 - \frac{1097471}{3923023104000}v^8 \\
&\quad - \frac{388206337}{2000741783040000}v^{10} - \frac{2296132327}{109168679854080000}v^{12} + \cdots, \\
c_1 &= -\frac{7337}{15120} + \frac{8183}{12960}v^2 - \frac{10571107}{119750400}v^4 + \frac{477221839}{65383718400}v^6 - \frac{28957817}{80061696000}v^8 \\
&\quad + \frac{368764213}{30780642816000}v^{10} - \frac{365875468709}{1419192838103040000}v^{12} + \cdots, \\
c_2 &= \frac{339}{112} - \frac{8183}{7200}v^2 + \frac{1040789}{4435200}v^4 - \frac{258736661}{12108096000}v^6 + \frac{18948373}{17435658240}v^8 \qquad (28)\\
&\quad - \frac{859009673}{24700515840000}v^{10} + \frac{425574909211}{473064279367680000}v^{12} + \cdots, \\
c_3 &= -\frac{29}{15120} + \frac{8183}{12960}v^2 - \frac{18132199}{119750400}v^4 + \frac{185140811}{13076743680}v^6 - \frac{2843353421}{3923023104000}v^8 \\
&\quad + \frac{9199663201}{400148356608000}v^{10} - \frac{293666512891}{473064279367680000}v^{12} + \cdots.
\end{aligned}
$$

Appendix C.

$$
\begin{aligned}
c_0 = {} &\big(-3\cos(2v) - 6v^2 + 3\cos(6v) + 22v\sin(3v) + 3v^2\cos(2v) - 18v^2\cos(3v) \\
&+ 6v^2\cos(4v) + 12v^2\cos(v) - 16v^4\cos(v) + 6\cos(3v) - 4v^4\cos(2v)
\end{aligned}
$$

$$
\begin{aligned}
&- 11v\sin(2v) + 6v^2\cos(5v) - 3v^2\cos(6v) - 12v^4 - 10v\sin(5v)\\
&+ 5v\sin(6v) - 6v\sin(4v) - 6\cos(5v)\big)\big/\\
&\big(-6v^4 - 3v^4\cos(3v) + 8v^4\cos(2v) + 2v^4\cos(v) - 2v^4\cos(4v) + v^4\cos(5v)\big),\\
c_1 = {}&-\big(6\cos(v) - 9\cos(2v) - 18v^2 + 9\cos(6v) + 10v\sin(3v) + 3v^2\cos(7v)\\
&+ 19v^2\cos(2v) + 3v^2\cos(3v) + 2v^2\cos(4v) + 24v\sin(v) + v^2\cos(v)\\
&+ 68v^4\cos(v) + 44v^4\cos(2v) - 37v\sin(2v) - 7v^2\cos(5v) - 3v^2\cos(6v)\\
&+ 36v^4 + 10v\sin(5v) + 12v^4\cos(3v) + 11v\sin(6v) - 8v\sin(7v)\\
&- 10v\sin(4v) - 6\cos(7v)\big)\big/\\
&\big(6v^4 + 3v^4\cos(3v) - 8v^4\cos(2v) - 2v^4\cos(v) + 2v^4\cos(4v) - v^4\cos(5v)\big),\\
c_2 = {}&\big(-3 + 3\cos(8v) + 3\cos(2v) + 15v^2 - 3\cos(6v) + 20v\sin(3v) - v^2\cos(7v)\\
&- 19v^2\cos(2v) - 9v^2\cos(3v) + 2v^2\cos(4v) + 2v\sin(v) + 5v^2\cos(v)\\
&+ 3v\sin(8v) - 108v^4\cos(v) + 6\cos(3v) - 60v^4\cos(2v) + 9v\sin(2v)\\
&+ 5v^2\cos(5v) + 3v^2\cos(6v) - v^2\cos(8v) - 72v^4 - 12v^4\cos(4v)\\
&- 12v\sin(5v) - 36v^4\cos(3v) - 7v\sin(6v) + 2v\sin(7v) - 4v\sin(4v)\\
&- 6\cos(5v)\big)\big/\\
&\big(6v^4 - 3v^4\cos(3v) + 8v^4\cos(2v) + 2v^4\cos(v) - 2v^4\cos(4v) + v^4\cos(5v)\big),\\
c_3 = {}&\big(-3 + 3\cos(8v) + 6\cos(v) - 9\cos(2v) - 9v^2 + 9\cos(6v) + 52v\sin(3v)\\
&+ 2v^2\cos(7v) + 3v^2\cos(2v) - 24v^2\cos(3v) + 10v^2\cos(4v) + 26v\sin(v)\\
&+ 18v^2\cos(v) + 3v\sin(8v) - 64v^4\cos(v) + 12\cos(3v) - 52v^4\cos(2v)\\
&- 39v\sin(2v) + 4v^2\cos(5v) - 3v^2\cos(6v) - v^2\cos(8v) - 24v^4\\
&- 4v^4\cos(4v) - 12v\sin(5v) - 12v^4\cos(3v) + 9v\sin(6v) - 4v^4\cos(5v)\\
&- 6v\sin(7v) - 20v\sin(4v) - 6\cos(7v) - 12\cos(5v)\big)\big/\\
&\big(6v^4 + 3v^4\cos(3v) - 8v^4\cos(2v) - 2v^4\cos(v) + 2v^4\cos(4v) - v^4\cos(5v)\big),
\end{aligned}
\tag{29}
$$

where $v = wh$.

Appendix D.

$$
\begin{aligned}
c_0 = {}&\frac{22081}{15120} - \frac{8183}{43200}v^2 + \frac{38261}{7983360}v^4 - \frac{53454109}{163459296000}v^6 - \frac{224519}{9686476800}v^8\\
&- \frac{7948002947}{2667655710720000}v^{10} - \frac{304389874157}{851515702861824000}v^{12} + \cdots,\\
c_1 = {}&-\frac{7337}{15120} + \frac{8183}{8640}v^2 - \frac{8517617}{39916800}v^4 + \frac{121277771}{6538371840}v^6 - \frac{64580539}{62270208000}v^8\\
&+ \frac{13296432923}{533531142144000}v^{10} - \frac{38809673941}{22767799541760000}v^{12} + \cdots,
\end{aligned}
$$

$$c_2 = \frac{339}{112} - \frac{8183}{4800}v^2 + \frac{2711669}{4435200}v^4 - \frac{78584357}{672672000}v^6 + \frac{1967211203}{145297152000}v^8 - \frac{310087862587}{296406190080000}v^{10} + \frac{994742061737}{17520899235840000}v^{12} + \cdots,$$
$$c_3 = -\frac{29}{15120} + \frac{8183}{8640}v^2 - \frac{16078709}{39916800}v^4 + \frac{3223501717}{32691859200}v^6 - \frac{5439466481}{435891456000}v^8 + \frac{546451320323}{533531142144000}v^{10} - \frac{17918689431103}{327506039562240000}v^{12} + \cdots. \tag{30}$$

Appendix E.

$$c_0 = \Bigg(-12\cos\left(\frac{11}{2}v\right) + 26v^2\cos\left(\frac{11}{2}v\right) + 56v^2\cos\left(\frac{9}{2}v\right) + 12\cos\left(\frac{5}{2}v\right) + 12\cos\left(\frac{7}{2}v\right) - 12\cos\left(\frac{9}{2}v\right) - 12v^2\cos\left(\frac{3}{2}v\right) - 6v^3\sin\left(\frac{7}{2}v\right) - 60v^3\sin\left(\frac{5}{2}v\right) - 24v^3\sin\left(\frac{3}{2}v\right) + 12v^3\sin\left(\frac{1}{2}v\right) - 12v^2\cos\left(\frac{1}{2}v\right) - 86v^2\cos\left(\frac{5}{2}v\right) - 20v^2\cos\left(\frac{7}{2}v\right) + 27v\sin\left(\frac{7}{2}v\right) + 45v\sin\left(\frac{5}{2}v\right) + 30v^3\sin\left(\frac{9}{2}v\right) + 12v^3\sin\left(\frac{11}{2}v\right) - 27v\sin\left(\frac{11}{2}v\right) - 45v\sin\left(\frac{9}{2}v\right)\Bigg) \Bigg/ \Bigg(24v^5\sin\left(\frac{3}{2}v\right) - 3v^5\sin\left(\frac{9}{2}v\right) - 9v^5\sin\left(\frac{7}{2}v\right) + 18v^5\sin\left(\frac{1}{2}v\right)\Bigg)$$

$$c_1 = -\Bigg(24\cos\left(\frac{11}{2}v\right) - 109v^2\cos\left(\frac{11}{2}v\right) - 57v^2\cos\left(\frac{13}{2}v\right) + 2v^2\cos\left(\frac{9}{2}v\right) - 24\cos\left(\frac{5}{2}v\right) + 72v\sin\left(\frac{13}{2}v\right) + 12\cos\left(\frac{7}{2}v\right) - 36\cos\left(\frac{3}{2}v\right) - 12\cos\left(\frac{9}{2}v\right) + 309v^2\cos\left(\frac{3}{2}v\right) - 144v\sin\left(\frac{3}{2}v\right) - 18v^3\sin\left(\frac{13}{2}v\right) + 12v^3\sin\left(\frac{7}{2}v\right) + 30v^3\sin\left(\frac{5}{2}v\right) + 150v^3\sin\left(\frac{3}{2}v\right) + 120v^3\sin\left(\frac{1}{2}v\right) + 60v^2\cos\left(\frac{1}{2}v\right) + 25v^2\cos\left(\frac{5}{2}v\right) + 10v^2\cos\left(\frac{7}{2}v\right) + 36\cos\left(\frac{13}{2}v\right) + 45v\sin\left(\frac{7}{2}v\right) - 45v\sin\left(\frac{5}{2}v\right) - 12v^3\sin\left(\frac{9}{2}v\right) - 42v^3\sin\left(\frac{11}{2}v\right) + 99v\sin\left(\frac{11}{2}v\right) - 27v\sin\left(\frac{9}{2}v\right)\Bigg) \Bigg/ \tag{31}$$

$$\left(-24v^5\sin\left(\frac{3}{2}v\right)+3v^5\sin\left(\frac{9}{2}v\right)+9v^5\sin\left(\frac{7}{2}v\right)-18v^5\sin\left(\frac{1}{2}v\right)\right),$$

$$c_2=-\left(4v^3\sin\left(\frac{15}{2}v\right)-12\cos\left(\frac{11}{2}v\right)+17v^2\cos\left(\frac{11}{2}v\right)+17v^2\cos\left(\frac{13}{2}v\right)\right.$$
$$+76v^2\cos\left(\frac{9}{2}v\right)-12\cos\left(\frac{15}{2}v\right)+14v^2\cos\left(\frac{15}{2}v\right)+12\cos\left(\frac{5}{2}v\right)$$
$$-15v\sin\left(\frac{13}{2}v\right)+24\cos\left(\frac{7}{2}v\right)-24\cos\left(\frac{9}{2}v\right)+27v^2\cos\left(\frac{3}{2}v\right)$$
$$-15v\sin\left(\frac{3}{2}v\right)+6v^3\sin\left(\frac{13}{2}v\right)+12\cos\left(\frac{1}{2}v\right)-66v^3\sin\left(\frac{5}{2}v\right)$$
$$-34v^3\sin\left(\frac{3}{2}v\right)+12v^3\sin\left(\frac{1}{2}v\right)-21v\sin\left(\frac{15}{2}v\right)-130v^2\cos\left(\frac{1}{2}v\right)$$
$$+51v\sin\left(\frac{1}{2}v\right)-149v^2\cos\left(\frac{5}{2}v\right)-16v^2\cos\left(\frac{7}{2}v\right)+54v\sin\left(\frac{7}{2}v\right)$$
$$+54v\sin\left(\frac{5}{2}v\right)+24v^3\sin\left(\frac{9}{2}v\right)+6v^3\sin\left(\frac{11}{2}v\right)-18v\sin\left(\frac{11}{2}v\right)$$
$$\left.-90v\sin\left(\frac{9}{2}v\right)\right)\Bigg/$$
$$\left(-8v^5\sin\left(\frac{3}{2}v\right)-6v^5\sin\left(\frac{1}{2}v\right)+3v^5\sin\left(\frac{7}{2}v\right)+v^5\sin\left(\frac{9}{2}v\right)\right),$$

$$c_3=\left(3v^3\sin\left(\frac{15}{2}v\right)+24\cos\left(\frac{11}{2}v\right)-3v^3\sin\left(\frac{17}{2}v\right)+12\cos\left(\frac{17}{2}v\right)\right.$$
$$-148v^2\cos\left(\frac{11}{2}v\right)-46v^2\cos\left(\frac{13}{2}v\right)+132v^2\cos\left(\frac{9}{2}v\right)-24\cos\left(\frac{15}{2}v\right)$$
$$+13v^2\cos\left(\frac{15}{2}v\right)-24\cos\left(\frac{5}{2}v\right)+81v\sin\left(\frac{13}{2}v\right)+72\cos\left(\frac{7}{2}v\right)$$
$$-60\cos\left(\frac{3}{2}v\right)+18v\sin\left(\frac{17}{2}v\right)-72\cos\left(\frac{9}{2}v\right)+634v^2\cos\left(\frac{3}{2}v\right)$$
$$-279v\sin\left(\frac{3}{2}v\right)-12v^3\sin\left(\frac{13}{2}v\right)+12\cos\left(\frac{1}{2}v\right)+42v^3\sin\left(\frac{7}{2}v\right)$$
$$-72v^3\sin\left(\frac{5}{2}v\right)+108v^3\sin\left(\frac{3}{2}v\right)+162v^3\sin\left(\frac{1}{2}v\right)-27v\sin\left(\frac{15}{2}v\right)$$
$$-86v^2\cos\left(\frac{1}{2}v\right)+171v\sin\left(\frac{1}{2}v\right)-11v^2\cos\left(\frac{17}{2}v\right)-272v^2\cos\left(\frac{5}{2}v\right)$$
$$+24v^2\cos\left(\frac{7}{2}v\right)+60\cos\left(\frac{13}{2}v\right)+198v\sin\left(\frac{7}{2}v\right)+18v\sin\left(\frac{5}{2}v\right)$$

$$+30v^3\sin\left(\frac{9}{2}v\right)-48v^3\sin\left(\frac{11}{2}v\right)+162v\sin\left(\frac{11}{2}v\right)-234v\sin\left(\frac{9}{2}v\right)\Bigg)\Bigg/ \left(24v^5\sin\left(\frac{3}{2}v\right)-3v^5\sin\left(\frac{9}{2}v\right)-9v^5\sin\left(\frac{7}{2}v\right)+18v^5\sin\left(\frac{1}{2}v\right)\right),$$

where $v = wh$.

Appendix F.

$$\begin{aligned}
c_0 &= \frac{22081}{15120}-\frac{8183}{32400}v^2+\frac{163217}{59875200}v^4-\frac{18674219}{20432412000}v^6-\frac{847002619}{7846046208000}v^8 \\
&\quad -\frac{10634141009}{666913927680000}v^{10}-\frac{4881472343381}{2128789257154560000}v^{12}+\cdots, \\
c_1 &= -\frac{7337}{15120}+\frac{8183}{6480}v^2-\frac{23499361}{59875200}v^4+\frac{126960761}{4086482400}v^6-\frac{2671623259}{1120863744000}v^8 \\
&\quad -\frac{489026521}{19054683648000}v^{10}-\frac{30694336017227}{2128789257154560000}v^{12}+\cdots, \\
c_2 &= \frac{339}{112}-\frac{8183}{3600}v^2+\frac{7724309}{6652800}v^4-\frac{257511533}{756756000}v^6+\frac{37885490177}{871782912000}v^8 \\
&\quad -\frac{96624716203}{24700515840000}v^{10}+\frac{13771078022381}{78844046561280000}v^{12}+\cdots, \\
c_3 &= -\frac{29}{15120}+\frac{8183}{6480}v^2-\frac{46182637}{59875200}v^4+\frac{1267336361}{4086482400}v^6-\frac{816823794001}{7846046208000}v^8 \\
&\quad +\frac{18857047381}{1067062284288}v^{10}-\frac{4406209046546399}{2128789257154560000}v^{12}+\cdots.
\end{aligned} \tag{32}$$

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