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Sixth algebraic order trigonometrically fitted predictor–corrector methods for the numerical solution of the radial Schrödinger equation

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Our new trigonometrically fitted predictor–corrector (P–C) schemes presented here are based on the well known Adams–Bashforth–Moulton methods: the predictor is based on the fifth order Adams–Bashforth scheme and the corrector on the sixth order Adams–Moulton scheme. We tested the efficiency of our newly developed schemes against well known methods, with excellent results. The numerical experiments showed that at least one of our schemes is noticeably more efficient compared to other methods, some of which are specially designed for this type of problem. It is also worth mentioning that this is the first time that sixth algebraic order trigonometrically fitted Adams–Bashforth–Moulton P–C schemes are used to efficiently solve the radial Schrödinger equation.

KEY WORDS: trigonometric fitting, Adams–Bashforth–Moulton, predictor–corrector methods, Schrödinger equation

1. Introduction

Equations or systems of equations of the form

$$\mathbf{y}'(\mathbf{x}) = \mathbf{f}(\mathbf{x}, \mathbf{y}), \quad \mathbf{y}(\mathbf{x_0}) = \mathbf{y_0}, \tag{1}$$

are used to mathematical model problems in physical chemistry and chemical physics, celestial mechanics, quantum mechanics, electronics, materials sciences

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and elsewhere. A class of equations that deserves special attention is the one with oscillatory/periodic solution (see [1,2]).

During the last two decades there have been extensive investigations regarding the numerical solution of the above equation (indicatively see [10–23] and references therein). One of the better processes, first introduced by Lyche [21], for the development of efficient methods for the numerical integration of first order initial value problems with oscillating or periodic solution is the exponential and the trigonometric fitting technique. In a previous paper of ours [5], we had applied trigonometric fitting to a lower algebraic order Adams–Bashforth–Moulton P–C scheme for the solution of (1), with excellent results. We have also applied trigonometric fitting to quite different types of predictor–corrector methods, like the Explicit Advanced Step-point or EAS methods (see Ref. [3]), which had been introduced in their non-trigonometrically fitted form in Ref. [4]. However, until our recent paper [6], it appears that nobody had previously successfully attempted to use trigonometrically fitted P–C schemes for the efficient solution of the radial Schrödinger equation. In this paper we further develop our new trigonometrically fitted P–C methods for the numerical solution of the resonance problem of the Schrödinger equation.

The one-dimensional Schrödinger equation has the form:

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

Models of this type, which represent a boundary value problem, occur frequently in chemistry and theoretical physics, (see for example [14]). It is known from the literature that during the last decades many numerical methods have been constructed for the approximate solution of the Schrödinger equation (see indicatively [9–15]). The aim and the scope of the above activity was the development of fast and reliable methods. The developed methods could be divided into two main categories:

- Methods with constant coefficients.
- Methods with coefficients dependent on the frequency of the problem.[1]

This paper is structured as follows: In Section 2 we develop a new family of trigonometrically fitted schemes and we also investigate and briefly discuss the stability of our new schemes. In Section 3 we proceed to the numerical experimentations. Finally, in Section 4 we present the concluding remarks.

[1] In the case of the Schrödinger equation the frequency of the problem is equal to: $\sqrt{|l(l+1)/r^2 + V(r) - k^2|}$.

2. A family of trigonometrically fitted sixth algebraic order P–C schemes

The P–C family of methods appearing below has been widely used (e.g., by Shampine and Gordon [7]):

$$\overline{y}_{n+1} = y_n + h \sum_{i=0}^{k-1} b_i \nabla^i f_n,$$
$$y_{n+1} = y_n + h \sum_{i=0}^{k} \beta_i \nabla^i \overline{f}_{n+1}. \tag{3}$$

In (3) the corrector is always one order higher than the predictor and the overall algebraic order of the scheme is determined by the corrector's order. From the general case (3), after expressing the backward differences in terms of f_{n-i}, we can obtain the following sixth algebraic order five-step scheme:

$$\overline{y}_{n+1} = y_n + h \left(a_0 f_n + a_1 f_{n-1} + a_2 f_{n-2} + a_3 f_{n-3} + a_4 f_{n-4}\right),$$
$$y_{n+1} = y_n + h \left(c_0 \overline{f}_{n+1} + c_1 f_n + c_2 f_{n-1} + c_3 f_{n-2} + c_4 f_{n-3} + c_5 f_{n-4}\right), \tag{4}$$

where in terms of f_{n-i}, a_i, $i = 0(1)4$ are the known Adams–Bashforth coefficients and the c_i, $i = 0(1)5$ coefficients correspond to the Adams–Moulton coefficients for (3) above, as well as for $w = 0$, see equation (B.1) in Appendix B.

2.1. *First member of the family*

2.1.1. *Development of the method*

In order for the above method (4) to be exact for any linear combination of the functions

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

the following system of equations must hold:

$$\begin{aligned}
-1 + \cos(h\,v) = {} & -(-2\,c_3 \cos(h\,v)\sin(h\,v) - c_2 \sin(h\,v) + c_0\, h\, a_0\, v \\
& -4\cos(h\,v)^2 c_4 \sin(h\,v) + h\,v\,c_0\,a_1 \cos(h\,v) - 8\cos(h\,v)^2 c_0\, h\, a_4\, v \\
& +4\,c_5 \cos(h\,v)\sin(h\,v) + 2\cos(h\,v)^2 c_0\, h\, a_2\, v + 4\,h\,v\,c_0\,a_3 \cos(h\,v)^3 \\
& +8\cos(h\,v)^4 c_0\, h\, a_4\, v - 3\,h\,v\,c_0\,a_3 \cos(h\,v) + c_4 \sin(h\,v) \\
& -c_0\, h\, a_2\, v + c_0\, h\, a_4\, v - 8\cos(h\,v)^3 c_5 \sin(h\,v))h\,v, \qquad (6) \\
\sin(h\,v) = {} & (4\cos(h\,v)^2 h\,v\,c_0\,a_3 \sin(h\,v) + h\,v\,c_0\,a_1 \sin(h\,v) \\
& +2\,h\,v\,c_0\,a_2 \cos(h\,v)\sin(h\,v) + 2\cos(h\,v)^2 c_3 - h\,v\,c_0\,a_3 \sin(h\,v) \\
& +8\cos(h\,v)^4 c_5 - 4\,h\,v\,c_0\,a_4 \cos(h\,v)\sin(h\,v) + c_2 \cos(h\,v) \\
& +8\cos(h\,v)^3 h\,v\,c_0\,a_4 \sin(h\,v) + 4\cos(h\,v)^3 c_4 - 8\,c_5 \cos(h\,v)^2
\end{aligned}$$

$$+c_0 + c_1 - c_3 + c_5 - 3\,c_4 \cos(h\,v))h\,v, \tag{7}$$

$$1 = c_0 + c_1 + c_2 + c_3 + c_4 + c_5, \tag{8}$$

$$\begin{aligned} 1 = {} & 2\,c_0\,a_0 + 2\,c_0\,a_1 + 2\,c_0\,a_2 + 2\,c_0\,a_3 + 2\,c_0\,a_4 \\ & -2\,c_2 - 4\,c_3 - 6\,c_4 - 8\,c_5, \end{aligned} \tag{9}$$

$$\begin{aligned} 1 = {} & -6\,c_0\,a_1 + 48\,c_5 + 27\,c_4 + 12\,c_3 \\ & -12\,c_0\,a_2 + 3\,c_2 - 18\,c_0\,a_3 - 24\,c_0\,a_4, \end{aligned} \tag{10}$$

$$\begin{aligned} 1 = {} & 192\,c_0\,a_4 + 108\,c_0\,a_3 + 48\,c_0\,a_2 + 12\,c_0\,a_1 \\ & -108\,c_4 - 256\,c_5 - 4\,c_2 - 32\,c_3. \end{aligned} \tag{11}$$

We note here that in the above system the equations (8)–(11) are produced from the requirement that method (4) is accurate for any linear combination of the functions 1, x, x^2, x^3, x^4. The equations (6) and (7) are produced from the requirement that method (4) is accurate for any linear combination of the functions $\cos(\pm v\,x)$, $\sin(\pm v\,x)$. Assuming the known Adams–Bashforth coefficients in terms of f_{n-i}:

$$a_0 = \frac{1901}{720}, \quad a_1 = -\frac{1387}{360}, \quad a_2 = \frac{109}{30}, \quad a_3 = -\frac{637}{360}, \quad a_4 = \frac{251}{720} \tag{12}$$

the solution of this system of equations is given in Appendix A.

For small values of w the formulae given by (A.1) are subject to heavy cancelations. In this case the Taylor series expansions, presented in Appendix B, should be used.

In figure 1 we present the behavior of the quantities $c[i] = c_i,\ i = 0(1)5$, where $c_i,\ i = 0(1)5$ are given by (A.1). It is easy to see that for $4 < w < 8$ and $12 < w < 14$ (for the coefficient c_0) and for $6.2 < w < 6.4$ (for the coefficients $c_j,\ j = 1(1)5$ is better to use Taylor series expansions.

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

$$\mathrm{L.T.E} = \frac{1}{2903040}\,h^7\left(274451\,w^2\,y_n^{(5)} - 315875\,y_n^{(6)} - 41424\,y_n^{(7)}\right) + O\left(h^8\right), \tag{13}$$

where $y_n^{(5)}$ is the fifth derivative of y at x_n, $y_n^{(6)}$ is the sixth derivative of y at x_n and $y_n^{(7)}$ is the seventh derivative of y at x_n. We note here that in order to produce equation (13) we express the quantities $y_{n+1},\ y_{n-1},\ y_{n-2},\ y_{n-3},\ y_{n-4}$ and $f_{n+1},\ f_{n-1},\ f_{n-2},\ f_{n-3},\ f_{n-4}$ around the point x_n and then we substitute the expressions into (4).

Since $w = vh$, it can be seen that when $v \to 0$ our trigonometrically fitted method becomes the original predictor–corrector method for the relevant algebraic order and step-number.

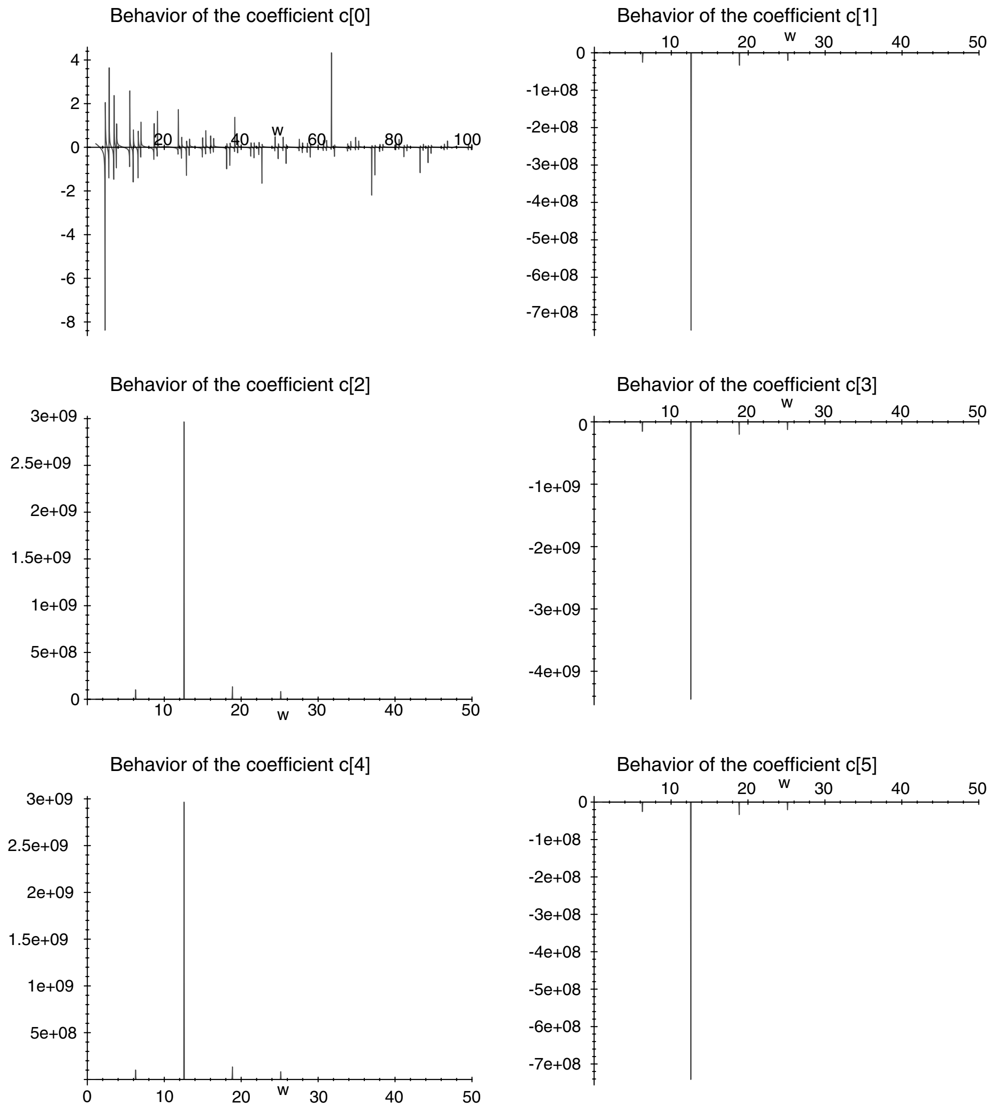

Figure 1. Behavior of the coefficients $c_i,\ i = 0(1)5$ given by (A.1) for several values of v.

2.1.2. Stability analysis of the method

Applying scheme (4) with the coefficients $a_0 = \frac{1901}{720}$, $a_1 = -\frac{1387}{360}$, $a_2 = \frac{109}{30}$, $a_3 = -\frac{637}{360}$ and $a_4 = \frac{251}{720}$ to the scalar test equation

$$y' = \lambda\, y, \qquad \text{where } \lambda \in \mathcal{C} \tag{14}$$

we obtain the following difference equation

$$y_{n+1} - A_0(H)\, y_n + A_1(H)\, y_{n-1} + A_2(H)\, y_{n-2} + A_3(H)\, y_{n-3} + A_4(H)\, y_{n-4} = 0, \tag{15}$$

where

$$\begin{aligned} A_0(H) &= 1 + c_0\, H + \frac{1901}{720}\, c_0\, H^2 + H\, c_1, \\ A_1(H) &= \frac{1387}{360}\, c_0\, H^2 - H\, c_2, \\ A_2(H) &= -\frac{109}{30}\, c_0\, H^2 - H\, c_3, \quad A_3 = \frac{637}{360}\, c_0\, H^2 - H\, c_4, \\ A_4 &= -\frac{251}{720}\, c_0\, H^2 - H\, c_5. \end{aligned} \tag{16}$$

The characteristic equation of (15) is given by

$$r^5 - A_0(H)\, r^4 + A_1(H)\, r^3 + A_2(H)\, r^2 + A_3(H)\, r + A_4(H) = 0. \tag{17}$$

By solving the above equation in H and using the boundary locus technique [8] and substituting $r = \exp(\mathrm{i}\theta)$, where $\mathrm{i} = \sqrt{-1}$, we can plot the regions of absolute stability for $\theta \in [0, 2\pi]$. In figure 2 we present the region of absolute stability for the original case (i.e., method (4) without trigonometric fitting). In figure 3 we present the regions of absolute stability for the trigonometrically fitted case and for $w = 1$, $w = 2$, $w = 5$ and $w = 10$.

As we can see from figure 3, it appears that the larger the frequency w becomes, the region of absolute stability also has gains in certain instances. Among other things, it remains to be investigated how w influences the region of absolute stability.

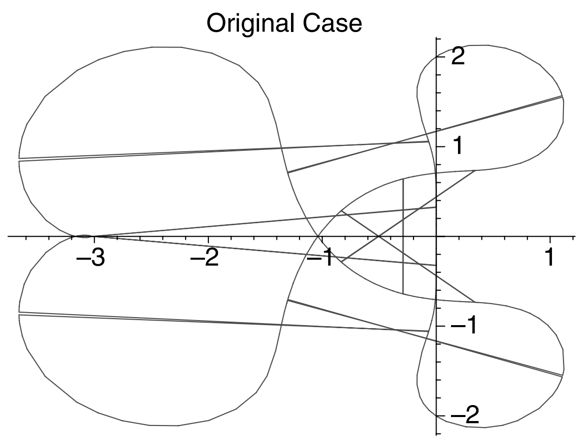

Figure 2. Stability region for the original case.

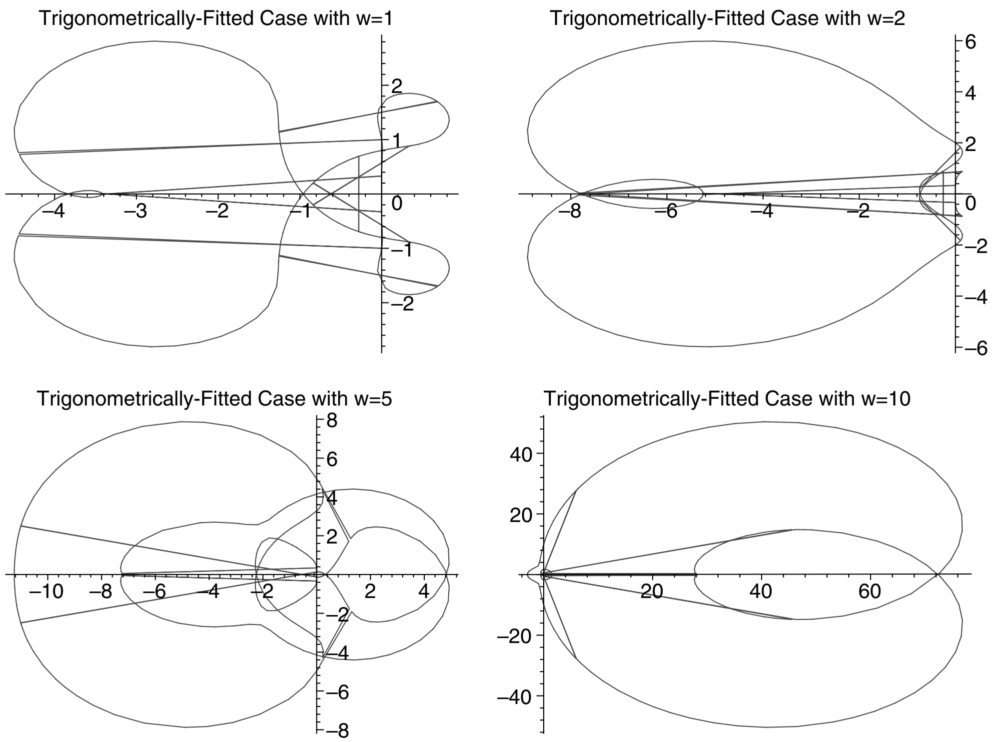

Figure 3. Stability region for the second member of the trigonometrically fitted case and for $w = 1$ (above left), $w = 2$ (above right), $w = 5$ (below left) and $w = 10$ (below right).

2.2. Second member of the family

2.2.1. Development of the method

In order for the above method (4) to be exact for any linear combination of the functions

$$\{1,\ x,\ x^2,\ \cos(\pm v\,x),\ \sin(\pm v\,x),\ x\cos(\pm v\,x),\ x\sin(\pm v\,x)\} \tag{18}$$

the following system of equations must hold:

$$\begin{aligned} -1+\cos(h\,v) = {} & -(h\,v\,c_0\,a_0 + h\,v\,c_0\,a_1\cos(h\,v) + 2\,h\,v\,c_0\,a_2\cos(h\,v)^2 \\ & +4\,h\,v\,c_0\,a_3\cos(h\,v)^3 + 8\,h\,v\,c_0\,a_4\cos(h\,v)^4 \\ & -h\,v\,c_0\,a_2 - 3\,h\,v\,c_0\,a_3\cos(h\,v) \\ & -8\cos(h\,v)^2\,h\,v\,c_0\,a_4 + h\,v\,c_0\,a_4 \\ & -c_2\sin(h\,v) - 2\,c_3\cos(h\,v)\sin(h\,v) \\ & -4\,c_4\sin(h\,v)\cos(h\,v)^2 + c_4\sin(h\,v) \\ & -8\sin(h\,v)\,c_5\cos(h\,v)^3 + 4\,c_5\cos(h\,v)\sin(h\,v))h\,v, \end{aligned} \tag{19}$$

$$\begin{aligned}
\sin(hv) = {} & (c_2\cos(hv) - 8\cos(hv)^2 c_5 + c_5 + 2c_3\cos(hv)^2 \\
& + 8\sin(hv)hvc_0a_4\cos(hv)^3 + 8c_5\cos(hv)^4 \\
& - c_3 + c_0 + c_1 + hvc_0a_1\sin(hv) + 4c_4\cos(hv)^3 \\
& + 2hvc_0a_2\cos(hv)\sin(hv) - hvc_0a_3\sin(hv) \\
& - 4hvc_0a_4\cos(hv)\sin(hv) - 3c_4\cos(hv) \\
& + 4hvc_0a_3\sin(hv)\cos(hv)^2)hv, \qquad (20)
\end{aligned}$$

$$\begin{aligned}
\cos(hv)x + \cos(hv)h - x = {} & (4h^2c_0a_4v^2 + hc_0a_2v^2x + 4c_4\cos(hv)^3 \\
& - 3c_4\cos(hv) + c_2v\sin(hv)x - c_4v\sin(hv)x \\
& + 3hc_4v\sin(hv) - hc_2v\sin(hv) - 8\cos(hv)^2c_5 \\
& - hc_0a_4v^2x + h^2c_0a_1v^2\cos(hv) \\
& - 12hc_4v\sin(hv)\cos(hv)^2 - 2hc_0a_2v^2x\cos(hv)^2 \\
& - 9h^2c_0a_3v^2\cos(hv) - 4hc_3v\cos(hv)\sin(hv) \\
& - 4c_5v\cos(hv)\sin(hv)x - hc_0a_1v^2\cos(hv)x \\
& + 16hc_5v\cos(hv)\sin(hv) + 3hc_0a_3v^2\cos(hv)x \\
& + 4h^2c_0a_2v^2\cos(hv)^2 + 8hc_0a_4v^2x\cos(hv)^2 \\
& - 4hc_0a_3v^2\cos(hv)^3x + 4\cos(hv)^2c_4v\sin(hv)x \\
& + 2c_3v\cos(hv)\sin(hv)x + 12h^2c_0a_3v^2\cos(hv)^3 \\
& + c_5 - 32h^2c_0a_4v^2\cos(hv)^2 + c_2\cos(hv) \\
& + 2hvc_0a_1\sin(hv) - 2hvc_0a_3\sin(hv) \\
& + 16\sin(hv)hvc_0a_4\cos(hv)^3 - hc_0a_0xv^2 \\
& + 8hvc_0a_3\sin(hv)\cos(hv)^2 - c_3 + c_0 + c_1 \\
& + 32\cos(hv)^4h^2c_0a_4v^2 - 8\cos(hv)^4hc_0a_4v^2x \\
& - 8hvc_0a_4\cos(hv)\sin(hv) - 2h^2c_0a_2v^2 \\
& + 8\cos(hv)^3c_5v\sin(hv)x - 32\cos(hv)^3hc_5v\sin(hv) \\
& + 4hvc_0a_2\cos(hv)\sin(hv) + 2c_3\cos(hv)^2 \\
& + 8c_5\cos(hv)^4)h, \qquad (21)
\end{aligned}$$

$$\begin{aligned}
\sin(hv)(x+h) = {} & -h(-2hc_3v + 4hc_5v - 2hvc_0a_0 \\
& + 2hvc_0a_2 - 2hvc_0a_4 + c_2\sin(hv) - c_4\sin(hv) \\
& + hc_2v\cos(hv) - 8hvc_0a_3\cos(hv)^3 \\
& + 6hvc_0a_3\cos(hv) + 16\cos(hv)^2hvc_0a_4 \\
& - 2hvc_0a_1\cos(hv) \\
& - 4hvc_0a_2\cos(hv)^2 + 4c_4\sin(hv)\cos(hv)^2 \\
& - c_1xv - 4c_5\cos(hv)\sin(hv) \\
& + 32\cos(hv)^4hc_5v - 8\cos(hv)^4c_5vx \\
& + 32\cos(hv)^3h^2c_0a_4v^2\sin(hv)
\end{aligned}$$

$$
\begin{aligned}
&-8\cos(h\,v)^3\,h\,c_0\,a_4\,v^2\sin(h\,v)\,x\\
&-c_0\,x\,v-16\,h\,v\,c_0\,a_4\cos(h\,v)^4\\
&+8\sin(h\,v)\,c_5\cos(h\,v)^3-c_5\,v\,x\\
&+4\,h\,c_0\,a_4\,v^2\cos(h\,v)\sin(h\,v)\,x\\
&+2\,c_3\cos(h\,v)\sin(h\,v)+c_3\,v\,x\\
&+4\,h^2\,c_0\,a_2\,v^2\cos(h\,v)\sin(h\,v)\\
&-h\,c_0\,a_1\,v^2\sin(h\,v)\,x-3\,h^2\,c_0\,a_3\,v^2\sin(h\,v)\\
&-2\,h\,c_0\,a_2\,v^2\cos(h\,v)\sin(h\,v)\,x\\
&+3\,c_4\,v\cos(h\,v)\,x-9\,h\,c_4\,v\cos(h\,v)\\
&-2\cos(h\,v)^2\,c_3\,v\,x+h^2\,c_0\,a_1\,v^2\sin(h\,v)\\
&-16\,h^2\,c_0\,a_4\,v^2\cos(h\,v)\sin(h\,v)\\
&+h\,c_0\,a_3\,v^2\sin(h\,v)\,x\\
&-4\,h\,c_0\,a_3\,v^2\sin(h\,v)\,x\cos(h\,v)^2\\
&-c_2\,v\cos(h\,v)\,x+8\,c_5\,v\,x\cos(h\,v)^2\\
&+4\,h\,c_3\,v\cos(h\,v)^2\\
&-32\,h\,c_5\,v\cos(h\,v)^2+12\cos(h\,v)^3\,h\,c_4\,v\\
&-4\cos(h\,v)^3\,c_4\,v\,x\\
&+12\cos(h\,v)^2\,h^2\,c_0\,a_3\,v^2\sin(h\,v)),
\end{aligned}
\tag{22}
$$

$$
1=c_0+c_1+c_2+c_3+c_4+c_5, \tag{23}
$$

$$
\begin{aligned}
1=\;&2\,c_0\,a_0+2\,c_0\,a_1+2\,c_0\,a_2\\
&+2\,c_0\,a_3+2\,c_0\,a_4-2\,c_2-4\,c_3-6\,c_4-8\,c_5,
\end{aligned}
\tag{24}
$$

where $w = v\,h$. We note here that in the above system the equations (23) and (24) are produced from the requirement that method (4) is accurate for any linear combination of the functions 1, x, x^2. The equations (19–22) are produced from the requirement that method (4) is accurate for any linear combination of the functions

$$
\cos(\pm v\,x),\ \sin(\pm v\,x),\ x\cos(\pm v\,x),\ x\sin(\pm v\,x). \tag{25}
$$

Assuming the known Adams–Bashforth coefficients in terms of f_{n-i} given by (12) the solution of this system of equations is given in Appendix C.

For small values of w the formulae given by (A.1) are subject to heavy cancellations. In this case the Taylor series expansions presented in Appendix D should be used.

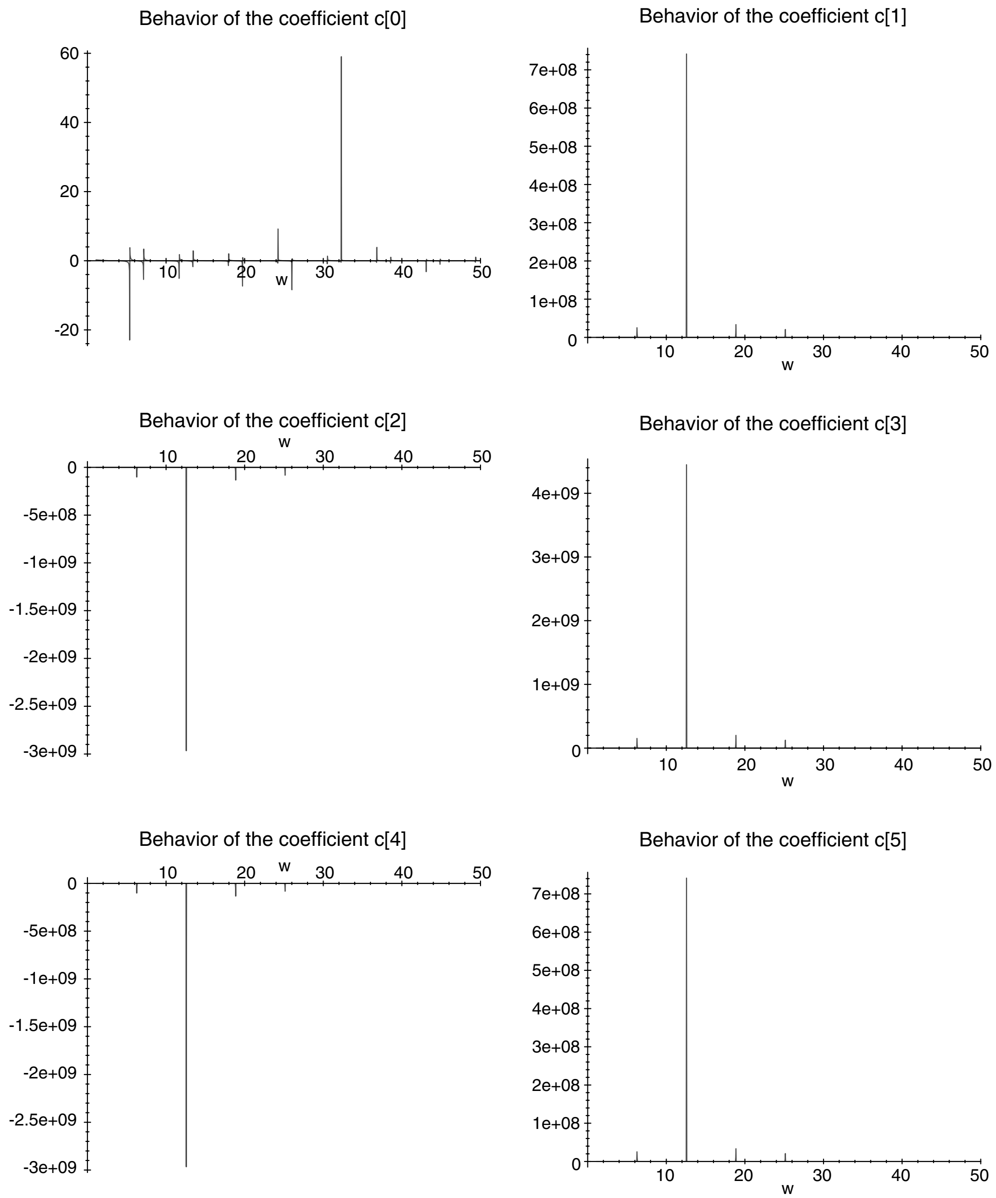

Figure 4. Behavior of the coefficients $c_i,\ i = 0(1)5$ given by (A.1) for several values of v.

In figure 4 we present the behavior of the quantities $c[i] = c_i,\ i = 0(1)5$, where $c_i,\ i = 0(1)5$ are given by (A.1). It is easy to see that for $4.5 < w < 7.5$ and $11.5 < w < 14$ (for the coefficient c_0) and for $6.2 < w < 6.4$ (for the coefficients $c_j,\ j = 1(1)5$ is better to use Taylor series expansions.

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

$$\text{L.T.E} = \frac{1}{2903040}\, h^7 \left(274451\, w^4\, y_n^{(3)} + 548902\, w^2\, y_n^{(5)} - 315875\, y_n^{(6)} - 41424\, y_n^{(7)}\right) + O\left(h^8\right), \tag{26}$$

where $y_n^{(3)}$ is the third derivative of y at x_n, $y_n^{(5)}$ is the fifth derivative of y at x_n, $y_n^{(6)}$ is the sixth derivative of y at x_n and $y_n^{(7)}$ is the seventh derivative of y at x_n. We note here that in order to produce equation (13) we express the quantities y_{n+1}, y_{n-1}, y_{n-2}, y_{n-3}, y_{n-4} and f_{n+1}, f_{n-1}, f_{n-2}, f_{n-3}, f_{n-4} around the point x_n and then we substitute the expressions into (4).

Since $w = vh$, it can be seen that when $v \to 0$ our trigonometrically fitted method becomes the original predictor–corrector method for the relevant algebraic order and step-number.

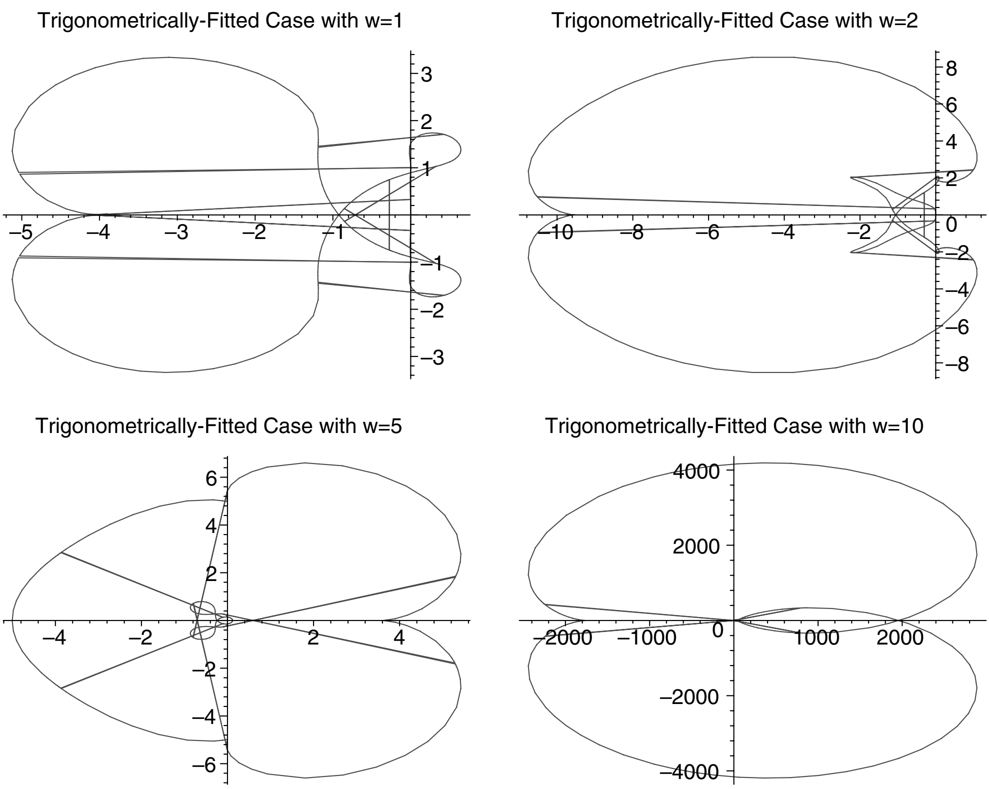

Figure 5. Stability region for the second member of the trigonometrically-fitted case and for $w = 1$ (above left), $w = 2$ (above right), $w = 5$ (below left) and $w = 10$ (below right).

2.2.2. Stability analysis of the method

We follow the same procedure as in the fist method of the family. We apply the scheme (4) with the coefficients $a_0 = \frac{1901}{720}$, $a_1 = -\frac{1387}{360}$, $a_2 = \frac{109}{30}$, $a_3 = -\frac{637}{360}$ and $a_4 = \frac{251}{720}$ to the scalar test equation (14) and we obtain the difference equation (15) and (16). The characteristic equation of (15) and (16) is given by (17).

By solving the above equation in H and using the boundary locus technique [8] and substituting $r = \exp(\mathrm{i}\theta)$, where $\mathrm{i} = \sqrt{-1}$, we can plot the regions of absolute stability for $\theta \in [0, 2\pi]$. In figure 5 we present the regions of absolute stability for the trigonometrically fitted case and for $w = 1$, $w = 2$, $w = 5$ and $w = 10$.

As we can see from figure 5, the larger the frequency w, the larger the region of absolute stability. As a matter of fact it appears that for appropriate w our trigonometrically fitted scheme has huge gains in absolute stability. Such large regions of absolute stability place our scheme in an advantageous position and thus it could be used to efficiently solve a much larger selection of problems, in comparison to other relevant methods with considerably smaller stability regions.

3. Numerical illustrations

In this section we present some numerical results to illustrate the performance of our new methods. Consider the numerical integration of the Schrödinger equation as given by (2)

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]y(r)$$

using the well-known Woods–Saxon potential (see [10,14,26,27]) which is given by

$$V(r) = V_w(r) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{27}$$

with $z = \exp[(r - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$. In figure 6 we give a graph of this potential. Below we provide certain important definitions for (2):

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

$$y(0) = 0 \tag{28}$$

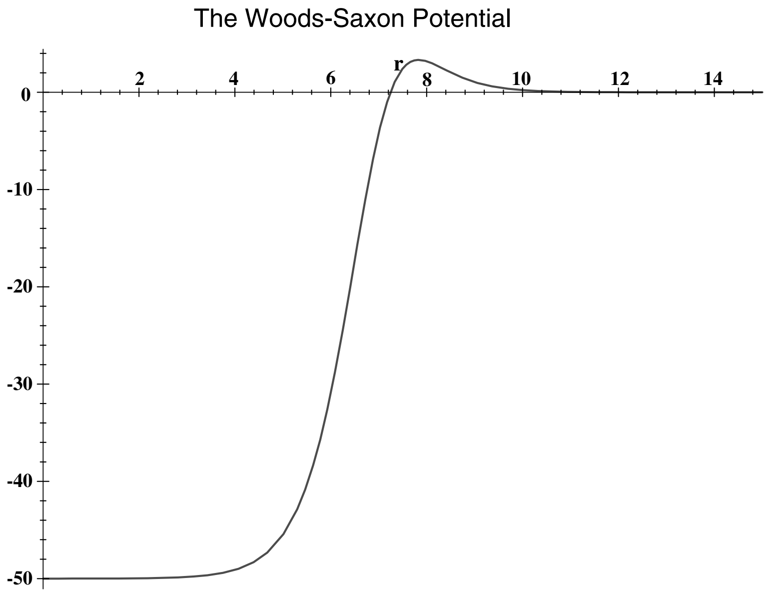

Figure 6. The Woods-Saxon potential.

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

In the case of negative eigenenergies (i.e., when $E \in [-50, 0]$) we have the well-known *bound-states problem* while in the case of positive eigenenergies (i.e., when $E \in (0, 1000]$) we have the well-known *resonance problem* (see [9,17,27]).

3.1. Resonance problem

In the asymptotic region the equation (2) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{29}$$

for x greater than some value X.

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)], \end{aligned} \tag{30}$$

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

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{31}$$

for x_1 and x_2 distinct points on the asymptotic region (for which we have that x_1 is the right-hand end point of the interval of integration and $x_2 = x_1 - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

Since the problem is treated as an initial-value problem, one needs y_j, $j = 0(1)5$ before starting a five-step methods. From the initial condition, $y_0 = 0$. The values y_k, $k = 1(1)3$ are computed using the a high order Runge–Kutta method of Dormand et al. [25]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l from the above relation.

3.1.1. The Woods–Saxon potential

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (2) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods–Saxon one (27).

One can investigate the problem considered here, following two procedures. The first procedure consists of finding the *phase shift* $\delta(E) = \delta_l$ for $E \in [1, 1000]$. The second procedure consists of finding those E, for $E \in [1, 1000]$, at which δ equals $\pi/2$. In our case we follow the first procedure i.e., we try to find the phase shifts for given energies. The obtained phase shift is then compared to the analytic value of $\pi/2$.

The above problem is the so-called *resonance problem* when *the positive eigenenergies lie under the potential barrier*. We solve this problem, using the technique fully described in [5].

The boundary conditions for this problem are:

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

The domain of numerical integration is [0, 15]. The w we use is: if $r > 6.5$ then $w = \sqrt{E - 50}$ and if $r \leqslant 6.5$ then $w = \sqrt{E}$.

For comparison purposes in our numerical illustration we use:

- the well known Numerov's method (which we call Method [a]),
- the explicit Numerov-type method of Chawla [24] (Method [b]),
- the original Adams–Bashforth–Moulton P–C multistep method (4) of fifth order (Method [c]),
- the well known Adams–Bashforth–Moulton P–C multistep method of sixth order (Method [d]),
- the well known Adams–Bashforth–Moulton P–C multistep method of seventh order (Method [e]) and

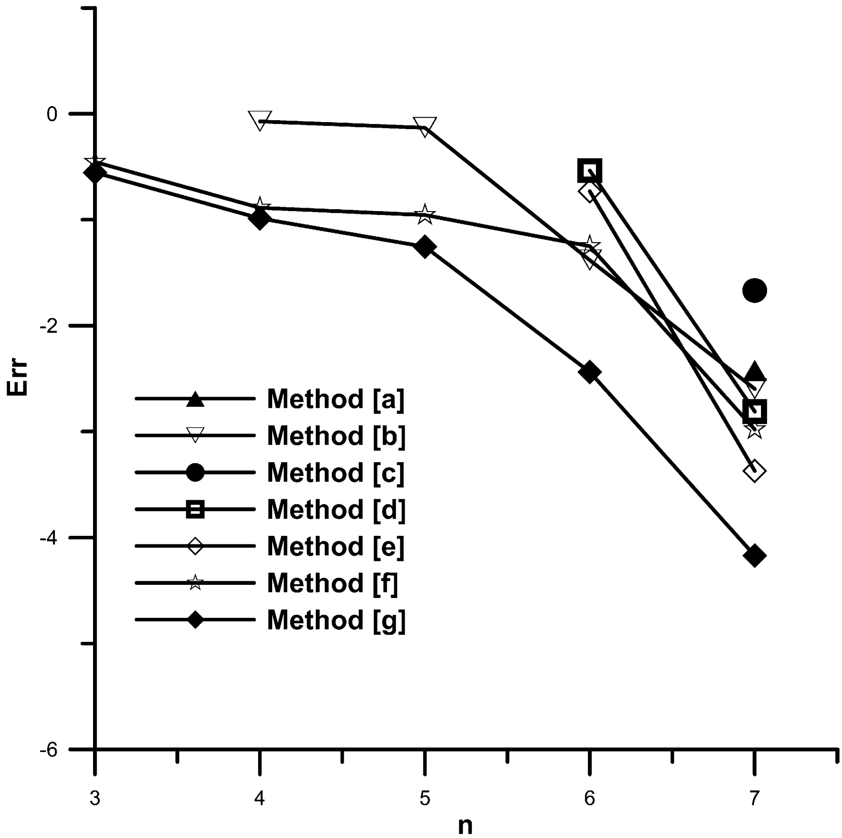

Figure 7. Error Err for several values of n for the eigenvalue $E_3 = 989.701916$.

- the first family member of the newly developed trigonometrically predictor–corrector multistep method (Method [f]),
- the second family member of the new developed trigonometrically predictor–corrector multistep method (Method [g]).

The numerical results obtained for the seven methods, with stepsizes equal to $1/2^n$ for several values of n, were compared with the analytic solution of the Woods–Saxon potential resonance problem, rounded to six decimal places. In figure 7 we may see the errors $\mathrm{Err} = -\log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$ of the highest eigenenergy $E_3 = 989.701916$ for several values of n.

4. Conclusions

In this paper have introduced a new approach for developing efficient methods for the numerical solution of the Schrödinger type equations. Using this new approach we have developed two trigonometrically fitted predictor–corrector multistep methods of algebraic order six.

From the numerical results we can draw the following points:

- Methods [a] and [c], i.e., the Numerov's method and the original P–C multistep method (4) perform very badly and basically they appear unable to solve the problem.
- The well known Adams–Bashforth–Moulton P–C multistep methods of sixth and seventh order respectively, i.e., Methods [d] and [e], just manage to solve the problem, but only with very small stepsizes (for large ns). As expected, the seventh order performs a little better.
- Method [b], i.e., the explicit Numerov-type method of Chawla [24], behaves respectably and achieves a solution from a relatively early point.
- Finally, our new trigonometrically fitted P–C schemes are overall more efficient than the other methods. In particular, the second scheme performs noticeably better than any of the other methods used, including our newly developed first P–C scheme.

Using our two new P–C schemes, in the near future we intend to publish a further paper, in which we will apply these methods to the solution of the bound states problem of the Schrödinger equation.

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

$$c_0 = -\frac{15}{4}\,\frac{48\cos(w)^3 - 24\cos(w)^2 + 55w\cos(w)\sin(w) - 36\cos(w) - 25w\sin(w) + 12}{(269\cos(w)^2 w - 270\cos(w)\sin(w) - 253w\cos(w) + 29w + 225\sin(w))\,w},$$

$$\begin{aligned}
c_1 = {} & \frac{1}{192}(138240\cos(w)^5 + 104555\cos(w)^4 w^2 + 12048\sin(w)\cos(w)^4 w \\
& -328320\cos(w)^4 + 129600\cos(w)^3 - 297046\cos(w)^3 w^2 \\
& +3000\sin(w)\cos(w)^3 w + 286656\cos(w)^2 w^2 - 4476w\cos(w)^2\sin(w) \\
& +198720\cos(w)^2 - 159840\cos(w) - 100754w^2\cos(w) - 48960w\cos(w)\sin(w) \\
& +4429w^2 + 42708w\sin(w) + 21600)/((269w\cos(w)^4 - 270\sin(w)\cos(w)^3 \\
& -791\cos(w)^3 w + 804\cos(w)^2 w + 765\sin(w)\cos(w)^2 - 720\cos(w)\sin(w) \\
& -311w\cos(w) + 29w + 225\sin(w))w),
\end{aligned}$$

$$\begin{aligned}
c_2 = {} & -\frac{1}{48}(51840\cos(w)^5 + 12048\sin(w)\cos(w)^4 w + 17937\cos(w)^4 w^2 \\
& -112320\cos(w)^4 + 21600\cos(w)^3 - 42344\cos(w)^3 w^2 - 9060\sin(w)\cos(w)^3 w
\end{aligned}$$

$$
\begin{aligned}
&-7806\,w\cos(w)^2\sin(w)+27768\cos(w)^2\,w^2+90720\cos(w)^2-51840\cos(w)\\
&-612\,w^2\cos(w)-6120\,w\cos(w)\sin(w)+15258\,w\sin(w)-4909\,w^2)/\\
&((\cos(w)^2-2\cos(w)+1)\,w(269\cos(w)^2\,w-270\cos(w)\sin(w)\\
&-253\,w\cos(w)+29\,w+225\sin(w))),\\
c_3={}&-\frac{1}{96}(-69120\cos(w)^5+1603\cos(w)^4\,w^2-36144\sin(w)\cos(w)^4\,w\\
&+120960\cos(w)^4+43200\cos(w)^3+70560\sin(w)\cos(w)^3\,w\\
&-35914\cos(w)^3\,w^2+82320\cos(w)^2\,w^2-61992\,w\cos(w)^2\sin(w)\\
&-164160\cos(w)^2+47520\cos(w)+59040\,w\cos(w)\sin(w)-62230\,w^2\cos(w)\\
&+20701\,w^2-44424\,w\sin(w)+21600)/((269\,w\cos(w)^4-270\sin(w)\cos(w)^3\\
&-791\cos(w)^3\,w+804\cos(w)^2\,w+765\sin(w)\cos(w)^2-720\cos(w)\sin(w)\\
&-311\,w\cos(w)+29\,w+225\sin(w))w),\\
c_4={}&\frac{1}{48}(-8640\cos(w)^5+4320\cos(w)^4-12048\sin(w)\cos(w)^4\,w+8963\cos(w)^4\,w^2\\
&+32400\cos(w)^3-36756\cos(w)^3\,w^2+31560\sin(w)\cos(w)^3\,w-36720\cos(w)^2\\
&-37194\,w\cos(w)^2\sin(w)+52632\cos(w)^2\,w^2-2160\cos(w)-30488\,w^2\cos(w)\\
&+28620\,w\cos(w)\sin(w)+10800-15258\,w\sin(w)+7809\,w^2)/\\
&((\cos(w)^2-2\cos(w)+1)\,w(269\cos(w)^2\,w-270\cos(w)\sin(w)-253\,w\cos(w)\\
&+29\,w+225\sin(w))),\\
c_5={}&-\frac{1}{192}(-17280\cos(w)^4+13805\cos(w)^4\,w^2-12048\sin(w)\cos(w)^4\,w\\
&-50994\cos(w)^3\,w^2+36600\sin(w)\cos(w)^3\,w+43200\cos(w)^3\\
&-47724\,w\cos(w)^2\sin(w)-25920\cos(w)^2+67104\cos(w)^2\,w^2\\
&-36086\,w^2\cos(w)+34560\,w\cos(w)\sin(w)-12960\cos(w)-15708\,w\sin(w)\\
&+12960+8331\,w^2)/((\cos(w)^2-2\cos(w)+1)\,w(269\cos(w)^2\,w\\
&-270\cos(w)\sin(w)-253\,w\cos(w)+29\,w+225\sin(w))),
\end{aligned}
\tag{A.1}
$$

where $w = v\,h$.

Appendix B

$$
\begin{aligned}
c_0 = {}&\frac{95}{288}-\frac{16691}{435456}\,w^2+\frac{617963}{658409472}\,w^4-\frac{6747760249}{273766658457600}\,w^6\\
&-\frac{1630503557167}{26905787193212928000}\,w^8-\frac{543718683891689}{40681550236137947136000}\,w^{10}\\
&-\frac{1532464198122612586 21}{2875616059991646931255296 00000}\,w^{12}+\cdots
\end{aligned}
$$

$$
\begin{aligned}
c_1 = {} & \frac{1427}{1440} + \frac{120821}{1244160}\,w^2 - \frac{111345817}{65840947200}\,w^4 + \frac{36456178571}{1095066633830400}\,w^6 \\
& + \frac{708972974579}{1956784523142758400}\,w^8 + \frac{617293894360919}{3254524018891035770880}\,w^{10} \\
& + \frac{1935617462985481288 99}{2300492847993317545004236800 00}\,w^{12} + \cdots \\
c_2 = {} & -\frac{133}{240} - \frac{11197}{2177280}\,w^2 - \frac{43144933}{16460236800}\,w^4 + \frac{31021423919}{273766658457600}\,w^6 \\
& - \frac{907539121207}{1076231487728517120}\,w^8 + \frac{470143473422459}{813631004722758942720 0}\,w^{10} \\
& + \frac{112931093325974388343}{575123211998329386251059200 00}\,w^{12} + \cdots \\
c_3 = {} & \frac{241}{720} - \frac{800959}{4354560}\,w^2 + \frac{283925549}{32920473600}\,w^4 - \frac{160541874247}{547533316915200}\,w^6 \\
& + \frac{796313823367}{827870375175782400}\,w^8 - \frac{499573557610151}{3254524018891035770880}\,w^{10} \\
& - \frac{645286119602445682271}{115024642399665877250211840000}\,w^{12} + \cdots \\
c_4 = {} & -\frac{173}{1440} + \frac{203039}{1088640}\,w^2 - \frac{30097577}{4115059200}\,w^4 + \frac{16190056291}{68441664614400}\,w^6 \\
& - \frac{726798012217}{1345289359660646400}\,w^8 + \frac{253465539328537}{203407751180689735680 0}\,w^{10} \\
& + \frac{665443782845589117 41}{143780802999582346562764800 00}\,w^{12} + \cdots \\
c_5 = {} & \frac{3}{160} - \frac{489533}{8709120}\,w^2 + \frac{135839383}{65840947200}\,w^4 - \frac{71507985413}{1095066633830400}\,w^6 \\
& + \frac{12905456687173}{107623148772851712000}\,w^8 - \frac{5613029470462429}{162726200944551788544000}\,w^{10} \\
& - \frac{873019991472611466 73}{676615543527446336765952000 00}\,w^{12} + \cdots
\end{aligned}
\tag{B.1}
$$

Appendix C

$$
\begin{aligned}
c_0 = {} & -\frac{45}{2}(-8\,w\cos(w)^4 + 8\sin(w)\cos(w)^3 + 8\,w\cos(w)^3 + 14\,w\cos(w)^2 \\
& -4\sin(w)\cos(w)^2 - 10\,w\cos(w) + 5\,w^2\cos(w)\sin(w) - 6\cos(w)\sin(w) \\
& -4\,w + 5\,w^2\sin(w) + 2\sin(w))\big/((-269\sin(w)\cos(w)^2 + 16\,w\cos(w)^2 \\
& +208\cos(w)\sin(w) + 343\,w\cos(w) - 224\,w - 74\sin(w))w^2),
\end{aligned}
$$

$$c_1 = \frac{1}{32}(-8592\,w - 4602\,w^3 + 1958\sin(w) + 20298\,w^2\cos(w)\sin(w)$$
$$+5756\sin(w)\cos(w)^2 + 6244\,w\cos(w) - 10260\cos(w)\sin(w)$$
$$+15680\sin(w)\cos(w)^3 - 22712\,w\cos(w)^3 + 25336\,w\cos(w)^4 + 19668\,w\cos(w)^2$$
$$-34426\sin(w)\cos(w)^2\,w^2 - 2170\sin(w)\cos(w)^3\,w^2 + 30419\sin(w)\cos(w)^4\,w^2$$
$$+15208\sin(w)\cos(w)^6\,w^2 - 28368\sin(w)\cos(w)^5\,w^2 + 3752\sin(w)\cos(w)^6$$
$$-5420\sin(w)\cos(w)^5 - 11466\sin(w)\cos(w)^4 - 36412\,w\cos(w)^6$$
$$-12204\cos(w)^5\,w + 9505\cos(w)^5\,w^3 + 28672\cos(w)^7\,w - 27092\cos(w)^3\,w^3$$
$$+5682\cos(w)^2\,w^3 + 18667\cos(w)\,w^3 - 4201\,w^2\sin(w))/((-269\sin(w)\cos(w)^5$$
$$+16\cos(w)^5\,w + 477\sin(w)\cos(w)^4 + 327\,w\cos(w)^4 - 13\sin(w)\cos(w)^3$$
$$-583\,w\cos(w)^3 - 403\sin(w)\cos(w)^2 - 103\,w\cos(w)^2 + 282\cos(w)\sin(w)$$
$$+567\,w\cos(w) - 74\sin(w) - 224\,w)w^2),$$

$$c_2 = -\frac{1}{16}(-3650\,w + 6935\cos(w)^4\,w^3 + 3545\,w^3 + 158\sin(w)$$
$$+13828\,w^2\cos(w)\sin(w) + 5396\sin(w)\cos(w)^2 + 6746\,w\cos(w)$$
$$-3060\cos(w)\sin(w) - 880\sin(w)\cos(w)^3 + 21324\,w\cos(w)^3 + 4302\,w\cos(w)^4$$
$$-8852\,w\cos(w)^2 - 19204\sin(w)\cos(w)^2\,w^2 + 10272\sin(w)\cos(w)^3\,w^2$$
$$-13919\sin(w)\cos(w)^4\,w^2 + 12120\sin(w)\cos(w)^5\,w^2 - 2008\sin(w)\cos(w)^6$$
$$+3220\sin(w)\cos(w)^5 - 2826\sin(w)\cos(w)^4 + 25112\,w\cos(w)^6$$
$$-46990\cos(w)^5\,w + 2008\cos(w)^7\,w - 13594\cos(w)^3\,w^3 + 6028\cos(w)^2\,w^3$$
$$-754\cos(w)\,w^3 - 6337\,w^2\sin(w))/((-269\sin(w)\cos(w)^4 + 16\,w\cos(w)^4$$
$$+746\sin(w)\cos(w)^3 + 311\,w\cos(w)^3 - 894\,w\cos(w)^2 - 759\sin(w)\cos(w)^2$$
$$+791\,w\cos(w) + 356\cos(w)\sin(w) - 74\sin(w) - 224\,w)w^2),$$

$$c_3 = -\frac{1}{16}(1484\,w - 4994\cos(w)^4\,w^3 - 4208\,w^3 - 158\sin(w) - 184\,w^2\cos(w)\sin(w)$$
$$+4\sin(w)\cos(w)^2 + 10892\,w\cos(w) + 3104\cos(w)\sin(w) + 4016\sin(w)\cos(w)^7$$
$$-4016\,w\cos(w)^8 - 12432\sin(w)\cos(w)^3 - 48336\,w\cos(w)^3 + 50404\,w\cos(w)^4$$
$$-16016\,w\cos(w)^2 - 7066\sin(w)\cos(w)^2\,w^2 + 22322\sin(w)\cos(w)^3\,w^2$$
$$+15661\sin(w)\cos(w)^4\,w^2 - 424\sin(w)\cos(w)^6\,w^2 - 25898\sin(w)\cos(w)^5\,w^2$$
$$-7312\sin(w)\cos(w)^6 + 5312\sin(w)\cos(w)^5 + 7466\sin(w)\cos(w)^4$$
$$-31856\,w\cos(w)^6 + 37156\cos(w)^5\,w + 119\cos(w)^5\,w^3 + 288\cos(w)^7\,w$$
$$+3968\cos(w)^3\,w^3 + 5962\cos(w)^2\,w^3 - 7327\cos(w)\,w^3 + 5309\,w^2\sin(w))/$$
$$((-269\sin(w)\cos(w)^5 + 16\cos(w)^5\,w + 477\sin(w)\cos(w)^4 + 327\,w\cos(w)^4$$
$$-13\sin(w)\cos(w)^3 - 583\,w\cos(w)^3 - 403\sin(w)\cos(w)^2 - 103\,w\cos(w)^2$$
$$+282\cos(w)\sin(w) + 567\,w\cos(w) - 74\sin(w) - 224\,w)w^2)$$

$$
\begin{aligned}
c_4 = {} & \frac{1}{16}(2002\,w + 3185\cos(w)^4\,w^3 - 4705\,w^3 - 158\sin(w) - 1868\,w^2\cos(w)\sin(w) \\
& -8276\sin(w)\cos(w)^2 + 5782\,w\cos(w) + 3780\cos(w)\sin(w) \\
& +1600\sin(w)\cos(w)^3 + 19236\,w\cos(w)^3 + 35778\,w\cos(w)^4 - 33068\,w\cos(w)^2 \\
& -6556\sin(w)\cos(w)^2\,w^2 + 27808\sin(w)\cos(w)^3\,w^2 - 24921\sin(w)\cos(w)^4\,w^2 \\
& +5096\sin(w)\cos(w)^5\,w^2 + 2008\sin(w)\cos(w)^6 - 6100\sin(w)\cos(w)^5 \\
& +7146\sin(w)\cos(w)^4 + 12200\,w\cos(w)^6 - 39922\cos(w)^5\,w - 2008\cos(w)^7\,w \\
& -9606\cos(w)^3\,w^3 + 7052\cos(w)^2\,w^3 + 1914\cos(w)\,w^3 + 3681\,w^2\sin(w))/ \\
& ((-269\sin(w)\cos(w)^4 + 16\,w\cos(w)^4 + 746\sin(w)\cos(w)^3 + 311\,w\cos(w)^3 \\
& -894\,w\cos(w)^2 - 759\sin(w)\cos(w)^2 + 791\,w\cos(w) + 356\cos(w)\sin(w) \\
& -74\sin(w) - 224\,w)w^2), \\
c_5 = {} & -\frac{1}{32}(2624\,w - 5518\,w^3 + 202\sin(w) + 286\,w^2\cos(w)\sin(w) \\
& -7916\sin(w)\cos(w)^2 - 1844\,w\cos(w) + 2340\cos(w)\sin(w) \\
& +3760\sin(w)\cos(w)^3 + 21352\,w\cos(w)^3 + 12104\,w\cos(w)^4 - 18820\,w\cos(w)^2 \\
& -6294\sin(w)\cos(w)^2\,w^2 + 13970\sin(w)\cos(w)^3\,w^2 - 6699\sin(w)\cos(w)^4\,w^2 \\
& +2008\sin(w)\cos(w)^6\,w^2 - 4016\sin(w)\cos(w)^5\,w^2 + 2008\sin(w)\cos(w)^6 \\
& -6100\sin(w)\cos(w)^5 + 5706\sin(w)\cos(w)^4 + 4092\,w\cos(w)^6 \\
& -19508\cos(w)^5\,w + 1255\cos(w)^5\,w^3 - 6348\cos(w)^3\,w^3 + 4438\cos(w)^2\,w^3 \\
& +4013\cos(w)\,w^3 + 3985\,w^2\sin(w))/((-269\sin(w)\cos(w)^5 + 16\cos(w)^5\,w \\
& +477\sin(w)\cos(w)^4 + 327\,w\cos(w)^4 - 13\sin(w)\cos(w)^3 - 583\,w\cos(w)^3 \\
& -403\sin(w)\cos(w)^2 - 103\,w\cos(w)^2 + 282\cos(w)\sin(w) + 567\,w\cos(w) \\
& -74\sin(w) - 224\,w)w^2),
\end{aligned}
\tag{C.1}
$$

where $w = v\,h$.

Appendix D

$$
\begin{aligned}
c_0 = {} & \frac{95}{288} - \frac{16691}{217728}w^2 + \frac{4441291}{823011840}w^4 - \frac{667102693}{8555208076800}w^6 \\
& + \frac{161743808609}{76436895435264000}w^8 - \frac{160492149731219}{1271298444879310848000}w^{10} \\
& - \frac{4157762749700361349}{345626930287457563852800000}w^{12} + \cdots
\end{aligned}
$$

$$\begin{aligned}
c_1 &= \frac{1427}{1440} + \frac{120821}{622080} w^2 - \frac{848384329}{16460236800} w^4 + \frac{236767896359}{136883329228800} w^6 \\
&\quad - \frac{14790812373479}{840805849787904000} w^8 + \frac{1082065512430667}{635649222439655424000} w^{10} \\
&\quad + \frac{3983594582040531541}{3594520074989558664069120000} w^{12} + \cdots \\
c_2 &= -\frac{133}{240} - \frac{11197}{1088640} w^2 + \frac{159111073}{8230118400} w^4 + \frac{119191515379}{68441664614400} w^6 \\
&\quad - \frac{210529105869239}{840805849787904000} w^8 + \frac{17291289653066651}{254259688975862169600 0} w^{10} \\
&\quad - \frac{6356238984788850172821}{1797260037494779332034560000} w^{12} + \cdots \\
c_3 &= \frac{241}{720} - \frac{800959}{2177280} w^2 + \frac{845622083}{8230118400} w^4 \\
&\quad - \frac{603625434817}{68441664614400} w^6 + \frac{788484410653}{1469940296832000} w^8 \\
&\quad - \frac{24861626265433117}{1271298444879310848000} w^{10} + \frac{1148437640691769738393}{1797260037494779332034560000} w^{12} + \cdots \\
c_4 &= -\frac{173}{1440} + \frac{203039}{544320} w^2 - \frac{693873277}{8230118400} w^4 \\
&\quad + \frac{402824638499}{68441664614400} w^6 - \frac{110085754079447}{420402924893952000} w^8 \\
&\quad + \frac{31864509400954033}{2542596889758621696000} w^{10} - \frac{2898689436188606263 31}{1797260037494779332034560000} w^{12} + \cdots \\
c_5 &= \frac{3}{160} - \frac{489533}{4354560} w^2 + \frac{137838751}{16460236800} w^4 - \frac{62875691393}{136883329228800} w^6 \\
&\quad - \frac{7300838386603}{840805849787904000} w^8 - \frac{85995606835367}{63564922243965542400} w^{10} \\
&\quad - \frac{1195977821097866623 51}{1057211786761634901196800000} w^{12} + \cdots
\end{aligned} \tag{D.1}$$

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