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The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor–Corrector methods

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In this paper, we develop new seventh order trigonometrically fitted Adams–Bashforth–Moulton predictor–corrector (P–C) algorithms. Our predictor is based on the sixth algebraic order Adams–Bashforth scheme and our corrector on the seventh algebraic order Adams–Moulton scheme. In order to assess the efficiency of our new methods, we contacted appropriate comparisons of our schemes against well known methods and the numerical experimentations demonstrated that our schemes behave more efficiently.

KEY WORDS: Trigonometric fitting, Predictor-Corrector methods, Schrödinger equation

1. Introduction

Equations or systems of equations of the form

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

are often used as the main mathematical model for problems in physical chemistry and chemical physics, celestial mechanics, electronics, quantum mechanics, nanotechnology, financial maths, materials sciences and elsewhere. The class of the above equations with oscillatory and/or periodic solution need special attention (see [1, 2]).

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During the last couple decades there has been much research activity towards the investigation of the numerical solution of the above equation (indicatively see [3–13] and also [14–37]). The exponential and the trigonometric fitting technique first introduced by Lyche [23] is one of the better processes for the development of efficient methods for the numerical integration of first order initial value problems with oscillating or periodic solution. In previous papers of ours [38, 39], we had applied trigonometric fitting to lower algebraic order Adams–Bashforth–Moulton P–C schemes for the solution of (1), with excellent results. We have also applied trigonometric fitting to quite different types of P–C methods, like the Explicit Advanced Step-point or EAS methods (see [40]), which had been introduced in their non-trigonometrically fitted form in [41]. A main characteristic of the methods developed in the literature for the numerical solution of (1) is that they belong to the type of multistep and hybrid approaches, to which P–C methods also belong. Interestingly, until our recent paper [42], it appears that there had been no previous successful attempts to use trigonometrically fitted P–C schemes for the efficient solution of the radial Schrödinger equation. In this paper, we develop seventh order algorithms of our trigonometrically fitted Adams–Bashforth–Moulton P–C methods, which we had previously developed in their sixth order in [43, 44]. With respect to exponential and trigonometric fitting, the reader could refer to [45, 46] for a glimpse of certain different numerical methods, which could be employed in the solution of similar problems.

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 theoretical physics and chemistry (see, e.g. [6]). During the last 20 years or so many numerical methods have been constructed for the approximate solution of the Schrödinger equation (see indicatively [3–7, 47]). The aim and the scope of the above activity was the development of fast and reliable methods and such 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 constructed as follows: In section 2, we develop the new seventh order trigonometrically fitted P–C schemes and we briefly discuss the stability of our new method. In section 3, we proceed to the numerical comparisons and results. In section 4, we make a few concluding remarks. After Section 4, four Appendices can be found with several equations.

[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 seventh order P–C schemes

The P–C family of methods which appears below has been widely used (e.g. [48]):

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

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 seventh algebraic order six-step scheme:

$$\overline{y}_{n+1} = y_n + h \sum_{i=0}^{5} a_i f_{n-i},$$
$$y_{n+1} = y_n + h \sum_{i=0}^{6} c_i g_{n-i+1}, \tag{4}$$

where,

- $g_{n+1} = \overline{f}_{n+1},\ g_{n-j} = f_{n-j},\ j = 0(1)5$
- in terms of $f_{n-i},\ a_i,\ i = 0(1)5$ are the known Adams–Bashforth coefficients and $c_i,\ i = 0(1)6$ the coefficients correspond to the Adams–Moulton coefficients for (3) above, as well as for $w = 0$ (see equation (22) in Appendix B).

2.1. *First member of the family: developing the new scheme*

In this instance and in contrast to the trigonometric functions we have used in previous investigations (e.g. [47]), we ask for the above method (4) to be exact for any linear combination of the following functions:

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

Hence, in order for (4) to be exact for any linear combination of the above trigonometric functions, the following system of equations must hold:

$$\begin{aligned}-1 + \cos(h\,w) = {} & -w\,h(-c_0\,h\,a_2\,w + c_0\,h\,a_4\,w - c_2 \sin(h\,w) + 4\,c_5 \cos(h\,w)\sin(h\,w) \\ & + c_0\,h\,a_0\,w + 16\cos(h\,w)^5\,h\,w\,c_0\,a_5 - 16\cos(h\,w)^4\,c_6 \sin(h\,w)\end{aligned}$$

$$
\begin{aligned}
&-4\,c_4 \sin(h\,w)\cos(h\,w)^2 - 8\,c_5 \cos(h\,w)^3 \sin(h\,w)\\
&+4\cos(h\,w)^3\, h\,w\,c_0\,a_3 - 20\cos(h\,w)^3\, h\,w\,c_0\,a_5\\
&-8\cos(h\,w)^2\, c_0\,h\,a_4\,w + 8\cos(h\,w)^4\, c_0\,h\,a_4\,w\\
&+2\,c_0\,h\,a_2\,w\cos(h\,w)^2 + 12\,c_6 \sin(h\,w)\cos(h\,w)^2\\
&+h\,w\,c_0\,a_1\cos(h\,w) - 3\,h\,w\,c_0\,a_3\cos(h\,w)\\
&+5\,h\,w\,c_0\,a_5\cos(h\,w) - 2\,c_3\cos(h\,w)\sin(h\,w)\\
&+c_4\sin(h\,w) - c_6\sin(h\,w))
\end{aligned}
$$

$$
\begin{aligned}
\sin(h\,w) = {}& w\,h(c_0 + c_1 - c_3 + c_5 + 16\cos(h\,w)^5\, c_6 + c_2\cos(h\,w)\\
&+h\,w\,c_0\,a_5\sin(h\,w) + 2\,h\,w\,c_0\,a_2\cos(h\,w)\sin(h\,w) - h\,w\,c_0\,a_3\sin(h\,w)\\
&-12\,h\,w\,c_0\,a_5\sin(h\,w)\cos(h\,w)^2 + 4\cos(h\,w)^2\, h\,w\,c_0\,a_3\sin(h\,w)\\
&+8\,h\,w\,c_0\,a_4\cos(h\,w)^3\sin(h\,w) + 4\,c_4\cos(h\,w)^3 - 8\,c_5\cos(h\,w)^2\\
&+8\,c_5\cos(h\,w)^4 - 20\,c_6\cos(h\,w)^3 + 2\,c_3\cos(h\,w)^2 + h\,w\,c_0\,a_1\sin(h\,w)\\
&+16\cos(h\,w)^4\, h\,w\,c_0\,a_5\sin(h\,w) - 4\,h\,w\,c_0\,a_4\cos(h\,w)\sin(h\,w)\\
&-3\,c_4\cos(h\,w) + 5\,c_6\cos(h\,w)\\
1 = {}& c_0 + c_1 + c_2 + c_3 + c_4 + c_5 + c_6\\
1 = {}& -2\,c_2 + 2\,c_0\,a_0 + 2\,c_0\,a_1 + 2\,c_0\,a_2 + 2\,c_0\,a_3 + 2\,c_0\,a_4 + 2\,c_0\,a_5\\
&-4\,c_3 - 6\,c_4 - 8\,c_5 - 10\,c_6\\
1 = {}& 3\,c_2 + 12\,c_3 + 27\,c_4 + 48\,c_5 + 75\,c_6 - 6\,c_0\,a_1 - 12\,c_0\,a_2 - 18\,c_0\,a_3\\
&-24\,c_0\,a_4 - 30\,c_0\,a_5\\
1 = {}& -32\,c_3 + 12\,c_0\,a_1 - 256\,c_5 - 500\,c_6 + 48\,c_0\,a_2 + 108\,c_0\,a_3 + 192\,c_0\,a_4\\
&+300\,c_0\,a_5 - 4\,c_2 - 108\,c_4\\
1 = {}& 80\,c_3 + 1280\,c_5 + 3125\,c_6 + 5\,c_2 + 405\,c_4 - 20\,c_0\,a_1 - 160\,c_0\,a_2\\
&-540\,c_0\,a_3 - 1280\,c_0\,a_4 - 2500\,c_0\,a_5.
\end{aligned} \tag{6}
$$

Assuming the known Adams-Bashforth coefficients in terms of f_{n-i}:

$$
\begin{aligned}
a_0 &= \frac{4277}{1440}, \quad a_1 = -\frac{2641}{480}, \quad a_2 = \frac{4991}{720},\\
a_3 &= -\frac{3649}{720}, \quad a_4 = \frac{959}{480}, \quad a_5 = -\frac{95}{288}
\end{aligned} \tag{7}
$$

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

For small values of w the formulae given in Appendix A by (21) are subject to heavy cancellations. In such a case the Taylor series expansions, which are given in Appendix B, should be used.

In figure 1, we present the behaviour of the quantities $c[i] = c_i,\ \ i = 0(1)6$, where $c_i,\ i = 0(1)6$ are given by (21). It is easy to see that for w in which we have cancellations it is appropriate to use the relevant Taylor series expansion.

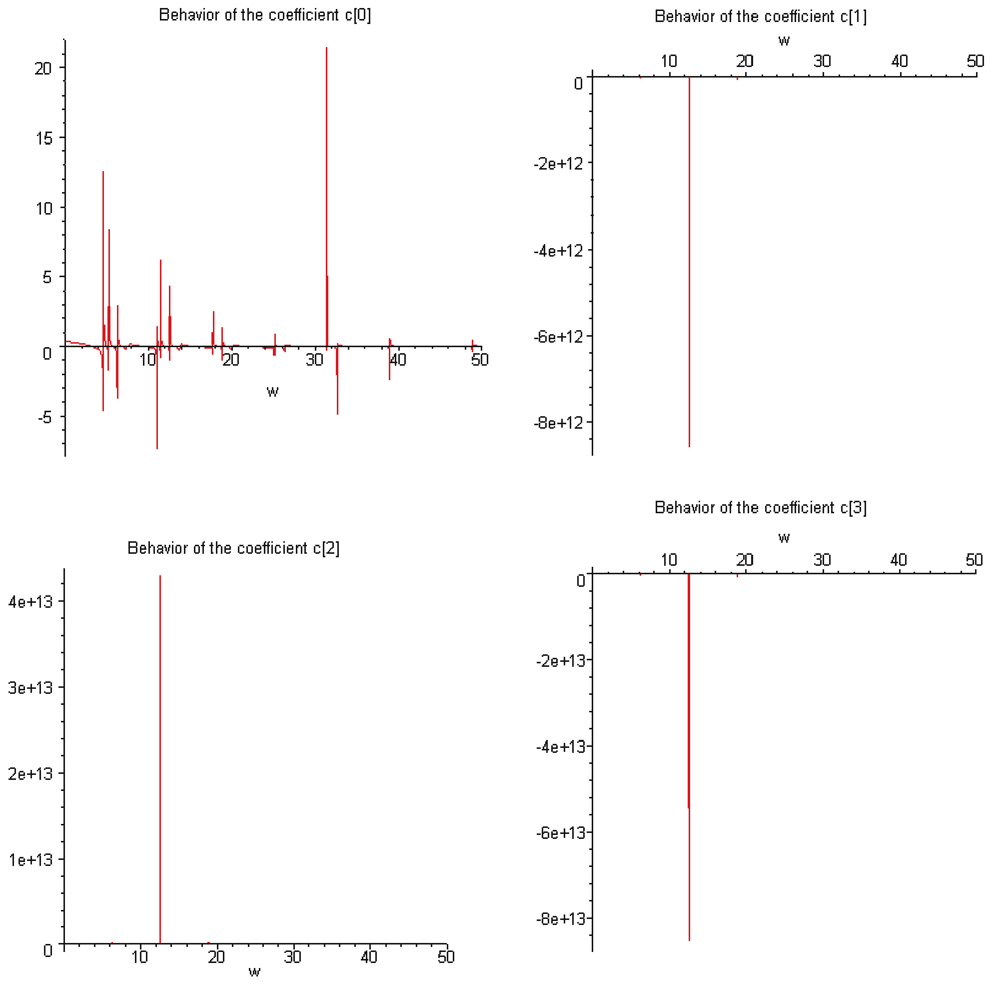

Figure 1. Behavior of the coefficients c_i, $i = 0(1)6$ given by (21) for several values of v.

The above method has the following local truncation error:

$$L.T.E = \frac{1}{3657830400} h^8 \left(322733569\, w^2\, y_n^{(6)} - 364313569\, y_n^{(7)} - 41580000\, y_n^{(8)}\right) + O\left(h^9\right), \tag{8}$$

where $y_n^{(6)}$ is the sixth derivative of y at x_n, $y_n^{(7)}$ is the seventh derivative of y at x_n and $y_n^{(8)}$ is the eighth derivative of y at x_n. We note here that in order to produce equation (8) we express the quantities y_{n+1}, y_{n-1}, y_{n-2}, y_{n-3}, y_{n-4}, y_{n-5} and f_{n+1}, f_{n-1}, f_{n-2}, f_{n-3}, f_{n-4}, f_{n-5} around the point x_n and then we substitute the expressions into (4).

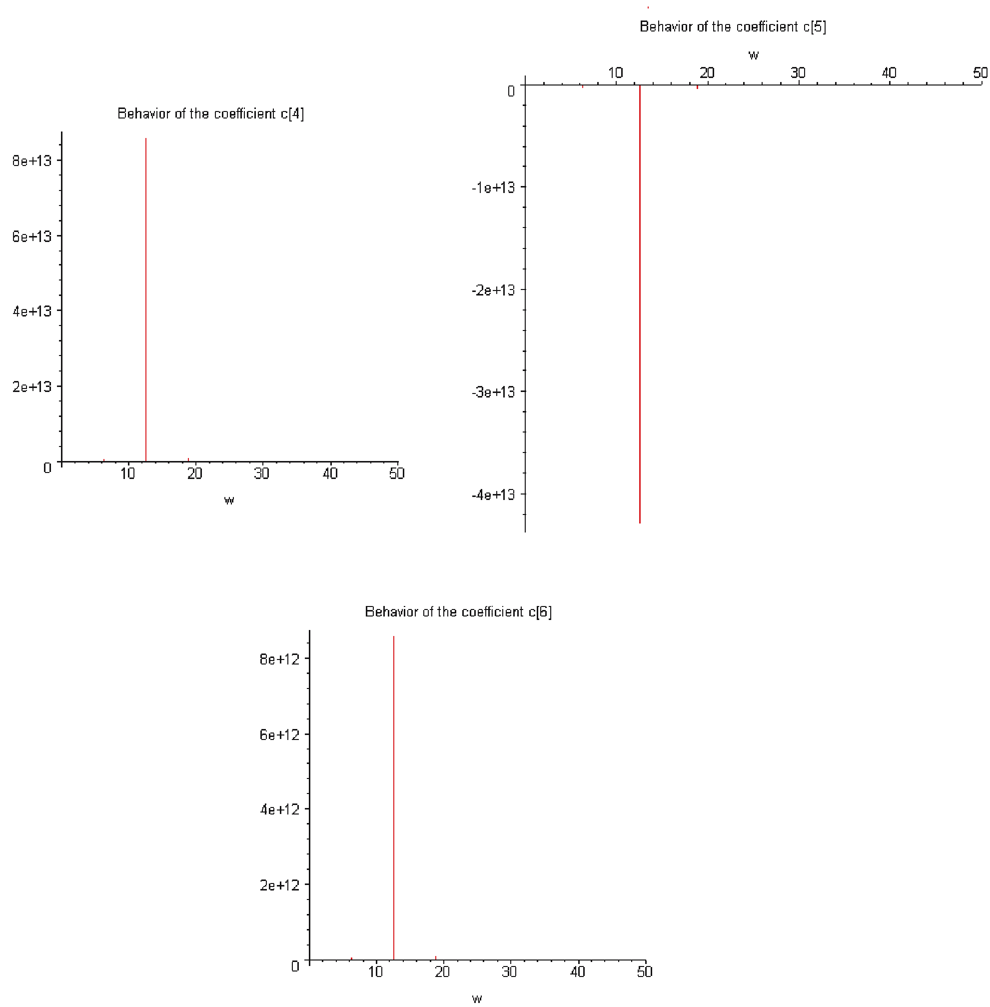

Figure 1. Continued.

Since $w = vh$, we see that when $v \to 0$ our trigonometrically fitted method becomes the original P–C method for the relevant algebraic order and step-number.

2.1.1. Stability analysis

Applying scheme (4) with the coefficients $a_0 = \frac{4277}{1440}$, $a_1 = -\frac{2641}{480}$, $a_2 = \frac{4991}{720}$, $a_3 = -\frac{3649}{720}$, $a_4 = \frac{959}{480}$, $a_5 = -\frac{95}{288}$ to the scalar test equation

$$y' = \lambda\, y, \qquad \text{where } \lambda \in \mathcal{C}, \tag{9}$$

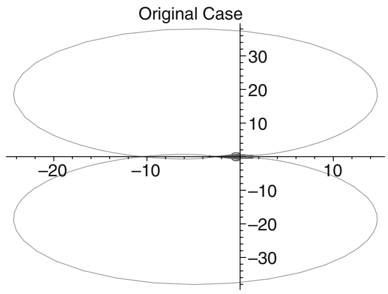

Figure 2. Stability region for the original Adams–Bashforth–Moulton method.

we obtain the following difference equation

$$y_{n+1} + A_0(H)\, y_n + A_1(H)\, y_{n-1} + A_2(H)\, y_{n-2} + A_3(H)\, y_{n-3} + A_4(H)\, y_{n-4} + A_5(H)\, y_{n-5} = 0, \tag{10}$$

where

$$A_0(H) = -1 - c_0\, H - \frac{4277}{1440}\, c_0\, H^2 - H\, c_1,$$
$$A_1(H) = \frac{2641}{480}\, c_0\, H^2 - H\, c_2,$$
$$A_2(H) = -\frac{4991}{720}\, c_0\, H^2 - H\, c_3, \qquad A_3 = \frac{3649}{720}\, c_0\, H^2 - H\, c_4,$$
$$A_4 = -\frac{959}{480}\, c_0\, H^2 - H\, c_5, \qquad A_5 = \frac{95}{288}\, c_0\, H^2 - H\, c_6. \tag{11}$$

The characteristic equation of (10) is given by

$$r^6 + A_0(H)\, r^5 + A_1(H)\, r^4 + A_2(H)\, r^3 + A_3(H)\, r^2 + A_4(H) r + A_5(H) = 0. \tag{12}$$

By solving the above equation in H, using the boundary locus technique [49] and substituting $r = \exp(i\,\theta)$, where $i = \sqrt{-1}$, 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 Adams–Bashforth–Moulton P–C case (i.e. method (4) without trigonometric fitting). In figure 3, we present the regions of absolute stability for the first member of the family of our new trigonometrically fitted case and for $w = 1$, $w = 2$, $w = 5$ and $w = 10$.

Among other things, it remains to be investigated how w influences the regions of absolute stability.

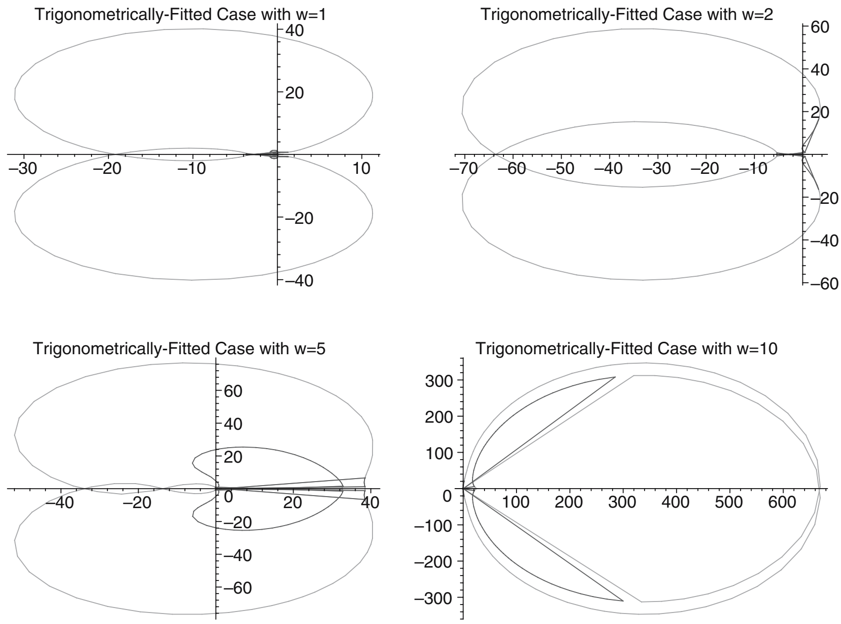

Figure 3. Stability region for the trigonometrically-fitted case and for $w = 1$ (above left), $w = 2$ (above right), $w = 5$ (below left) and $w = 10$ (below right).

2.2. Second member of the family: developing the new scheme

We base our analysis on the same method (4) mentioned above. In this instance, we ask for the above method (4) to be exact for any linear combination of the following functions:

$$\{1,\ x,\ x^2,\ x^3,\ \cos(\pm v x),\ \sin(\pm v x),\ x\cos(\pm v x),\ x\sin(\pm v x)\}. \tag{13}$$

Hence, in order for (4) to be exact for any linear combination of the above trigonometric functions, the following system of equations must hold:

$$\begin{aligned}-1+\cos(h\,w) = {} & -w\,h(c_0\,h\,a_0\,w - c_0\,h\,a_2\,w - 16\cos(h\,w)^4\,c_6\sin(h\,w) + c_0\,h\,a_4\,w\\ & -20\cos(h\,w)^3\,h\,w\,c_0\,a_5 + 4\,c_5\cos(h\,w)\sin(h\,w)\\ & -4\,c_4\sin(h\,w)\cos(h\,w)^2 + 12\,c_6\sin(h\,w)\cos(h\,w)^2\\ & +16\cos(h\,w)^5\,h\,w\,c_0\,a_5 - 8\,c_5\cos(h\,w)^3\sin(h\,w)\\ & -8\,c_0\,h\,a_4\,w\cos(h\,w)^2 + 8\,c_0\,h\,a_4\,w\cos(h\,w)^4\\ & +2\cos(h\,w)^2\,c_0\,h\,a_2\,w + 4\cos(h\,w)^3\,h\,w\,c_0\,a_3 + h\,w\,c_0\,a_1\cos(h\,w)\\ & -3\,h\,w\,c_0\,a_3\cos(h\,w) + 5\,h\,w\,c_0\,a_5\cos(h\,w) - c_2\sin(h\,w)\\ & -2\,c_3\cos(h\,w)\sin(h\,w) + c_4\sin(h\,w)\\ & -c_6\sin(h\,w)),\end{aligned}$$

$$\begin{aligned}\sin(h\,w) = w\,h(&c_0 + c_1 - c_3 + c_5 - 3\,c_4\cos(h\,w) - 4\,h\,w\,c_0\,a_4\cos(h\,w)\sin(h\,w)\\ &+16\cos(h\,w)^4\,h\,w\,c_0\,a_5\sin(h\,w) + h\,w\,c_0\,a_5\sin(h\,w) + 8\cos(h\,w)^4\,c_5\\ &+5\,c_6\cos(h\,w) - 12\cos(h\,w)^2\,h\,w\,c_0\,a_5\sin(h\,w)\\ &+8\,h\,w\,c_0\,a_4\cos(h\,w)^3\sin(h\,w)\\ &+4\,h\,w\,c_0\,a_3\sin(h\,w)\cos(h\,w)^2 - h\,w\,c_0\,a_3\sin(h\,w) + 16\cos(h\,w)^5\,c_6\\ &+h\,w\,c_0\,a_1\sin(h\,w) + 2\,h\,w\,c_0\,a_2\cos(h\,w)\sin(h\,w) + 2\,c_3\cos(h\,w)^2\\ &+4\cos(h\,w)^3\,c_4 - 20\cos(h\,w)^3\,c_6 - 8\cos(h\,w)^2\,c_5 + c_2\cos(h\,w))\end{aligned}$$

$$\begin{aligned}&\cos(h\,w)\,x + \cos(h\,w)\,h - x = -h(-c_0 - c_1 + c_3 - c_5 - c_6\,w\sin(h\,w)\,x\\ &\quad +h\,c_2\,w\sin(h\,w) + 5\,h\,c_6\,w\sin(h\,w) + 12\cos(h\,w)^2\,h\,c_4\,w\sin(h\,w)\\ &\quad -20\cos(h\,w)^3\,h\,c_0\,a_5\,w^2\,x - c_2\,w\sin(h\,w)\,x - 3\,h\,c_4\,w\sin(h\,w) + c_4\,w\sin(h\,w)\,x\\ &\quad -4\,h^2\,c_0\,a_4\,w^2 + 16\cos(h\,w)^5\,h\,c_0\,a_5\,w^2\,x - 16\cos(h\,w)^4\,c_6\,w\sin(h\,w)\,x\\ &\quad -80\cos(h\,w)^5\,h^2\,c_0\,a_5\,w^2 + 8\,h\,w\,c_0\,a_4\cos(h\,w)\sin(h\,w) - 8\cos(h\,w)^4\,c_5\\ &\quad -2\,h\,w\,c_0\,a_5\sin(h\,w) - 16\,h\,w\,c_0\,a_4\cos(h\,w)^3\sin(h\,w)\\ &\quad -8\,h\,w\,c_0\,a_3\sin(h\,w)\cos(h\,w)^2 + 2\,h\,w\,c_0\,a_3\sin(h\,w) - 2\,h\,w\,c_0\,a_1\sin(h\,w)\\ &\quad -4\,h\,w\,c_0\,a_2\cos(h\,w)\sin(h\,w) + 3\,c_4\cos(h\,w) - 5\,c_6\cos(h\,w) - 2\,c_3\cos(h\,w)^2\\ &\quad -4\cos(h\,w)^3\,c_4 + 20\cos(h\,w)^3\,c_6 + 8\cos(h\,w)^2\,c_5 - c_2\cos(h\,w)\\ &\quad +80\cos(h\,w)^4\,h\,c_6\,w\sin(h\,w) + 2\cos(h\,w)^2\,h\,c_0\,a_2\,w^2\,x\\ &\quad -32\cos(h\,w)^4\,h\,w\,c_0\,a_5\sin(h\,w) - 16\cos(h\,w)^5\,c_6\\ &\quad +24\cos(h\,w)^2\,h\,w\,c_0\,a_5\sin(h\,w) - h\,c_0\,a_2\,w^2\,x - 16\cos(h\,w)\,h\,c_5\,w\sin(h\,w)\\ &\quad -60\cos(h\,w)^2\,h\,c_6\,w\sin(h\,w) - \cos(h\,w)\,h^2\,c_0\,a_1\,w^2\\ &\quad +32\cos(h\,w)^3\,h\,c_5\,w\sin(h\,w) + 4\cos(h\,w)\,c_5\,w\sin(h\,w)\,x\\ &\quad -8\cos(h\,w)^3\,c_5\,w\sin(h\,w)\,x + 4\cos(h\,w)\,h\,c_3\,w\sin(h\,w) + h\,c_0\,a_0\,x\,w^2\\ &\quad +h\,c_0\,a_4\,w^2\,x - 25\cos(h\,w)\,h^2\,c_0\,a_5\,w^2 - 4\,c_4\,w\sin(h\,w)\,x\cos(h\,w)^2\\ &\quad +12\cos(h\,w)^2\,c_6\,w\sin(h\,w)\,x + 9\cos(h\,w)\,h^2 c_0 a_3 w^2 - 12\cos(h\,w)^3\,h^2\,c_0\,a_3\,w^2\\ &\quad +100\cos(h\,w)^3\,h^2\,c_0\,a_5\,w^2 + 5\cos(h\,w)\,h\,c_0\,a_5\,w^2\,x - 3\cos(h\,w)\,h\,c_0\,a_3\,w^2\,x\\ &\quad +4\cos(h\,w)^3\,h\,c_0\,a_3\,w^2\,x + \cos(h\,w)\,h\,c_0\,a_1\,w^2\,x - 8\,h\,c_0\,a_4\,w^2\,x\cos(h\,w)^2\\ &\quad +8\,h\,c_0\,a_4\,w^2\,x\cos(h\,w)^4 - 2\cos(h\,w) c_3 w\sin(h\,w)\,x - 4\cos(h\,w)^2 h^2 c_0 a_2\,w^2\\ &\quad +32\cos(h\,w)^2\,h^2\,c_0\,a_4\,w^2 - 32\cos(h\,w)^4\,h^2\,c_0\,a_4\,w^2 + 2\,h^2\,c_0\,a_2\,w^2),\end{aligned}$$

$$\begin{aligned}&\sin(h\,w)\,(x + h) = h(2\,c_0\,h\,a_0\,w - 2\,c_0 h\,a_2 w + 2\,c_0\,h\,a_4\,w - 2\,c_3\cos(h\,w)\sin(h\,w)\\ &\quad +c_0\,x\,w - 12\,h^2\,c_0\,a_3\,w^2\sin(h\,w)\cos(h\,w)^2 + c_1\,x\,w + 32\cos(h\,w)^5\,h\,w\,c_0\,a_5\\ &\quad +8\,h\,c_0\,a_4\,w^2\cos(h\,w)^3\sin(h\,w)\,x - 32\,h^2\,c_0\,a_4\,w^2\cos(h\,w)^3\sin(h\,w)\\ &\quad +4\cos(h\,w)^2\,h\,c_0\,a_3\,w^2\sin(h\,w)\,x + 60\cos(h\,w)^2\,h^2\,c_0\,a_5\,w^2\sin(h\,w)\end{aligned}$$

$$
\begin{aligned}
&-12h\,c_0\,a_5\,w^2\sin(h\,w)\,x\cos(h\,w)^2+hc_0a_1\,w^2\sin(h\,w)\,x-h\,c_0a_3w^2\sin(h\,w)\,x\\
&-16\cos(h\,w)^4\,c_6\sin(h\,w)-c_2\sin(h\,w)+c_4\sin(h\,w)-c_6\sin(h\,w)\\
&+4\,c_5\cos(h\,w)\sin(h\,w)-4\,c_4\sin(h\,w)\cos(h\,w)^2+12\,c_6\sin(h\,w)\cos(h\,w)^2\\
&-8\,c_5\cos(h\,w)^3\sin(h\,w)+hc_0\,a_5w^2\sin(h\,w)x-4\,h\,c_0a_4\,w^2\cos(h\,w)\sin(h\,w)\,x\\
&+3\,h^2\,c_0\,a_3\,w^2\sin(h\,w)-4\,h^2\,c_0\,a_2\,w^2\cos(h\,w)\sin(h\,w)-5\,h^2\,c_0\,a_5w^2\sin(h\,w)\\
&+16\,h^2\,c_0\,a_4\,w^2\cos(h\,w)\sin(h\,w)-h^2\,c_0\,a_1\,w^2\sin(h\,w)\\
&+2\,h\,c_0\,a_2\,w^2\cos(h\,w)\sin(h\,w)\,x-40\cos(h\,w)^3\,h\,w\,c_0\,a_5\\
&-16\,c_0\,h\,a_4\,w\cos(h\,w)^2+16\,c_0\,h\,a_4\,w\cos(h\,w)^4+4\cos(h\,w)^2\,c_0\,h\,a_2\,w\\
&+8\cos(h\,w)^3\,h\,w\,c_0\,a_3+2\,h\,w\,c_0\,a_1\cos(h\,w)-6\,h\,w\,c_0\,a_3\cos(h\,w)\\
&+10\,h\,w\,c_0\,a_5\cos(h\,w)-c_3\,w\,x+16\cos(h\,w)^5\,c_6\,w\,x-80\cos(h\,w)^5\,h\,c_6\,w\\
&-32\cos(h\,w)^4hc_5w+c_2w\cos(h\,w)\,x+2\,c_3\,w\,x\cos(h\,w)^2-4\cos(h\,w)^2\,h\,c_3\,w\\
&+32\cos(h\,w)^2\,h\,c_5\,w-20\,c_6\,w\cos(h\,w)^3\,x-12\,h\,c_4\,w\cos(h\,w)^3\\
&+4\,c_4\,w\cos(h\,w)^3\,x-h\,c_2\,w\cos(h\,w)+9\,h\,c_4\,w\cos(h\,w)-8\cos(h\,w)^2\,c_5\,w\,x\\
&+8\cos(h\,w)^4\,c_5\,w\,x+100\,h\,c_6\,w\cos(h\,w)^3-25\,h\,c_6\,w\cos(h\,w)\\
&-3\,c_4\,w\cos(h\,w)\,x+5\,c_6\,w\cos(h\,w)\,x+16\cos(h\,w)^4\,h\,c_0\,a_5\,w^2\sin(h\,w)\,x\\
&-80\cos(h\,w)^4\,h^2\,c_0\,a_5\,w^2\sin(h\,w)+2\,h\,c_3\,w-4\,h\,c_5\,w+c_5\,w\,x),\\
1&=c_0+c_1+c_2+c_3+c_4+c_5+c_6,\\
1&=2\,c_0\,a_0+2\,c_0\,a_1+2\,c_0\,a_2+2\,c_0\,a_3+2\,c_0\,a_4+2\,c_0\,a_5-2\,c_2-4\,c_3-6\,c_4-8\,c_5\\
&\quad-10\,c_6,\\
1&=3\,c_2+12\,c_3+27\,c_4+48\,c_5+75\,c_6-6\,c_0\,a_1-12\,c_0\,a_2-18\,c_0\,a_3-24\,c_0\,a_4\\
&\quad-30\,c_0\,a_5.
\end{aligned}
\tag{14}
$$

Assuming the known Adams–Bashforth coefficients in terms of f_{n-i} given by (7) the solution of this system of equations is given in Appendix C.

For small values of w the formulae given in Appendix C by (23) are subject to heavy cancellations. In such a case the Taylor series expansions, which are given in Appendix D, should be used.

In figure 4, we present the behavior of the quantities $c[i] = c_i,\ i = 0(1)6$, where $c_i,\ i = 0(1)6$ are given by (21). It is easy to see that for w in which we have cancellations it is appropriate to use the Taylor series expansion.

The above method has the following local truncation error:

$$
\begin{aligned}
L.T.E = \frac{1}{3657830400}\,h^8\Big(&322733569\,w^4\;y_n^{(4)}+645467138\,w^2\;y_n^{(6)}\\
&-364313569\,y_n^{(7)}-41580000\,y_n^{(8)}\Big)+O\Big(h^9\Big),
\end{aligned}
\tag{15}
$$

where $y_n^{(4)}$ is the fourth derivative of y at x_n, $y_n^{(6)}$ is the sixth derivative of y at x_n, $y_n^{(7)}$ is the seventh derivative of y at x_n and $y_n^{(8)}$ is the eighth derivative of y

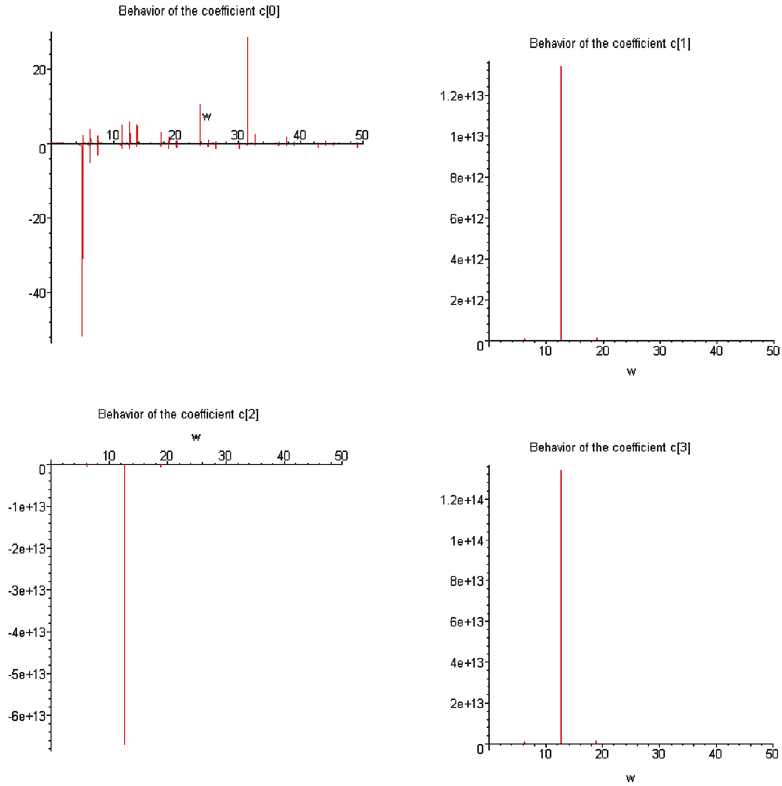

Figure 4. Behavior of the coefficients $c_i,\ i = 0(1)6$ given by (21) for several values of v.

at x_n. We note here that in order to produce equation (15) we express the quantities $y_{n+1},\ y_{n-1},\ y_{n-2},\ y_{n-3},\ y_{n-4},\ y_{n-5}$ and $f_{n+1},\ f_{n-1}, f_{n-2},\ f_{n-3},\ f_{n-4},\ f_{n-5}$ around the point x_n and then we substitute the expressions into (4).

Since $w = vh$, we see that when $v \to 0$ our trigonometrically fitted method becomes the original P–C method for the relevant algebraic order and step-number.

2.2.1. Stability remarks

Based on the stability analysis described above, applying the scheme (4) to the scalar test equation (9) we obtain the difference equation (10) with $A_j(H),\ j = 0(1)5$ given by (11). The characteristic equation of (10) is given by (12).

By solving the characteristic equation in H, using the boundary locus technique [13] and substituting $r = \exp(i\,\theta)$, where $i = \sqrt{-1}$, 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 second member of the family of our the new trigonometrically fitted case and for $w = 1$, $w = 2$, $w = 5$ and $w = 10$. In this instance also, it remains to be investigated how w influences the region of absolute stability.

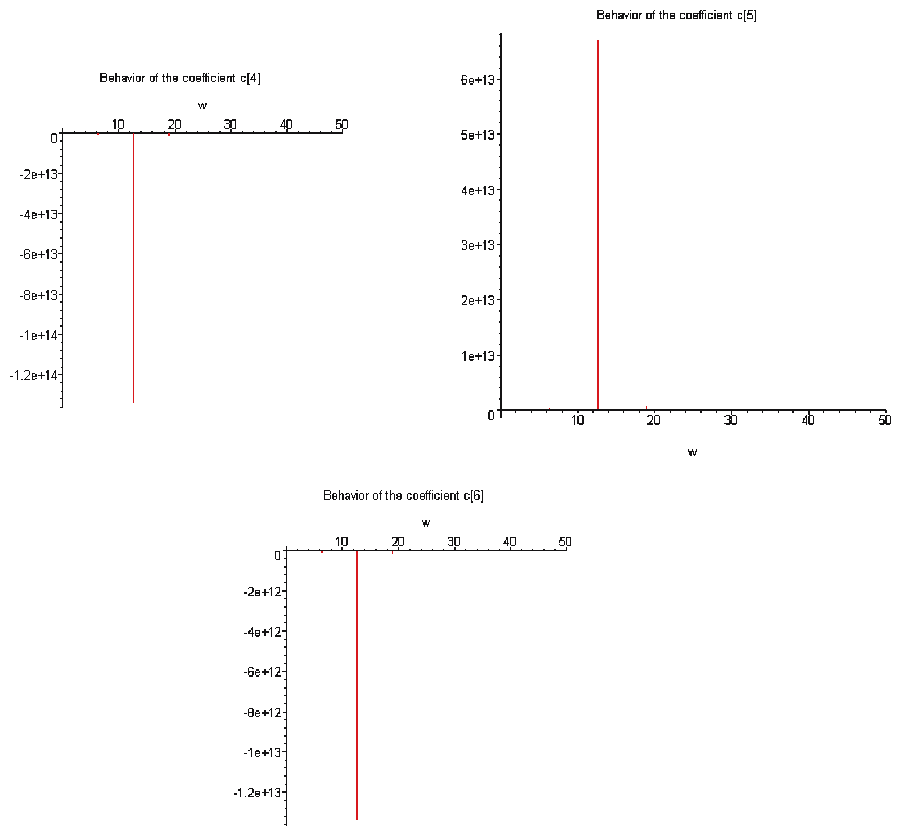

Figure 4. Continued.

3. Numerical comparisons and results

In order illustrate the performance of our scheme, we present here some numerical comparisons and results. 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 [15, 18, 27]) which is given by

$$V(r) = V_w(r) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{16}$$

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 $r \to \infty$

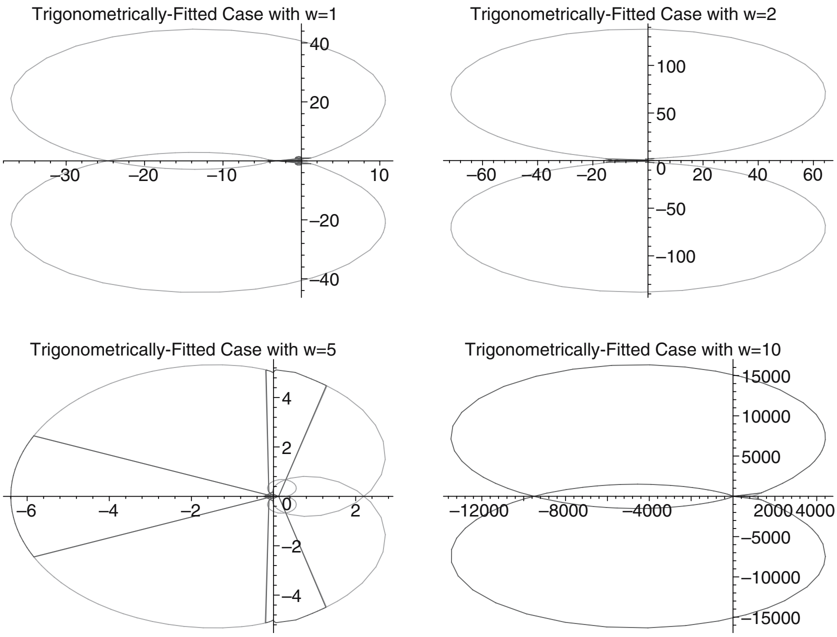

Figure 5. Stability region for the trigonometrically-fitted case and for $w = 1$ (above left), $w = 2$ (above right), $w = 5$ (below left) and $w = 10$ (below right).

- $E = k^2$ 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:

$$y(0) = 0 \tag{17}$$

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, 47, 50]).

3.1. Resonance problem

In the asymptotic region equation (2) effectively reduces to

$$y''(x) + (k^2 - \frac{l(l+1)}{x^2})y(x) = 0 \tag{18}$$

for x greater than some value X.

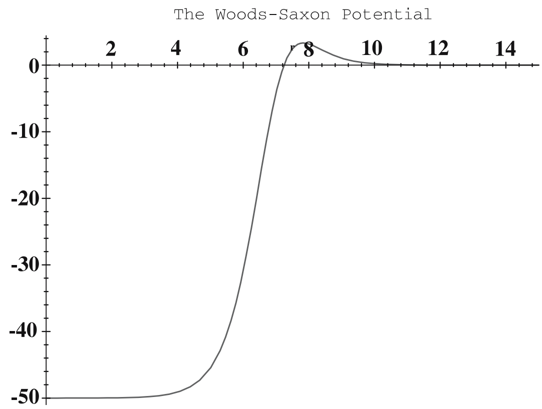

Figure 6. The Woods–Saxon potential.

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 $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)], \end{aligned} \tag{19}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{20}$$

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, $j = 0(1)3$ before starting a four-step method. 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 and Prince [51]. 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

In order to test the accuracy of our method 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 (16).

The problem considered here can be investigated via any of the 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 $\pi/2$. 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 described in [6].

The boundary conditions for this problem are:

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

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 original Adams–Bashforth–Moulton P–C multistep method (4) of seventh order (Method [a]),
- the well known Adams–Bashforth–Moulton P–C multistep method of eighth order (Method [b]),
- the first new trigonometrically fitted seventh order predictor-corrector multistep method developed in paragraph 2.1 of this paper (Method [c]) and
- the second new trigonometrically fitted seventh order P–C multistep method developed in paragraph 2.2 of this paper (Method [d]).

The numerical results obtained for the four methods, with stepsizes equal to $\frac{1}{2^n}$ 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 $\text{Err} = -\log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$ of the highest eigenenergy $E_3 = 989.701916$ for several values of n.

4. Concluding remarks

In this paper, we introduced new efficient trigonometrically fitted seventh order P–C methods for the numerical solution of the Schrödinger type equations.

From the numerical results we can draw the following points:

- Method [a], i.e. the original P–C multistep method (4) of order seven, performs less efficiently than the other methods.
- The well known Adams–Bashforth–Moulton P–C multistep method of eight order (Method [b]) manages to solve the problem better than Method [a].

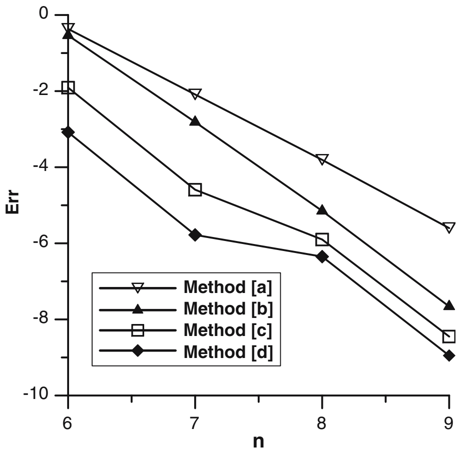

Figure 7. Error Err for several values of n for the eigenvalue $E_3 = 989.701916$.

- Finally, our new trigonometrically fitted P–C schemes [c] and [d] are overall more efficient than the other methods. The second algorithm [d] appears a little more efficient than scheme [c].

In the near future we intend to apply this method 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

$$
\begin{aligned}
c_0 = {} & (720\sin(4w) - 720\sin(2w) - 1901\,w\cos(3w) + 1181\,w\cos(w) + 622\,w\cos(2w) \\
& - 1342\,w)/(2880\,w\cos(w) - 2880\,w\cos(3w) - 3600\,w + 3600\,w\cos(2w) \\
& - 2376\,w^2\sin(3w) - 3240\,w^2\sin(w) + 3024\,w^2\sin(2w)), \\
c_1 = {} & (1036800 - 373938682\,w^2 - 16588800\cos(w) - 88128000\cos(3w) \\
& + 650978146\,w^2\cos(w) - 87651360\,w\sin(w) + 342000\,w\sin(6w) \\
& - 30067200\cos(5w) - 28177920\,w\sin(3w) + 80416080\,w\sin(2w) \\
& + 324000\,w\sin(5w) + 71539200\cos(4w) + 8130577\,w^2\cos(5w) \\
& + 195304333\,w^2\cos(3w) + 57024000\cos(2w) - 57838206\,w^2\cos(4w) \\
& + 1401840\,w\sin(4w) - 421599368\,w^2\cos(2w) + 5184000\cos(6w))/ \\
& (-166717440\,w^2 + 289267200\,w^2\cos(w) - 130636800\,w\sin(w)
\end{aligned}
$$

$$
\begin{aligned}
&-93312000\,w\sin(3\,w)+155520000\,w\sin(2\,w)-4147200\,w\sin(5\,w)\\
&+3421440\,w^2\cos(5\,w)+85536000\,w^2\cos(3\,w)-24883200\,w^2\cos(4\,w)\\
&+30067200\,w\sin(4\,w)-186624000\,w^2\cos(2\,w)),\\
c_2 = {}&(10368000+311116898\,w^2-10368000\cos(w)+129600000\cos(3\,w)\\
&-550644170\,w^2\cos(w)+57699360\,w\sin(w)-1710000\,w\sin(6\,w)\\
&+57024000\cos(5\,w)-19360800\,w\sin(3\,w)-19717200\,w\sin(2\,w)\\
&+671040\,w\sin(5\,w)-124416000\cos(4\,w)-8667173\,w^2\cos(5\,w)\\
&-176878865\,w^2\cos(3\,w)-51840000\cos(2\,w)+56567670\,w^2\cos(4\,w)\\
&+14272560\,w\sin(4\,w)+363321640\,w^2\cos(2\,w)-10368000\cos(6\,w))/\\
&(-166717440\,w^2+289267200\,w^2\cos(w)-130636800\,w\sin(w)\\
&-93312000\,w\sin(3\,w)+155520000\,w\sin(2\,w)-4147200\,w\sin(5\,w)\\
&+3421440\,w^2\cos(5\,w)+85536000\,w^2\cos(3\,w)-24883200\,w^2\cos(4\,w)\\
&+30067200\,w\sin(4\,w)-186624000\,w^2\cos(2\,w)),\\
c_3 = {}&(-15552000+28338334\,w^2+41472000\cos(w)-25920000\cos(3\,w)\\
&-38335990\,w^2\cos(w)-71946720\,w\sin(w)+1710000\,w\sin(6\,w)\\
&-25920000\cos(5\,w)-28008000\,w\sin(3\,w)+60238800\,w\sin(2\,w)\\
&-5914080\,w\sin(5\,w)+46656000\cos(4\,w)+1700741\,w^2\cos(5\,w)\\
&+2718065\,w^2\cos(3\,w)-25920000\cos(2\,w)-5902710\,w^2\cos(4\,w)\\
&+11108880\,w\sin(4\,w)+16665560\,w^2\cos(2\,w)+5184000\cos(6\,w))/\\
&(-83358720\,w^2+144633600\,w^2\cos(w)-65318400\,w\sin(w)\\
&-46656000\,w\sin(3\,w)+77760000\,w\sin(2\,w)-2073600\,w\sin(5\,w)\\
&+1710720\,w^2\cos(5\,w)+42768000\,w^2\cos(3\,w)-12441600\,w^2\cos(4\,w)\\
&+15033600\,w\sin(4\,w)-93312000\,w^2\cos(2\,w)),\\
c_4 = {}&(18144000-183709726\,w^2-57024000\cos(w)-25920000\cos(3\,w)\\
&+307916950\,w^2\cos(w)+90319680\,w\sin(w)-1710000\,w\sin(6\,w)\\
&+10368000\cos(5\,w)+59727600\,w\sin(3\,w)-93891600\,w\sin(2\,w)\\
&+8892720\,w\sin(5\,w)-7776000\cos(4\,w)+1487851\,w^2\cos(5\,w)\\
&+76996735\,w^2\cos(3\,w)+64800000\cos(2\,w)-17287050\,w^2\cos(4\,w)\\
&-26388720\,w\sin(4\,w)-190588760\,w^2\cos(2\,w)-2592000\cos(6\,w))/\\
&(-83358720\,w^2+144633600\,w^2\cos(w)-65318400\,w\sin(w)\\
&-46656000\,w\sin(3\,w)+77760000\,w\sin(2\,w)-2073600\,w\sin(5\,w)\\
&+1710720\,w^2\cos(5\,w)+42768000\,w^2\cos(3\,w)-12441600\,w^2\cos(4\,w)\\
&+15033600\,w\sin(4\,w)-93312000\,w^2\cos(2\,w)),\\
c_5 = {}&(-19699200+273088798\,w^2+66355200\cos(w)+57024000\cos(3\,w)\\
&-462996310\,w^2\cos(w)-104355360\,w\sin(w)+1710000\,w\sin(6\,w)
\end{aligned}
$$

$$
\begin{aligned}
&-1036800\cos(5\,w) - 80910720\,w\sin(3\,w) + 117668880\,w\sin(2\,w)\\
&-10775520\,w\sin(5\,w) - 15552000\cos(4\,w) - 3322123\,w^2\cos(5\,w)\\
&-122853535\,w^2\cos(3\,w) - 88128000\cos(2\,w) + 30627210\,w^2\cos(4\,w)\\
&+36249840\,w\sin(4\,w) + 290639960\,w^2\cos(2\,w) + 1036800\cos(6\,w))/\\
&(-166717440\,w^2 + 289267200\,w^2\cos(w) - 130636800\,w\sin(w)\\
&-93312000\,w\sin(3\,w) + 155520000\,w\sin(2\,w) - 4147200\,w\sin(5\,w)\\
&+3421440\,w^2\cos(5\,w) + 85536000\,w^2\cos(3\,w) - 24883200\,w^2\cos(4\,w)\\
&+30067200\,w\sin(4\,w) - 186624000\,w^2\cos(2\,w)),\\
c_6 = {}&(4147200 - 66241670\,w^2 - 14515200\cos(w) - 15552000\cos(3\,w)\\
&+112767614\,w^2\cos(w) + 22972320\,w\sin(w) - 342000\,w\sin(6\,w)\\
&-1036800\cos(5\,w) + 19170720\,w\sin(3\,w) - 26977680\,w\sin(2\,w)\\
&+2413440\,w\sin(5\,w) + 6220800\cos(4\,w) + 902975\,w^2\cos(5\,w)\\
&+30534467\,w^2\cos(3\,w) + 20736000\cos(2\,w) - 7860354\,w^2\cos(4\,w)\\
&-8617680\,w\sin(4\,w) - 71139832\,w^2\cos(2\,w))/(-166717440\,w^2\\
&+289267200\,w^2\cos(w) - 130636800\,w\sin(w) - 93312000\,w\sin(3\,w)\\
&+155520000\,w\sin(2\,w) - 4147200\,w\sin(5\,w) + 3421440\,w^2\cos(5\,w)\\
&+85536000\,w^2\cos(3\,w) - 24883200\,w^2\cos(4\,w) + 30067200\,w\sin(4\,w)\\
&-186624000\,w^2\cos(2\,w)),
\end{aligned}
\tag{21}
$$

where $w = v\,h$.

Appendix B

$$
\begin{aligned}
c_0 = {}&\frac{19087}{60480} - \frac{1872359}{50803200}\,w^2 + \frac{44765209}{52157952000}\,w^4 - \frac{40939605131}{1708694507520000}\,w^6\\
&-\frac{94119790991}{861182031790080000}\,w^8 - \frac{1127115752297323}{7515248530754764800000}\,w^{10} + \cdots\\
c_1 = {}&\frac{2713}{2520} + \frac{486125519}{3657830400}\,w^2 - \frac{1026745663}{417263616000}\,w^4 + \frac{7599656476933}{123026004541440000}\,w^6\\
&+\frac{3032118668141}{4769623560683520000}\,w^8 + \frac{239536068638024749}{541097894214343065600000}\,w^{10} + \cdots\\
c_2 = {}&-\frac{15487}{20160} - \frac{16339195}{146313216}\,w^2 - \frac{47619353}{83452723200}\,w^4 + \frac{1243298231363}{24605200908288000}\,w^6\\
&-\frac{19087667831777}{1240102125777152000}\,w^8 + \frac{3920933858197019}{10821957884286861312000000}\,w^{10} + \cdots\\
c_3 = {}&\frac{586}{945} - \frac{53113873}{365783040}\,w^2 + \frac{16229641}{1669054464}\,w^4 - \frac{838189960159}{2460520090828800}\,w^6
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{492441715217}{248020425155543040}w^8-\frac{3402930720944171}{21643915768573722624000}w^{10}+\cdots\\
c_4&=-\frac{6737}{20160}+\frac{17216971}{52254720}w^2-\frac{83543123}{5960908800}w^4+\frac{809253655073}{1757514350592000}w^6\\
&-\frac{1274675772107}{885787232698368000}w^8+\frac{17949919300901129}{772996991734775808000000}w^{10}+\cdots\\
c_5&=\frac{263}{2520}-\frac{804808757}{3657830400}w^2+\frac{3461191813}{417263616000}w^4-\frac{32745355281703}{123026004541440000}w^6\\
&+\frac{34448714596717}{620051062888857600000}w^8-\frac{57690436675357723}{4162291493956485120000000}w^{10}+\cdots\\
c_6&=-\frac{863}{60480}+\frac{187923721}{3657830400}w^2-\frac{28291211}{15454208000}w^4+\frac{7138601370227}{123026004541440000}w^6\\
&-\frac{503128902643}{5636827844444160000}w^8+\frac{166225602189011531}{5410978942143430656000000}w^{10}+\cdots \qquad (22)
\end{aligned}
$$

Appendix C

$$
\begin{aligned}
c_0 = {}&(60\cos(5w)-120\cos(3w)+60\cos(w)+60\,w\sin(5w)-360\,w\sin(3w)\\
&+300\sin(w)\,w+265\,w^2\cos(3w)+215\cos(w)\,w^2-120\,w\sin(4w)\\
&+120\,w\sin(2w)+650\,w^2\cos(2w)-170\,w^2)/(198\,w^2\cos(4w)\\
&+432\,w^2\cos(2w)-630\,w^2-72\,w^2\cos(3w)+72\cos(w)\,w^2+144\,w^3\sin(3w)\\
&-720\,w^3\sin(w)+1224\,w^3\sin(2w)),\\
c_1 = {}&(957984\,w-350714\,w^3\cos(5w)+3378318\,w^3\cos(3w)+429864\,w\cos(6w)\\
&+420672\sin(5w)-425640\sin(4w)+51324\,w^2\sin(8w)+2081498\,w^3\\
&+226681\,w^3\cos(6w)+3610780\sin(w)\,w^2+122568w\cos(w)-80736\sin(7w)\\
&-2380471\,w^2\sin(2w)-383616\sin(3w)+96768\,w\cos(8w)+774180\sin(2w)\\
&-225000\,w^2\sin(7w)-1825694\,w^2\sin(5w)+11580\sin(8w)+10260\sin(6w)\\
&-1421664\,w\cos(5w)-1489945\,w^3\cos(2w)-1232954\,w^3\cos(4w)\\
&+1324870\,w^2\sin(3w)+1493808\,w\cos(3w)-2869224\,w\cos(2w)\\
&+970261\,w^2\sin(6w)+774596\,w^2\sin(4w)-194712\,w\cos(7w)\\
&-3442324\cos(w)\,w^3-387360\sin(w)+1384608\,w\cos(4w))/(2405376\,w^3\\
&+41472\,w^3\cos(6w)-492480\,w^2\sin(5w)+580608\,w^2\sin(4w)\\
&-2778624\cos(w)\,w^3-57024\,w^2\sin(7w)+108864\,w^2\sin(3w)\\
&-1907712\,w^2\sin(2w)+248832\,w^2\sin(6w)+186624\,w^3\cos(5w)\\
&+2592000\,w^3\cos(3w)-1036800\,w^3\cos(2w)+2534976\sin(w)\,w^2\\
&-1410048\,w^3\cos(4w)),
\end{aligned}
$$

$$
\begin{aligned}
c_2 = -(&-1720968\, w+1302146w^3, \cos(5\, w)-341286w^3\cos(3\, w)-688992\, w\cos(6\, w)\\
&-483756\sin(5\, w) + 237624\sin(4\, w) - 136548\, w^2\sin(8\, w) + 3228114\, w^3\\
&-419919\, w^3\cos(6\, w) - 7304513\sin(w)\, w^2+1580844\, w\cos(w)+13008\sin(7\, w)\\
&+745963\, w^2\sin(2\, w) + 819588\sin(3\, w) - 324936\, w\cos(8\, w) - 566604\sin(2\, w)\\
&+204719\, w^2\sin(7\, w) + 1980789\, w^2\sin(5\, w) + 28716\sin(8\, w) - 7836\sin(6\, w)\\
&+1592988\, w\cos(5\, w) + 289231\, w^3\cos(2\, w) - 1023826\, w^3\cos(4\, w)\\
&-1272475\, w^2\sin(3\, w) - 3808380\, w\cos(3\, w) - 5700\, w\cos(9\, w)\\
&+3362208\, w\cos(2\, w) - 876337\, w^2\sin(6\, w) - 653540\, w^2\sin(4\, w)\\
&+640248\, w\cos(7\, w) + 1112740\cos(w)\, w^3 - 182340\sin(w) + 5700\sin(9\, w)\\
&-627312\, w\cos(4\, w))/(-2405376w^3-41472\, w^3\cos(6\, w)+492480w^2\sin(5\, w)\\
&-580608\, w^2\sin(4\, w) + 2778624\cos(w)\, w^3 + 57024\, w^2\sin(7\, w)\\
&-108864\, w^2\sin(3\, w) + 1907712\, w^2\sin(2\, w) - 248832\, w^2\sin(6\, w)\\
&-186624\, w^3\cos(5\, w) - 2592000\, w^3\cos(3\, w) + 1036800\, w^3\cos(2\, w)\\
&-2534976\sin(w)\, w^2 + 1410048\, w^3\cos(4\, w)),\\
c_3 = (&-1223160w+285764\, w^3\cos(5\, w)-148236\, w^3\cos(3\, w)+1409448\, w\cos(6\, w)\\
&-488388\sin(5\, w) + 450912\sin(4\, w) - 96000\, w^2\sin(8\, w) + 4843096\, w^3\\
&-202816\, w^3\cos(6\, w) - 9630727\sin(w)\, w^2 + 2825580\, w\cos(w)\\
&+205584\sin(7\, w) - 1756706\, w^2\sin(2\, w) + 540684\sin(3\, w)\\
&+4009672\cos(w)\, w^3-773100\sin(w)+17100\sin(9\, w)-599088w\cos(4\, w))/\\
&(-2405376\, w^3 - 41472\, w^3\cos(6\, w) + 492480\, w^2\sin(5\, w) - 580608\, w^2\sin(4\, w)\\
&+2778624\cos(w)\, w^3 + 57024\, w^2\sin(7\, w) - 108864\, w^2\sin(3\, w)\\
&+1907712\, w^2\sin(2\, w) - 248832\, w^2\sin(6\, w) - 186624\, w^3\cos(5\, w)\\
&-2592000\, w^3\cos(3\, w) + 1036800\, w^3\cos(2\, w) - 2534976\sin(w)\, w^2\\
&+1410048\, w^3\cos(4\, w)),\\
c_4 = (&72312\, w + 1131196\, w^3\cos(5\, w) - 3828\, w^3\cos(3\, w) - 2249256\, w\cos(6\, w)\\
&+695748\sin(5\, w) - 554592\sin(4\, w) - 18048\, w^2\sin(8\, w) - 4212376\, w^3\\
&-159200\, w^3\cos(6\, w) + 7408951\sin(w)\, w^2 - 1394796\, w\cos(w)\\
&-309264\sin(7\, w)+3904610\, w^2\sin(2\, w)-540684\sin(3\, w)-58536\, w\cos(8\, w)\\
&+6192\sin(2\, w) + 642171\, w^2\sin(7\, w) + 666679\, w^2\sin(5\, w) + 63312\sin(8\, w)\\
&+283248\sin(6\, w) + 193548\, w\cos(5\, w) + 2284928\, w^3\cos(2\, w)\\
&-2060552\, w^3\cos(4\, w) - 97421\, w^2\sin(3\, w) + 78468\, w\cos(3\, w)\\
&+17100\, w\cos(9\, w) + 205608\, w\cos(2\, w) - 1154822\, w^2\sin(6\, w)\\
&-291496\, w^2\sin(4\, w) + 1105680\, w\cos(7\, w) - 5274568\cos(w)\, w^3\\
&+462060\sin(w) - 17100\sin(9\, w) + 2029872\, w\cos(4\, w))/(-2405376\, w^3
\end{aligned}
$$

$$
\begin{aligned}
&-41472\,w^3\cos(6\,w)+492480\,w^2\sin(5\,w)-580608\,w^2\sin(4\,w)\\
&+2778624\cos(w)\,w^3+57024\,w^2\sin(7\,w)-108864\,w^2\sin(3\,w)\\
&+1907712\,w^2\sin(2\,w)-248832\,w^2\sin(6\,w)-186624\,w^3\cos(5\,w)\\
&-2592000\,w^3\cos(3\,w)+1036800\,w^3\cos(2\,w)-2534976\sin(w)\,w^2\\
&+1410048\,w^3\cos(4\,w)),\\
c_5 = {} &(290424\,w-691102\,w^3\cos(5\,w)+1722810\,w^3\cos(3\,w)+389280\,w\cos(6\,w)\\
&-587436\sin(5\,w)+30264\sin(4\,w)+34524\,w^2\sin(8\,w)+3985842\,w^3\\
&+152481\,w^3\cos(6\,w)-3947441\sin(w)\,w^2-202452\,w\cos(w)+64848\sin(7\,w)\\
&-3254789w^2\sin(2\,w)+819588\sin(3\,w)+69048w\cos(8\,w)-411084\sin(2\,w)\\
&-321025\,w^2\sin(7\,w)+31173\,w^2\sin(5\,w)-23124\sin(8\,w)+147684\sin(6\,w)\\
&+1240476\,w\cos(5\,w)-2584865\,w^3\cos(2\,w)+520142\,w^3\cos(4\,w)\\
&+2084597\,w^2\sin(3\,w)-552828\,w\cos(3\,w)-5700\,w\cos(9\,w)\\
&+1039776\,w\cos(2\,w)+464159\,w^2\sin(6\,w)-1006052\,w^2\sin(4\,w)\\
&-479496\,w\cos(7\,w)+1041892\cos(w)\,w^3-26820\sin(w)+5700\sin(9\,w)\\
&-1788528w\cos(4\,w))/(-2405376\,w^3-41472\,w^3\cos(6\,w)+492480\,w^2\sin(5\,w)\\
&-580608\,w^2\sin(4\,w)+2778624\cos(w)\,w^3+57024\,w^2\sin(7\,w)\\
&-108864\,w^2\sin(3\,w)+1907712\,w^2\sin(2\,w)-248832\,w^2\sin(6\,w)\\
&-186624\,w^3\cos(5\,w)-2592000\,w^3\cos(3\,w)+1036800\,w^3\cos(2\,w)\\
&-2534976\sin(w)\,w^2+1410048\,w^3\cos(4\,w)),\\
c_6 = {} &(-92640\,w+38950\,w^3\cos(5\,w)-1125714\,w^3\cos(3\,w)+312360\,w\cos(6\,w)\\
&+178752\sin(5\,w)+127320\sin(4\,w)-5700\,w^2\sin(8\,w)-1712326\,w^3\\
&-25175\,w^3\cos(6\,w)+1121308\sin(w)\,w^2+233160\,w\cos(w)+40224\sin(7\,w)\\
&+998489\,w^2\sin(2\,w)-383616\sin(3\,w)+203940\sin(2\,w)+34200\,w^2\sin(7\,w)\\
&-214622\,w^2\sin(5\,w)-5700\sin(8\,w)-145260\sin(6\,w)-751200\,w\cos(5\,w)\\
&+994487\,w^3\cos(2\,w)+328294\,w^3\cos(4\,w)-1135226\,w^2\sin(3\,w)\\
&+546864\,w\cos(3\,w)-678120\,w\cos(2\,w)+4453\,w^2\sin(6\,w)\\
&+647876\,w^2\sin(4\,w)-28824\,w\cos(7\,w)+672044\cos(w)\,w^3-24480\sin(w)\\
&+458400\,w\cos(4\,w))/(-2405376\,w^3-41472\,w^3\cos(6\,w)+492480\,w^2\sin(5\,w)\\
&-108864\,w^2\sin(3\,w)+1907712\,w^2\sin(2\,w)-248832\,w^2\sin(6\,w)\\
&-186624\,w^3\cos(5\,w)-2592000\,w^3\cos(3\,w)+1036800\,w^3\cos(2\,w)\\
&-2534976\sin(w)\,w^2+1410048\,w^3\cos(4\,w)),
\end{aligned}
\tag{23}
$$

where $w = v\,h$.

Appendix D

$$\begin{aligned}
c_0 &= \frac{19087}{60480} - \frac{1872359}{25401600} w^2 + \frac{115012297}{23471078400} w^4 - \frac{2985275429}{53396703360000} w^6 \\
&\quad + \frac{408815105267}{134559692467200000} w^8 - \frac{1870964050840153}{21136636492747776000000} w^{10} + \cdots \\
c_1 &= \frac{2713}{2520} + \frac{486125519}{1828915200} w^2 - \frac{3644194019}{67596705792} w^4 + \frac{8389942509271}{5126083522560000} w^6 \\
&\quad - \frac{42560025736859}{242207446440960000} w^8 + \frac{1030233953797576631}{380459456869459968000000} w^{10} + \cdots \\
c_2 &= -\frac{15487}{20160} - \frac{16339195}{73156608} w^2 + \frac{119925912961}{1689917644800} w^4 - \frac{51388420049}{205043340902400} w^6 \\
&\quad - \frac{2401507948363}{12110372322048000} w^8 + \frac{65934812893590127}{3043675654955679744 0000} w^{10} + \cdots \\
c_3 &= \frac{586}{945} - \frac{53113873}{182891520} w^2 + \frac{29156059087}{422479411200} w^4 - \frac{227308491589}{25630417612800} w^6 \\
&\quad + \frac{64459545756169}{96882978576384000} w^8 - \frac{138749344094561803}{608735130991135948800 0} w^{10} + \cdots \\
c_4 &= -\frac{6737}{20160} + \frac{17216971}{26127360} w^2 - \frac{2018521163}{12070840320} w^4 + \frac{4187839577}{332862566400} w^6 \\
&\quad - \frac{9356778369889}{13840425510912000} w^8 + \frac{128836706359567469}{434810807850811392000 0} w^{10} + \cdots \\
c_5 &= \frac{263}{2520} - \frac{804808757}{1828915200} w^2 + \frac{141448504823}{1689917644800} w^4 - \frac{27691715912551}{5126083522560000} w^6 \\
&\quad + \frac{24102770625197}{110094293836800000} w^8 - \frac{9553535782741243987}{7609189137389199360 00000} w^{10} + \cdots \\
c_6 &= -\frac{863}{60480} + \frac{187923721}{1828915200} w^2 - \frac{12581726221}{1689917644800} w^4 + \frac{1842039177689}{5126083522560000} w^6 \\
&\quad + \frac{11189560586669}{242207446440960000} w^8 + \frac{354648328766250679}{380459456869459968000000} w^{10} + \cdots \qquad (24)
\end{aligned}$$

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