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ORIGINAL PAPER

# A predictor–corrector explicit four-step method with vanished phase-lag and its first, second and third derivatives for the numerical integration of the Schrödinger equation

**Ibraheem Alolyan · T. E. Simos**

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**Abstract** A predictor–corrector explicit four-step method of sixth algebraic order is investigated in this paper. More specifically, we investigate the results of the elimination of the phase-lag and its first, second and third derivatives on the efficiency of the proposed method. The resultant method is studied theoretically and computationally. The theoretical investigation of the new hybrid method consists of: (1) the construction of the new method, (2) the definition (calculation) of the local truncation error, (3) the comparative local truncation error analysis (with other known methods of the same form), (4) the stability analysis using scalar test equation with frequency different than the frequency of the phase-lag analysis. Finally, we will study computationally the new obtained method. This study is based on the application of the new produced predictor–corrector explicit four-step method to the approximate solution of the resonance problem of the radial time independent Schrödinger equation.

**Keywords** Schrödinger equation · Predictor–corrector methods · Interval of periodicity · Phase-lag · Phase-fitted · Derivatives of the phase-lag

**Mathematics Subject Classification** 65L05

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## 1 Introduction

In this paper, we will investigate a new proposed predictor–corrector explicit four-step method of sixth algebraic order with vanished phase-lag and its first, second and third derivatives. The novelties of the new proposed method are:

1. The predictor and the corrector of the new scheme are based on optimal explicit four-step method
2. The embedding form of the proposed predictor–corrector explicit four-step method. It is easy for one to see that the left hand part of the method (combination of $y_{n+j},\ j = -2(1)2$) is the same for the predictor and the corrector.

Based on the above proposed new algorithm, we will study the effective numerical solution of problems of the form of the radial time independent Schrödinger equation:

$$q''(x) = \left[l(l+1)/x^2 + V(x) - k^2\right] q(x), \tag{1}$$

For the model described above, we have the following definitions:

– The function $Q(x) = l(l+1)/x^2 + V(x)$ is called *the effective potential*. For the effective potential, we have the following relation: $Q(x) \to 0$ as $x \to \infty$.
– $k^2$ is a real number which denotes *the energy*,
– $l$ is defined by user integer which denotes the *angular momentum*,
– $V$ is defined by user function denotes the *potential*.

Since the above described problem belongs to the boundary value problems, we need two boundary conditions. The first is given by the definition of the problem:

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

while the second boundary condition, for large values of $x$, is determined by physical considerations.

As we mentioned above, generally the problems with models given by a form similar to the radial Schrödinger equation belong to the category of the special second-order initial or boundary value problems of the form:

$$q''(x) = f(x, q(x)), \tag{3}$$

for which the solution has a periodic and/or oscillatory behavior.

*Remark 1* The mathematical models which describe the above category of problems consist of a system of second order ordinary differential equations of the form (3) in which the first derivative $q'$ does not appear explicitly. Problems for which their description lead to models with the characteristic occur in applied sciences

– astronomy,
– astrophysics,
– quantum mechanics,

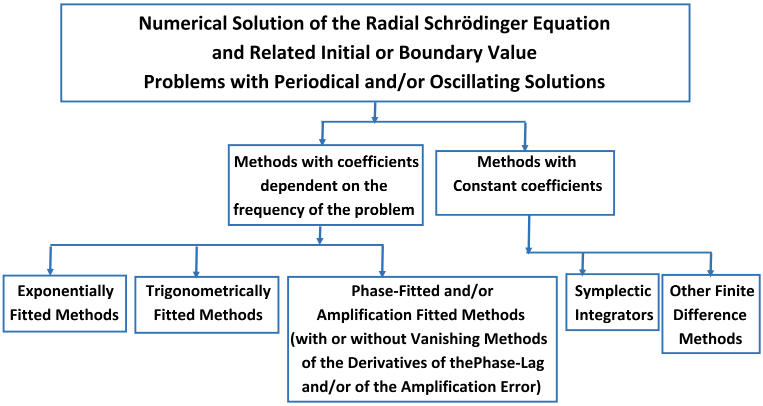



**Fig. 1** Main classes of the finite difference methods developed in the last decades

- quantum chemistry,
- celestial mechanics,
- electronics,
- physical chemistry,
- chemical physics, …, etc

For more details see [1–4].

*Remark 2* Last decades much research was taken place for the approximate solution of the above described problems. The aim and scope of the above mentioned research was the construction of :

- effective,
- fast and,
- reliable

algorithms (see for example [5–109]).

In Fig. 1, we present the main classes of finite difference methods which was the result of research and innovation which was done during the last decades.

In this paper, we will investigate a new methodology for the construction of efficient numerical algorithms for the problems with models of the form (3) which have periodic and/or oscillating solutions.

More specifically, we will investigate the case of predictor–corrector methods in which the predictor is an explicit four-step method and the corrector is the corresponding implicit four-step method. With this form, we can apply embedded form for the above mentioned predictor–corrector methods when we apply them to real problems.

The new methodology is based on the vanishing of the phase-lag and its derivatives in the whole method (when this is applied to the specific scalar test equation). The investigation will examine how this elimination of the phase-lag and its derivatives of the predictor–corrector method affects the efficiency of the resulting method.

We will finally investigate the effectiveness of the new produced predictor–corrector method compared with other well known methods of the literature.

*Remark 3* The algorithms produced using the above mentioned methodology can be applied effectively to the following categories of problems:

- problems with periodic solution and/or,
- problems with oscillating solution,
- problems the solutions of which contain the functions cos and sin
- problems the solutions of which contain combination of the the functions cos and sin

In this paper, we have established the following aims and scopes:

- The calculation of the coefficients of the new predictor–corrector four-step method in order to have
  1. the highest possible algebraic order,
  2. eliminated phase-lag,
  3. eliminated first derivative of the phase-lag,
  4. eliminated second derivative of the phase-lag,
  5. eliminated third derivative of the phase-lag,
- The study of the local truncation error. During this study, we will investigate the comparative local truncation error analysis of the new produced predictor–corrector four-step method with other methods of the same form.
- The study of the stability with scalar test equation using frequency different than the frequency of the scalar test equation for the phase-lag analysis.
- The study of the effectiveness of the new obtained predictor–corrector four-step method using the approximate solution of the resonance problem of the radial time independent Schrödinger equation.

The phase-lag and its derivatives will be based on the direct formula for the calculation of the phase-lag for any 2 m-method symmetric multistep method which was developed by Simos and his coworkers in [26] and [29].

In Fig. 2, we present the flowchart of the presentation of the analysis of the new proposed predictor–corrector method.

In Sect. 2, we present a description of the bibliography on the subject of this paper. The phase-lag analysis of symmetric $2\,m$-methods is presented in Sect. 3. The development of the new proposed explicit predictor–corrector four-step method is presented in Sect. 4. In Sect. 5, we calculate the local truncation error (LTE) of the obtained predictor–corrector method and we give a comparative local truncation error analysis with other similar methods. The stability analysis of the new produced predictor–corrector method is given in Sect. 6. We mention here that the frequency of the scalar test equation of the stability analysis is not equal with the frequency of the scalar test equation of the phase-lag analysis. Numerical experiments are given in Sect. 7. Finally, in Sect. 8, we present some remarks and conclusions.

## 2 Description of the bibliography

In this section, we present the recent bibliography on the research of this paper:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta Nyström type have been obtained in [5–12].

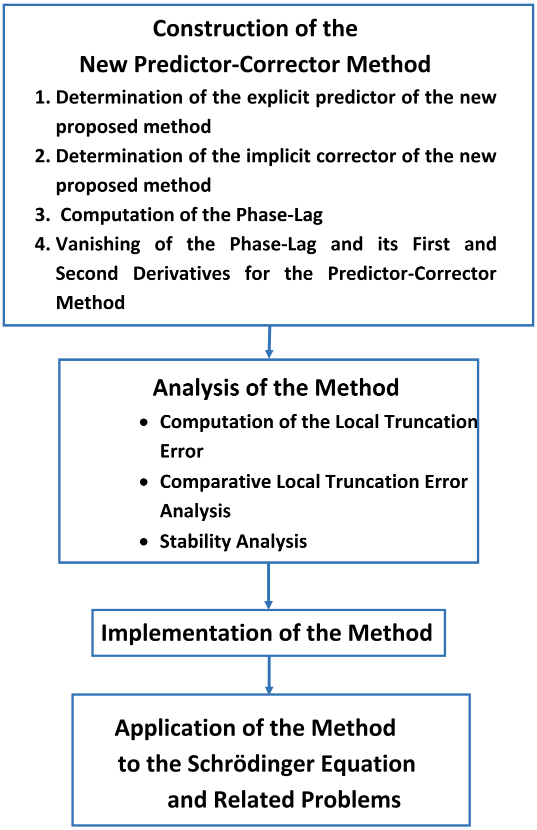



**Fig. 2** Flowchart of the presentation of the analysis of the new proposed hybrid type method.

- In [13–18], exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are constructed.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [23–51].
- Symplectic integrators are investigated in [52–81].
- Exponentially and trigonometrically multistep methods have been produced in [82–102].
- Nonlinear methods have been studied in [103] and [104]
- Review papers have been presented in [105–109]
- Special issues and Symposia in International Conferences have been developed on this subject (see [110–114])

## 3 Phase-lag analysis of symmetric 2 $m$-step methods

The aim and scope of the present paper is the investigation of the numerical solution of the initial or boundary value problem of the form:

$$q'' = f(x, q), \tag{4}$$

In order for the above mentioned problem to be solved using a multistep method with $m$ steps, we divide the interval $[a, b]$ into equally spaced intervals using $\{x_i\}_{i=0}^{p} \subset [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)p - 1$.

In this paper, we will investigate symmetric multistep methods, i.e.,

$$a_i = a_{m-i},\; b_i = b_{m-i},\; i = 0(1)\frac{p}{2}. \tag{5}$$

If we apply a symmetric $2\,m$-step method, that is for $i = -m(1)m$, to the scalar test equation

$$q'' = -w^2\, q, \tag{6}$$

the following difference equation is obtained

$$\begin{aligned} &A_m(v)\, q_{n+m} + \cdots + A_1(v)\, q_{n+1} + A_0(v)\, q_n \\ &\quad + A_1(v)\, q_{n-1} + \cdots + A_m(v)\, q_{n-m} = 0, \end{aligned} \tag{7}$$

where $v = w\, h$, $h$ is the step length and $A_0(v)$, $A_1(v)$, …, $A_m(v)$ are polynomials of $v$.

The associated characteristic equation is given by:

$$A_m(v)\, \lambda^m + \cdots + A_1(v)\, \lambda + A_0(v) + A_1(v)\, \lambda^{-1} + \cdots + A_m(v)\, \lambda^{-m} = 0 \tag{8}$$

**Theorem 1** *[26] and [29] The symmetric $2\,m$-step method with characteristic equation given by (8) has phase-lag order $k$ and phase-lag constant $c$ given by:*

$$\begin{aligned} &-c\, v^{k+2} + O\left(v^{k+4}\right) \\ &\quad = \frac{2\, A_m\,(v)\, \cos\,(m\, v) + \cdots + 2\, A_j\,(v)\, \cos\,(j\, v) + \cdots + A_0\,(v)}{2\, m^2\, A_m\,(v) + \cdots + 2\, j^2\, A_j\,(v) + \cdots + 2\, A_1\,(v)} \end{aligned} \tag{9}$$

*Remark 4* The formula (9) gives us a direct method for the computation of the phase-lag of any symmetric $2\,m$-step method.

*Remark 5* For the method which will be studied in this paper—for the predictor–corrector symmetric four-step method—the number $m = 2$ and the direct formula for the calculation of the phase-lag is given by:

$$-c\, v^{k+2} + O\left(v^{k+4}\right) = \frac{2\, A_2(v)\, \cos(2\, v) + 2\, A_1(v)\, \cos(v) + A_0(v)}{8\, A_2(v) + 2\, A_1(v)} \tag{10}$$

where $k$ is the phase-lag order and $c$ is the phase-lag constant.

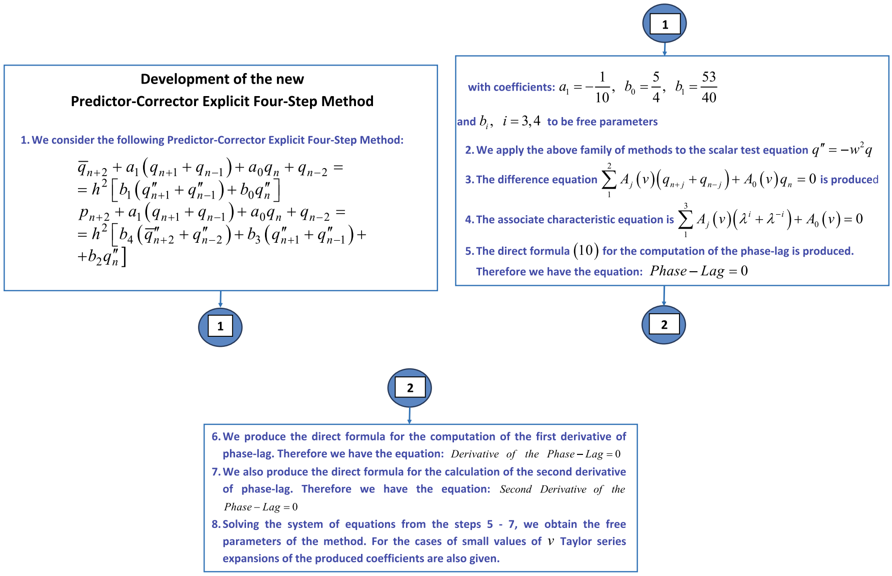



**Fig. 3** Flowchart of the construction of any method of the family

## 4 The new predictor–corrector method

We consider the following family of predictor–corrector explicit symmetric four-step methods for the numerical solution of initial or boundary value problems of the form $q'' = f(x, q)$:

$$
\begin{aligned}
\bar{q}_{n+2} &= -a_1\, q_{n+1} - a_0\, q_n - a_1\, q_{n-1} - q_{n-2} \\
&\quad + h^2\Big(b_1\, q''_{n+1} + b_0\, q''_n + b_1\, q''_{n-1}\Big) \\
&\quad q_{n+2} + a_1\, q_{n+1} + a_0\, q_n + a_1\, q_{n-1} + q_{n-2} \\
&= h^2\left[b_4\, \left(\bar{q}''_{n+2} + q''_{n-2}\right) + b_3\, \left(q''_{n+1} + q''_{n-1}\right) + b_2\, q''_n\right],
\end{aligned} \tag{11}
$$

where

$$
a_1 = -\frac{1}{10}, \ b_0 = \frac{5}{4}, \ b_1 = \frac{53}{40} \tag{12}
$$

and the coefficient $a_0$ and $b_i$, $i = 2(1)4$ are free parameters, $h$ is the step size of the integration, $n$ is the number of steps, $q_n$ is the approximation of the solution on the point $x_n$, $x_n = x_0 + n\,h$ and $x_0$ is the initial value point.

In the flowchart of Fig. 3, we present the development of the new proposed method.

Based on the above flowchart and applying the above mentioned method (11) to the scalar test equation (6), we get the difference equation (7) with $m = 2$ and $A_j(v)$, $j = 0, 1, 2$ given by:

$$A_2(v) = 1,\ A_1(v) = -\frac{1}{10} + v^2 \left( b_4 \left( \frac{1}{10} - \frac{53\,v^2}{40} \right) + b_3 \right)$$
$$A_0(v) = a_0 + v^2 \left( b_4 \left( -a_0 \frac{5}{4}\,v^2 \right) + b_2 \right) \tag{13}$$

We require the above method (11) to have vanished the phase-lag and its first, second and third derivatives. Therefore, we obtain the following system of equations [using the formula (10) and (13)]:

$$\text{Phase} - \text{Lag} = -\frac{T_0}{T_{denom}} = 0 \tag{14}$$
$$\text{First Derivative of the Phase} - \text{Lag} = \frac{T_1}{T_{denom}^2} = 0 \tag{15}$$
$$\text{Second Derivative of the Phase} - \text{Lag} = \frac{T_2}{T_{denom}^3} = 0 \tag{16}$$
$$\text{Third Derivative of the Phase} - \text{Lag} = \frac{T_3}{T_{denom}^4} = 0 \tag{17}$$

where

$$T_{denom} = 53\,v^4\,b_4 - 40\,v^2\,b_3 - 4\,v^2\,b_4 - 156$$

$$\begin{aligned}
T_0 = & -53\,\cos(v)\,v^4 b_4 - 25\,v^4 b_4 + 40\,\cos(v)\,v^2 b_3 \\
& + 4\,\cos(v)\,b_4 v^2 - 20\,v^2 a_0 b_4 + 20\,v^2 b_2 + 80\,(\cos(v))^2 \\
& - 40 - 4\,\cos(v) + 20\,a_0 \\
T_1 = & -24080\,v^3 b_4 + 624\,\sin(v) + 8480\,\sin(v)\cos(v)\,v^4 b_4 \\
& - 6400\,\sin(v)\cos(v)\,v^2 b_3 - 640\,\sin(v)\cos(v)\,v^2 b_4 \\
& + 4240\,\sin(v)\,v^6 b_3 b_4 - 320\,\sin(v)\,v^4 b_3 b_4 \\
& - 24960\,\sin(v)\cos(v) + 3200\,v b_3 + 320\,b_4 v + 6240\,v b_2 - 200\,v^5 {b_4}^2 \\
& + 4240\,v^3 a_0 b_4 - 2000\,v^5 b_3 b_4 - 2120\,v^5 a_0 {b_4}^2 + 2120\,v^5 b_2 b_4 \\
& + 1280\,\cos(v)\,b_4 v - 608\,\sin(v)\,b_4 v^2 - 6400\,v a_0 b_4 + 12800\,\cos(v)\,v b_3 \\
& - 6080\,\sin(v)\,v^2 b_3 + 8056\,\sin(v)\,v^4 b_4 - 16\,\sin(v)\,v^4 {b_4}^2 \\
& - 33920\,\cos(v)\,v^3 b_4 - 2809\,\sin(v)\,v^8 {b_4}^2 + 424\,\sin(v)\,v^6 {b_4}^2 \\
& - 1600\,\sin(v)\,v^4 {b_3}^2 - 1600\,v a_0 b_3 + 16960\,(\cos(v))^2\,v^3 b_4 \\
& - 6400\,(\cos(v))^2\,v b_3 - 640\,(\cos(v))^2\,v b_4 \\
T_2 = & -3893760 + 310400\,(\cos(v))^2\,v^4 {b_4}^2 + 512000\,(\cos(v))^2\,v^4 {b_3}^2 \\
& - 5291520\,(\cos(v))^2\,v^4 b_4 - 768000\,(\cos(v))^2\,v^2 {b_3}^2 \\
& + 898880\,(\cos(v))^2\,v^8 {b_4}^2 - 7680\,(\cos(v))^2\,v^2 {b_4}^2 \\
& + 3993600\,(\cos(v))^2\,v^2 b_3 - 7537920\,(\cos(v))^2\,v^2 b_4 \\
& - 4630080\,(\cos(v))^2\,v^6 {b_4}^2 + 76800\,v^2 b_3 b_4 - 192000\,v^2 a_0 {b_3}^2
\end{aligned}$$

$$
\begin{aligned}
&+748800\,v^2b_2b_3-76800\,v^2a_0{b_4}^2-1223664\,\cos(v)\,v^4b_4\\
&-1984320\,v^2a_0b_4-641600\,v^4b_3b_4+678400\,v^6b_3b_4\\
&-3968640\,v^4b_2b_4+4044960\,v^4a_0{b_4}^2+399360\,\sin(v)\,b_4v\\
&+3993600\,\sin(v)\,vb_3+15360\,\cos(v)\,v^2{b_4}^2-10583040\,\sin(v)\,v^3b_4\\
&+1536000\,\cos(v)\,v^2{b_3}^2+10240\,\sin(v)\,v^3{b_4}^2+923520\,\cos(v)\,v^2b_3\\
&-153600\,(\cos(v))^2\,v^2b_3b_4+3155200\,(\cos(v))^2\,v^4b_3b_4\\
&-1356800\,(\cos(v))^2\,v^6b_3b_4-399360\,\sin(v)\cos(v)\,vb_4\\
&-3595520\,\sin(v)\cos(v)\,v^7{b_4}^2+407040\,\sin(v)\cos(v)\,v^5{b_4}^2\\
&-1024000\,\sin(v)\cos(v)\,v^3{b_3}^2-10240\,\sin(v)\cos(v)\,v^3{b_4}^2\\
&+10583040\,\sin(v)\cos(v)\,v^3b_4+1024000\,\sin(v)\,v^3{b_3}^2\\
&-605632\,\cos(v)\,v^4{b_4}^2-407040\,\sin(v)\,v^5{b_4}^2+492800\,\cos(v)\,v^4{b_3}^2\\
&+8858208\,\cos(v)\,v^6{b_4}^2+16000\,v^6b_3{b_4}^2-97344\,\cos(v)\\
&+7787520\,(\cos(v))^2+80000\,v^6{b_3}^2b_4-1123600\,v^6a_0{b_4}^2+8480\,v^6a_0{b_4}^3\\
&+318000\,v^8b_3{b_4}^2-337080\,v^8b_2{b_4}^2+337080\,v^8a_0{b_4}^3+64\,\cos(v)\,v^6{b_4}^3\\
&+64000\,\cos(v)\,v^6{b_3}^3+3595520\,\sin(v)\,v^7{b_4}^2+865172\,\cos(v)\,v^8{b_4}^2\\
&+33708\,\cos(v)\,v^{10}{b_4}^3-148877\,\cos(v)\,v^{12}{b_4}^3-2544\,\cos(v)\,v^8{b_4}^3\\
&+74880\,v^2b_2b_4-8480\,v^6b_2{b_4}^2+15966912\,\cos(v)\,b_4v^2\\
&-3993600\,\sin(v)\cos(v)\,vb_3-49920\,b_4-499200\,b_3\\
&-973440\,b_2+307200\,\cos(v)\,v^2b_3b_4+204800\,\sin(v)\,v^3b_3b_4\\
&-6007040\,\cos(v)\,v^4b_3b_4-4070400\,\sin(v)\,v^5b_3b_4\\
&-1305920\,\cos(v)\,v^6b_3b_4+1920\,\cos(v)\,v^6b_3{b_4}^2+19200\,\cos(v)\,v^6{b_3}^2b_4\\
&-50880\,\cos(v)\,v^8b_3{b_4}^2-254400\,\cos(v)\,v^8{b_3}^2b_4+337080\,\cos(v)\,v^{10}b_3{b_4}^2\\
&-787200\,v^2a_0b_3b_4+763200\,v^4a_0b_3b_4-84800\,v^6b_2b_3b_4\\
&+84800\,v^6a_0b_3{b_4}^2+998400\,b_4a_0+2645760\,v^4b_4\\
&+11069760\,b_4v^2-61600\,v^4{b_4}^2-256000\,v^4{b_3}^2+6449040\,v^6{b_4}^2\\
&+249600\,a_0b_3-449440\,v^8{b_4}^2-204800\,\sin(v)\cos(v)\,v^3b_3b_4\\
&+4070400\,\sin(v)\cos(v)\,v^5b_3b_4-199680\,\cos(v)\,b_4+800\,v^6{b_4}^3\\
&-1996800\,\cos(v)\,b_3+384000\,v^2{b_3}^2+3840\,v^2{b_4}^2+31800\,v^8{b_4}^3\\
&+998400\,(\cos(v))^2\,b_3+99840\,(\cos(v))^2\,b_4-1996800\,v^2b_3
\end{aligned}
$$

$$
\begin{aligned}
T_3=\;&491212800\,va_0b_3b_4+934502400\,\sin(v)\cos(v)\,b_3\\
&+757186560\,\cos(v)\,v^3{b_4}^2-4952862720\,(\cos(v))^2\,v^3b_4\\
&+95846400\,\sin(v)\,v^2b_3b_4+23961600\,v^3b_2b_3b_4-571687680\,(\cos(v))^2\,v^{11}{b_4}^3\\
&+1537084800\,(\cos(v))^2\,v^9{b_4}^3-135951360\,(\cos(v))^2\,v^7{b_4}^3\\
&+3365406720\,(\cos(v))^2\,v^7{b_4}^2+8032527360\,(\cos(v))^2\,v^5{b_4}^2\\
&+6635520\,(\cos(v))^2\,v^5{b_4}^3+122880000\,(\cos(v))^2\,v^5{b_3}^3\\
&-122880000\,(\cos(v))^2\,v^3{b_3}^3-122880\,(\cos(v))^2\,v^3{b_4}^3\\
&+958464000\,(\cos(v))^2\,v^3{b_3}^2-371404800\,(\cos(v))^2\,v^3{b_4}^2
\end{aligned}
$$

$$
\begin{aligned}
&+ 479232000\ (\cos(v))^2\, v b_3{}^2 + 4792320\ (\cos(v))^2\, v b_4{}^2 \\
&- 344064000\, v^5 b_3{}^2 b_4 - 66969600\, v^5 b_3 b_4{}^2 + 18432000\, v^3 b_3{}^2 b_4 \\
&- 539328000\, v^9 b_3 b_4{}^2 + 325632000\, v^7 b_3{}^2 b_4 - 1682703360\ \cos(v)\, v^7 b_4{}^2 \\
&- 118041600\ \sin(v)\, v^8 b_3{}^2 b_4 + 113817600\ \sin(v)\, v^4 b_3{}^2 \\
&+ 2393164800\, v^3 b_3 b_4 - 16636538880\ \cos(v)\, v^5 b_4{}^2 \\
&- 3618201600\ (\cos(v))^2\, v^3 b_3 b_4 + 9809920\ \sin(v)\cos(v)\, v^6 b_4{}^3 \\
&- 1809699840\ \sin(v)\cos(v)\, v^6 b_4{}^2 + 133939200\ (\cos(v))^2\, v^5 b_3 b_4{}^2 \\
&- 3809894400\ (\cos(v))^2\, v^5 b_3 b_4 - 3686400\ (\cos(v))^2\, v^3 b_3 b_4{}^2 \\
&- 36864000\ (\cos(v))^2\, v^3 b_3{}^2 b_4 + 688128000\ (\cos(v))^2\, v^5 b_3{}^2 b_4 \\
&- 191692800\ \cos(v)\, v b_3 b_4 + 1652541696\ \sin(v)\, v^6 b_4{}^2 \\
&+ 95846400\ (\cos(v))^2\, v\, b_3 b_4 + 1450792320\ \sin(v)\cos(v)\, v^{10} b_4{}^3 \\
&+ 5393280\ \sin(v)\, v^{12} b_3 b_4{}^3 - 50880000\, v^9 b_3{}^2 b_4{}^2 - 10176000\, v^9 b_3 b_4{}^3 \\
&+ 1843200\, v^3 b_3 b_4{}^2 + 2025838080\ \sin(v)\, v^8 b_3 b_4{}^2 - 934502400\, v\, b_3 \\
&+ 1904947200\ \cos(v)\, v^5 b_3 b_4 - 206572800\ \sin(v)\cos(v)\, v^8 b_4{}^3 \\
&+ 841351680\ \sin(v)\cos(v)\, v^8 b_4{}^2 - 47923200\, v\, b_3 b_4 \\
&- 479232000\ \cos(v)\, v^3 b_3{}^2 - 1320960000\ \cos(v)\, v^5 b_3{}^2 b_4 \\
&- 24883200\, v^3 a_0 b_3 b_4{}^2 - 1682703360\, v^7 b_4{}^2 - 5529600\ \sin(v)\cos(v)\, v^4 b_3 b_4{}^2 \\
&- 2396160\, v b_4{}^2 - 15185664\ \sin(v) - 262348800\ \cos(v)\, v^5 b_3 b_4{}^2 \\
&- 2476431360\ \sin(v)\cos(v)\, v^4 b_4 + 1869004800\ (\cos(v))^2\, v\, b_3 \\
&+ 61440\, v^3 b_4{}^3 - 239616000\, v b_3{}^2 - 301616640\ \sin(v)\, v^6 b_3 b_4 \\
&- 612218880\ \sin(v)\, v^4 b_3 b_4 + 244108800\, v^3 b_4{}^2 + 55296000\ \sin(v)\, v^4 b_3{}^2 b_4 \\
&+ 2429706240\ \sin(v)\cos(v) + 10240\ \sin(v)\, v^8 b_3 b_4{}^3 - 93450240\ \sin(v)\, b_4 \\
&- 934502400\ \sin(v)\, b_3 - 11397120\, v^7 b_4{}^3 - 2083154400\, v^9 b_4{}^3 \\
&- 508800\, v^9 b_4{}^4 - 6741600\, v^{11} b_4{}^4 + 40960000\ \sin(v)\cos(v)\, v^6 b_3{}^3 \\
&- 184320\ \sin(v)\cos(v)\, v^4 b_4{}^3 + 285843840\, v^{11} b_4{}^3 + 61440000\, v^3 b_3{}^3 \\
&- 3317760\, v^5 b_4{}^3 - 61440000\, v^5 b_3{}^3 + 93450240\ \sin(v)\cos(v)\, b_4 \\
&- 184320000\ \sin(v)\cos(v)\, v^4 b_3{}^3 - 952473600\, v^3 a_0 b_3 b_4 \\
&+ 2663331840\ (\cos(v))^2\, v\, b_4 - 13568000\ \sin(v)\, v^{10} b_3{}^3 b_4 \\
&+ 667545600\, v^5 a_0 b_3 b_4{}^2 - 2082009600\ \sin(v)\cos(v)\, v^8 b_3 b_4{}^2 \\
&+ 989184000\ \sin(v)\cos(v)\, v^6 b_3{}^2 b_4 - 479232000\ \sin(v)\cos(v)\, v^2 b_3{}^2 \\
&+ 2476431360\ \cos(v)\, v^3 b_4 + 196608000\ \sin(v)\cos(v)\, v^6 b_3 b_4{}^2 \\
&- 1269964800\ \sin(v)\cos(v)\, v^6 b_3 b_4 - 479232000\, v^3 b_3{}^2 \\
&+ 162816000\, v^5 a_0 b_3{}^2 b_4 + 325632000\ \cos(v)\, v^7 b_3{}^2 b_4 \\
&+ 7523942400\ \cos(v)\, v^3 b_3 b_4 + 1904947200\, v^5 b_3 b_4 \\
&- 53932800\, v^9 a_0 b_3 b_4{}^3 - 162816000\ \sin(v)\cos(v)\, v^8 b_3{}^2 b_4 \\
&+ 619107840\, v a_0 b_4 + 5393280\, v^9 b_2 b_4{}^3 + 357304800\, v^9 a_0 b_4{}^3 \\
&+ 5529600\ \sin(v)\, v^4 b_3 b_4{}^2 + 73728000\ \cos(v)\, v^3 b_3{}^2 b_4
\end{aligned}
$$

$$
\begin{aligned}
&+7443311616\,\sin(v)\,b_4v^2-95281280\,\sin(v)\cos(v)\,v^{12}{b_4}^3\\
&-5393280\,v^9a_0{b_4}^4-67416000\,v^{11}b_3{b_4}^3-23820320\,\sin(v)\,v^{14}b_3{b_4}^3\\
&+71460960\,v^{11}b_2{b_4}^3+2476431360\,v^3b_4-651264000\,(\cos(v))^2\,v^7{b_3}^2b_4\\
&-1424640000\,(\cos(v))^2\,v^7b_3{b_4}^2+2103379200\,v^5a_0{b_4}^2\\
&-71460960\,v^{11}a_0{b_4}^4-9739264\,\sin(v)\,v^6{b_4}^3+29696000\,\sin(v)\,v^6{b_3}^3\\
&-323596800\,v^7a_0b_3{b_4}^2-934502400\,\cos(v)\,v\,b_3\\
&+26966400\,\sin(v)\,v^{12}{b_3}^2{b_4}^2+2653900800\,\cos(v)\,v^7b_3{b_4}^2\\
&+140175360\,\sin(v)\,v^2b_3+262133760\,\cos(v)\,v^7{b_4}^3\\
&+203764224\,\sin(v)\,v^8{b_4}^3-2912371200\,\cos(v)\,v^9{b_4}^3\\
&-634982400\,v^5b_2b_3b_4+1078656000\,(\cos(v))^2\,v^9b_3{b_4}^2-3609515520\,b_4v\\
&+256\,\sin(v)\,v^8{b_4}^4+2560000\,\sin(v)\,v^8{b_3}^4-1413578688\,\sin(v)\,v^{10}{b_4}^3\\
&+285843840\,\cos(v)\,v^{11}{b_4}^3-13568\,\sin(v)\,v^{10}{b_4}^4-69078928\,\sin(v)\,v^{12}{b_4}^3\\
&+269664\,\sin(v)\,v^{12}{b_4}^4-11755111680\,v^5{b_4}^2-2382032\,\sin(v)\,v^{14}{b_4}^4\\
&+7890481\,\sin(v)\,v^{16}{b_4}^4-46725120\,v\,b_2b_4+47923200\,va_0{b_4}^2\\
&-467251200\,vb_2b_3+119808000\,va_0{b_3}^2-62360064\,\sin(v)\,v^4{b_4}^2\\
&-5046312960\,\cos(v)\,b_4v+3095539200\,v^3b_2b_4+1198080\,v^3b_2{b_4}^2\\
&+119808000\,v^3b_2{b_3}^2-3190786560\,v^3a_0{b_4}^2-1228800\,v^3a_0{b_4}^3\\
&-30720000\,v^3a_0{b_3}^3+65126400\,v^5a_0{b_4}^3-63498240\,v^5b_2{b_4}^2\\
&-4792320\,\sin(v)\cos(v)\,v^2{b_4}^2+2103379200\,v^7b_2{b_4}^2-2135738880\,v^7a_0{b_4}^3\\
&-9584640\,\cos(v)\,v{b_4}^2-81408000\,v^7b_3{b_4}^2-958464000\,\cos(v)\,v{b_3}^2\\
&+4792320\,\sin(v)\,v^2{b_4}^2+479232000\,\sin(v)\,v^2{b_3}^2\\
&-55296000\,\sin(v)\cos(v)\,v^4{b_3}^2b_4-967987200\,\sin(v)\,v^6{b_3}^2b_4\\
&+184320\,\sin(v)\,v^4{b_4}^3+184320000\,\sin(v)\,v^4{b_3}^3+245760\,\cos(v)\,v^3{b_4}^3\\
&-13086720\,\cos(v)\,v^5{b_4}^3+245760000\,\cos(v)\,v^3{b_3}^3\\
&-61440000\,\cos(v)\,v^5{b_3}^3-194488320\,\sin(v)\,v^6b_3{b_4}^2\\
&+1024000\,\sin(v)\,v^8{b_3}^3b_4+1869004800\,\sin(v)\cos(v)\,v^2b_3\\
&-407040\,\sin(v)\,v^{10}b_3{b_4}^3+199821024\,\sin(v)\,v^8{b_4}^2\\
&-7242393600\,\sin(v)\cos(v)\,v^2b_4+68290560\,\sin(v)\cos(v)\,v^4{b_4}^2\\
&+479232000\,\sin(v)\cos(v)\,v^4{b_3}^2-185732352\,\sin(v)\,v^4b_4\\
&-129024000\,v^3a_0{b_3}^2b_4+156405120\,\sin(v)\,v^{10}b_3{b_4}^2\\
&+7372800\,\cos(v)\,v^3b_3{b_4}^2+53932800\,v^9b_2b_3{b_4}^2+153600\,\sin(v)\,v^8{b_3}^2{b_4}^2\\
&-539328000\,\cos(v)\,v^9b_3{b_4}^2+730828800\,\sin(v)\cos(v)\,v^4b_3b_4\\
&-95846400\,\sin(v)\cos(v)\,v^2b_3b_4+215731200\,\sin(v)\cos(v)\,v^{10}b_3{b_4}^2\\
&-4070400\,\sin(v)\,v^{10}{b_3}^2{b_4}^2
\end{aligned}
$$

Based on the above system of equations (14)-(17) and solving this system we obtain the coefficients of the proposed predictor–corrector explicit four-step method:

$$a_0 = \frac{T_4}{T_5},\ b_2 = \frac{T_6}{T_7},$$
$$b_3 = \frac{T_8}{T_9},\ b_4 = \frac{T_{10}}{T_{11}} \tag{18}$$

where

$$\begin{aligned}
T_4 = &-9954 + 500\,v^5 \sin(4\,v) + 2000\,v^5 \sin(2\,v) - 7155\,v^2 \cos(5\,v)\\
&- 5168\,v^3 \sin(2\,v) - 20772\,v \sin(4\,v) + 1644\,v^3 \sin(4\,v) + 32088\,v \sin(2\,v)\\
&+ 12975 \cos(v)\,v^4 - 530\,v^4 \cos(5\,v) + 132135\,v \sin(v)\\
&- 146755\,v^3 \sin(v) + 3710\,v^5 \sin(v) - 24360\,v^2 \cos(2\,v) + 89760\,v^2 \cos(3\,v)\\
&- 106845 \cos(v)\,v^2 + 3000\,v^4 \cos(2\,v) + 6335\,v^4 \cos(3\,v) + 5565\,v \sin(5\,v)\\
&- 69480\,v \sin(3\,v) + 12000\,v^2 \cos(4\,v) - 265\,v^5 \sin(5\,v)\\
&+ 3445\,v^5 \sin(3\,v) - 1325\,v^3 \sin(5\,v) + 30600\,v^3 \sin(3\,v)\\
&+ 1250\,v^4 \cos(4\,v) - 900 \cos(v) + 2904\,v^2 + 18000 \cos(2\,v) + 7750\,v^4\\
&-8046 \cos(4\,v) + 10440 \cos(3\,v) - 9540 \cos(5\,v)\\
T_5 = &-9000 + 9540 \cos(3\,v) + 2915\,v^3 \sin(3\,v) + 265\,v^4 \cos(3\,v)\\
&- 19875\,v \sin(3\,v) + 6000\,v^2 \cos(2\,v) - 11925\,v^2 \cos(3\,v)\\
&+ 24645 \cos(v)\,v^2 + 85065\,v \sin(v) + 9275\,v^3 \sin(v) + 2915 \cos(v)\,v^4\\
&+ 6000\,v \sin(2\,v) - 1000\,v^3 \sin(2\,v) - 9540 \cos(v) + 9000 \cos(2\,v)\\
T_6 = &-2266704 - 31800\,v^4 \cos(8\,v) - 3008120\,v^5 \sin(7\,v) + 3021000\,v^3 \sin(8\,v)\\
&- 616560\,v^4 \cos(7\,v) - 1952255 \sin(v)\,v^9 - 20185 \cos(v)\,v^8\\
&- 4891752 \cos(6\,v) - 13864488 \cos(2\,v)\,v^6 - 109757576\,v^6\\
&+ 3501225\,v^6 \cos(5\,v) + 710200\,v^5 \sin(8\,v) + 3470018\,v^5 \sin(6\,v)\\
&- 12243000\,v^8 + 954000\,v \sin(8\,v) - 80950576\,v^5 \sin(4\,v)\\
&+ 126110074\,v^5 \sin(2\,v) - 89618940\,v^2 \cos(5\,v) - 274092168\,v^3 \sin(2\,v)\\
&- 32106816\,v \sin(4\,v) + 112812672\,v^3 \sin(4\,v) - 31631544\,v \sin(2\,v)\\
&- 190800\,v^6 \cos(8\,v) - 656905\,v^7 \sin(7\,v) - 170637540 \cos(v)\,v^4\\
&+ 20848950\,v^4 \cos(5\,v) - 74462940\,v \sin(v) - 271536780\,v^3 \sin(v)\\
&+ 962914360\,v^5 \sin(v) - 159597486\,v^2 \cos(2\,v) - 203935140\,v^2 \cos(3\,v)\\
&+ 276584220 \cos(v)\,v^2 + 258190098\,v^4 \cos(2\,v) - 142974690\,v^4 \cos(3\,v)\\
&- 1976760\,v \sin(5\,v) - 16493040\,v \sin(3\,v) - 12868812\,v^2 \cos(4\,v)\\
&+ 7295840\,v^5 \sin(5\,v) - 384520240\,v^5 \sin(3\,v) + 159404250\,v^3 \sin(5\,v)\\
&-228553890\,v^3 \sin(3\,v) - 254392956\,v^4 \cos(4\,v) - 2710800 \cos(v)\\
&+ 206492076\,v^2 + 4027752 \cos(2\,v) - 213838668\,v^4 + 841104 \cos(4\,v)\\
&+ 6791040 \cos(3\,v) - 5896800 \cos(5\,v) + 16969860\,v^2 \cos(7\,v)\\
&+ 1816560 \cos(7\,v) + 2289600 \cos(8\,v) + 14045\,v^9 \sin(7\,v)\\
&- 42135\,v^9 \sin(5\,v) - 21200\,v^8 \cos(8\,v) + 715500\,v^8 \cos(6\,v)
\end{aligned}$$

$$- 24106575\, v^7 \sin(3\,v) + 2088200\, v^8 \cos(4\,v) - 5803500\, v^8 \cos(2\,v)$$
$$- 2008435\, v^9 \sin(3\,v) - 395025\, v^8 \cos(3\,v) + 6427848\, v^6 \cos(6\,v)$$
$$- 7342600\, v^6 \cos(4\,v) + 651065\, v^7 \sin(5\,v) - 742000\, v^9 \sin(4\,v)$$
$$- 53000\, v^9 \sin(6\,v) - 2173000\, v^9 \sin(2\,v) - 64898842\, v^7 \sin(2\,v)$$
$$- 16260616\, v^7 \sin(4\,v) + 31800\, v^7 \sin(8\,v) + 1170318\, v^7 \sin(6\,v)$$
$$+ 911305\, v^8 \cos(5\,v) - 114495\, v^8 \cos(7\,v) + 30676392\, v \sin(6\,v)$$
$$+ 58873455\, \sin(v)\, v^7 + 27242345\, \cos(v)\, v^6 + 2671200\, v^2 \cos(8\,v)$$
$$- 16601520\, v^3 \sin(7\,v) + 19848174\, v^4 \cos(6\,v) + 19117980\, v \sin(7\,v)$$
$$- 144846685\, v^6 \cos(3\,v) - 11895432\, v^3 \sin(6\,v) + 734795\, v^6 \cos(7\,v)$$
$$- 36696978\, v^2 \cos(6\,v)$$

$$T_7 = 5702270\, \sin(v)\, v^9 + 29469780\, \cos(v)\, v^8 + 64872000\, \cos(2\,v)\, v^6$$
$$- 15582000\, v^6 + 24059085\, v^6 \cos(5\,v) - 212000\, v^8 - 13356000\, v^5 \sin(4\,v)$$
$$+ 41976000\, v^5 \sin(2\,v) + 22896000\, v^3 \sin(2\,v) - 11448000\, v^3 \sin(4\,v)$$
$$- 95966640\, \cos(v)\, v^4 - 23258520\, v^4 \cos(5\,v) + 28334880\, v^3 \sin(v)$$
$$+ 503809830\, v^5 \sin(v) + 125928000\, v^4 \cos(2\,v) + 119225160\, v^4 \cos(3\,v)$$
$$+ 33750135\, v^5 \sin(5\,v) - 211000275\, v^5 \sin(3\,v) - 6067440\, v^3 \sin(5\,v)$$
$$+ 667440\, v^3 \sin(3\,v) - 12402000\, v^4 \cos(4\,v) - 113526000\, v^4$$
$$+ 1713490\, \cos(v)\, v^{10} + 14045\, v^{10} \cos(5\,v) + 294945\, v^{10} \cos(3\,v)$$
$$+ 266855\, v^9 \sin(5\,v) + 4351710\, v^7 \sin(3\,v) + 1484000\, v^8 \cos(4\,v)$$
$$+ 6360000\, v^8 \cos(2\,v) + 3272485\, v^9 \sin(3\,v) - 11127010\, v^8 \cos(3\,v)$$
$$- 18762000\, v^6 \cos(4\,v) - 9522510\, v^7 \sin(5\,v) - 106000\, v^9 \sin(4\,v)$$
$$- 1060000\, v^9 \sin(2\,v) - 3180000\, v^7 \sin(2\,v) + 7950000\, v^7 \sin(4\,v)$$
$$- 2162930\, v^8 \cos(5\,v) + 105263340\, \sin(v)\, v^7 + 121230810\, \cos(v)\, v^6$$
$$- 105730215\, v^6 \cos(3\,v)$$

$$T_8 = -19380\, v + 30789\, v^2 \sin(3\,v) - 2120\, v^6 \sin(2\,v) + 18840\, v \cos(4\,v)$$
$$- 22730\, v^4 \sin(2\,v) - 3405\, v^4 \sin(4\,v) + 53\, v^5 \cos(3\,v)$$
$$- 530\, v^6 \sin(4\,v) - 12479\, v^3 \cos(3\,v) + 3240\, v^2 \sin(4\,v)$$
$$+ 17040\, v \cos(3\,v) + 540\, v \cos(2\,v) + 35183\, v^3 \cos(v) - 88800\, v^3 \cos(2\,v)$$
$$+ 45240\, v^2 \sin(2\,v) - 17040\, \cos(v)\, v + 583\, v^5 \cos(v) + 9643\, v^4 \sin(v)$$
$$- 46983\, v^2 \sin(v) + 25300\, v^3 \cos(4\,v) + 8371\, v^4 \sin(3\,v)$$
$$+ 2915\, v^5 \cos(4\,v) - 9540\, v^5 \cos(2\,v) - 720\, \sin(2\,v) + 360\, \sin(4\,v)$$
$$+ 54\, \sin(v) - 18\, \sin(3\,v) - 18815\, v^5 + 114740\, v^3$$

$$T_9 = -19875\, v^4 \sin(3\,v) + 6000\, v^5 \cos(2\,v) + 9275\, v^6 \sin(v)$$
$$+ 24645\, v^5 \cos(v) + 85065\, v^4 \sin(v) - 9540\, v^3 \cos(v) + 9000\, v^3 \cos(2\,v)$$
$$+ 2915\, \cos(v)\, v^7 + 265\, v^7 \cos(3\,v) + 2915\, v^6 \sin(3\,v) - 9000\, v^3$$
$$+ 9540\, v^3 \cos(3\,v) - 11925\, v^5 \cos(3\,v) + 6000\, v^4 \sin(2\,v) - 1000\, v^6 \sin(2\,v)$$

$$T_{10} = -240\,v^3 \sin(v) - 80\,v^3 \sin(3\,v) - 1000\,\cos(v)\,v^2 + 4\,v^2 \cos(2\,v) + 40\,v^2 \cos(3\,v) + 720\,v \sin(v) - 240\,v \sin(3\,v) + 20\,v^2 + 240\,\cos(v) + 12\,\cos(2\,v) - 240\,\cos(3\,v) - 12$$

$$T_{11} = 53\,\cos(2\,v)\,v^6 - 200\,v^5 \sin(v) + 424\,v^5 \sin(2\,v) + 265\,v^6 + 600\,\cos(v)\,v^4 - 1113\,v^4 \cos(2\,v) - 600\,v^3 \sin(v) - 636\,v^3 \sin(2\,v) + 2385\,v^4$$

The formulae (18) can be subject to heavy cancelations for small values of $|w|$. The following Taylor series expansions should be used in the above described cases of possible cancellations:

$$a_0 = -\frac{9}{5} + \frac{31349\,v^8}{13440000} - \frac{3134167\,v^{10}}{24192000000} + \frac{22573535749\,v^{12}}{1117670400000000} - \frac{87003316039\,v^{14}}{670602240000000000} - \frac{294315005972879\,v^{16}}{4068320256000000000000} - \frac{9882192843770741993\,v^{18}}{373471799500800000000000000} + \cdots$$

$$b_2 = \frac{661}{400} - \frac{31349\,v^2}{560000} + \frac{4113931\,v^4}{144000000} - \frac{411203026699\,v^6}{46569600000000} + \frac{15610274821489\,v^8}{2794176000000000} - \frac{43564232338357763\,v^{10}}{5085400320000000000} + \frac{306364669720057073\,v^{12}}{171003571200000000000000} - \frac{2835570879535988410796599\,v^{14}}{1365973106674176000000000000000} + \frac{4297550052912878512736328\,89\,v^{16}}{819583864004505600000000000000000} + \frac{282609540661137476046925325\,9927\,v^{18}}{26390600420945080320000000000000000000} + \cdots$$

$$b_3 = \frac{317}{300} + \frac{31349\,v^2}{840000} - \frac{2717999\,v^4}{189000000} - \frac{8371477613\,v^6}{34927200000000} - \frac{1589768766407\,v^8}{2095632000000000} - \frac{1526020314848017\,v^{10}}{2860537680000000000} + \frac{1200344410089318\,61\,v^{12}}{194516562240000000000000} + \frac{34784937597638432348867\,v^{14}}{28457773055712000000000000000} + \frac{29472349929137160287708503\,v^{16}}{102447983000563200000000000000000} + \frac{137692044468396422063206886\,7011\,v^{18}}{29689425473563215360000000000000000000} + \cdots$$

$$b_4 = \frac{161}{2400} - \frac{31349\,v^2}{3360000} + \frac{583417\,v^4}{6048000000} - \frac{2910518999\,v^6}{279417600000000} + \frac{257387450539\,v^8}{16765056000000000} + \frac{4511203337283911\,v^{10}}{915372057600000000000}$$

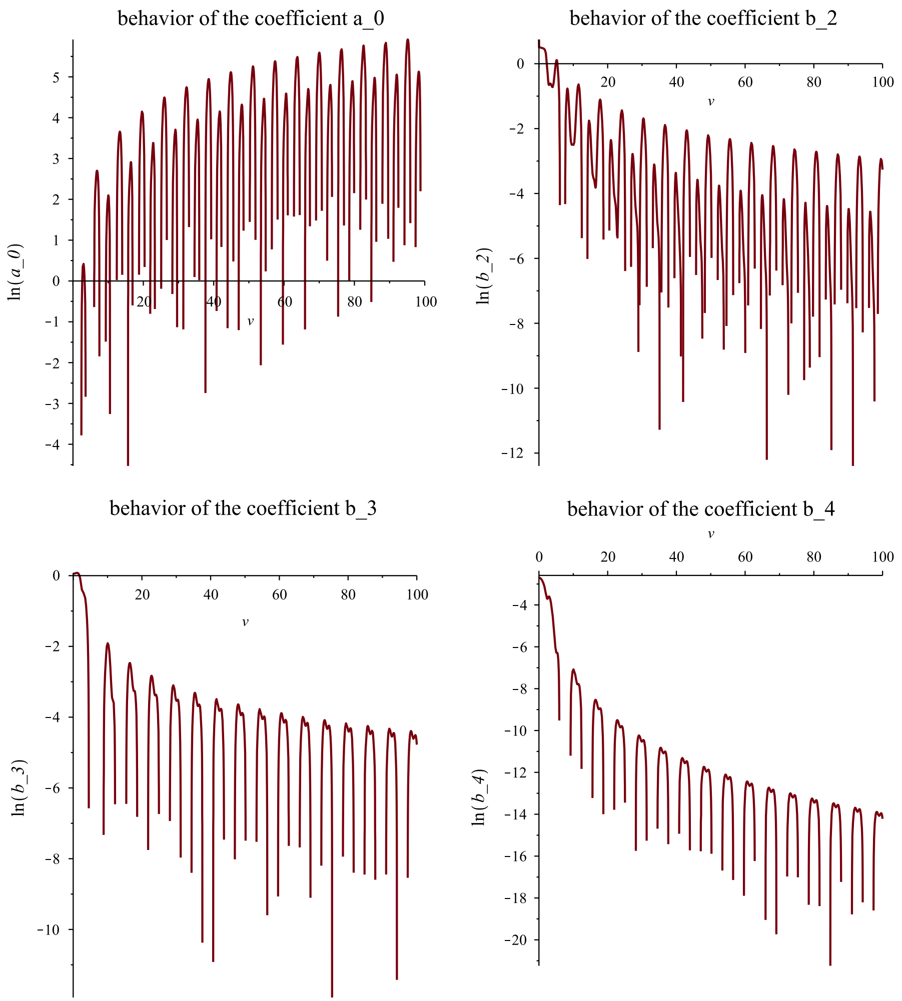



**Fig. 4** Behavior of the coefficients of the new proposed method given by (18) for several values of $v = w\,h$.

$$+\frac{316379820544874759\,v^{12}}{345807221760000000000000}+\frac{2038098525792045208855 1\,v^{14}}{16070271843225600000000000000}$$
$$+\frac{7100043582019690707850771\,v^{16}}{546389242669670400000000000000000}$$
$$+\frac{3210214356358167177762915109 81\,v^{18}}{475030807577011445760000000000000000000}+\cdots \tag{19}$$

Figure 4 shows the behavior of the coefficients $b_2$, $b_3$ and $b_4$.

The proposed method is the method (11) with the coefficients given by (18)–(19).

The local truncation error of this new proposed method (mentioned as $PCMeth$) is given by:

$$LTE_{PCMeth} = \frac{31349\,h^8}{13440000}\left(q_n^{(8)} + 4\,w^2\,q_n^{(6)} + 6\,w^4\,q_n^{(4)} + 4w^6\,q_n^{(2)} + w^8\,q_n\right) + O\left(h^{10}\right) \tag{20}$$

where $q_n^{(j)}$ is the $j$-th derivative of $q_n$.

## 5 Comparative error analysis

The following methods will be studied in this section:

5.1 Classical predictor–corrector explicit four-step method, i.e. the method (11) with constant coefficients

$$LTE_{CL} = \frac{31349\,h^8}{13440000}\,q_n^{(8)} + O\left(h^{10}\right) \tag{21}$$

5.2 The predictor–corrector explicit four-step method with vanished phase-lag and its first and second derivatives developed in Sect. 4

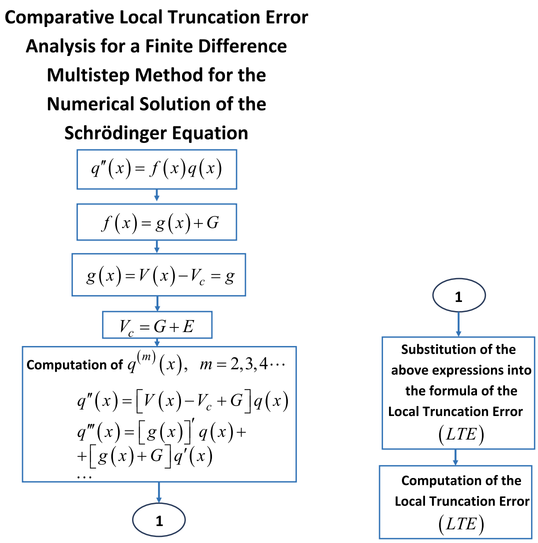
$$LTE_{PCMeth} = \frac{31349\,h^8}{13440000}\left(q_n^{(8)} + 4\,w^2\,q_n^{(6)} + 6\,w^4\,q_n^{(4)} + 4w^6\,q_n^{(2)} + w^8\,q_n\right) + O\left(h^{10}\right) \tag{22}$$

Our comparative Local Truncation Error Analysis is based on the Flowchart mentioned in the Fig. 5.

The Local Truncation Error formulae for the error analysis are produced using the algorithm mentioned on the flowchart and the following formulae:

$$\begin{aligned}
q_n^{(2)} &= \left(V(x) - V_c + G\right)\,q(x)\\
q_n^{(3)} &= \left(\frac{d}{dx}g\,(x)\right)q\,(x) + (g\,(x) + G)\,\frac{d}{dx}q\,(x)\\
q_n^{(4)} &= \left(\frac{d^2}{dx^2}g\,(x)\right)q\,(x) + 2\,\left(\frac{d}{dx}g\,(x)\right)\frac{d}{dx}q\,(x)\\
&\quad + \,(g\,(x) + G)^2\,q\,(x)\\
q_n^{(5)} &= \left(\frac{d^3}{dx^3}g\,(x)\right)q\,(x) + 3\,\left(\frac{d^2}{dx^2}g\,(x)\right)\frac{d}{dx}q\,(x)\\
&\quad + 4\,(g\,(x) + G)\,q\,(x)\,\frac{d}{dx}g\,(x) + (g\,(x) + G)^2\,\frac{d}{dx}q\,(x)
\end{aligned}$$

**Fig. 5** Flowchart for the comparative error analysis




$$q_n^{(6)} = \left(\frac{d^4}{dx^4} g(x)\right) q(x) + 4\left(\frac{d^3}{dx^3} g(x)\right) \frac{d}{dx} q(x)$$
$$+7\,(g(x)+G)\,q(x)\,\frac{d^2}{dx^2} g(x) + 4\left(\frac{d}{dx} g(x)\right)^2 q(x)$$
$$+6\,(g(x)+G)\left(\frac{d}{dx} q(x)\right) \frac{d}{dx} g(x) + (g(x)+G)^3\, q(x)$$

$$q_n^{(7)} = \left(\frac{d^5}{dx^5} g(x)\right) q(x) + 5\left(\frac{d^4}{dx^4} g(x)\right) \frac{d}{dx} q(x)$$
$$+11\,(g(x)+G)\,q(x)\,\frac{d^3}{dx^3} g(x) + 15\left(\frac{d}{dx} g(x)\right) q(x)\,\frac{d^2}{dx^2} g(x)$$
$$+13\,(g(x)+G)\left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x) + 10\left(\frac{d}{dx} g(x)\right)^2 \frac{d}{dx} q(x)$$
$$+9\,(g(x)+G)^2\, q(x)\,\frac{d}{dx} g(x) + (g(x)+G)^3\, \frac{d}{dx} q(x)$$

$$q_n^{(8)} = \left(\frac{d^6}{dx^6} g(x)\right) q(x) + 6\left(\frac{d^5}{dx^5} g(x)\right) \frac{d}{dx} q(x)$$
$$+16\,(g(x)+G)\,q(x)\,\frac{d^4}{dx^4} g(x) + 26\left(\frac{d}{dx} g(x)\right) q(x)\,\frac{d^3}{dx^3} g(x)$$
$$+24\,(g(x)+G)\left(\frac{d}{dx} q(x)\right) \frac{d^3}{dx^3} g(x) + 15\left(\frac{d^2}{dx^2} g(x)\right)^2 q(x)$$
$$+48\left(\frac{d}{dx} g(x)\right)\left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x) + 22\,(g(x)+G)^2\, q(x)\,\frac{d^2}{dx^2} g(x)$$

$$+\,28\,\left(g\left(x\right)+G\right)q\left(x\right)\left(\frac{d}{dx}g\left(x\right)\right)^{2}$$
$$+\,12\,\left(g\left(x\right)+G\right)^{2}\left(\frac{d}{dx}q\left(x\right)\right)\frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^{4}q\left(x\right)$$
$$\ldots$$

Two cases for the value of $E$ are of interest in our study:

- The Energy is closed to the potential, i.e., $G = V_c - E \approx 0$. Consequently, the terms of the Local Truncation Error which have powers of $G$ (i.e. $G^j$, $j \neq 0$) are approximately equal to zero. Therefore, in this case we take into account only the terms of the formulae of the Local Truncation Error which are free of $G$. As a result of the above analysis all the numerical methods of the same family, and for these values of $G$ (i.e. approximately equal to zero), are of comparable accuracy. This is because for this case the terms of the formulae of the Local Truncation Error which are free of $G$ are the **same** for the numerical methods of the same family (cases of the classical methods (methods with constant coefficients) and cases of the methods with vanished the phase-lag and its derivatives).
- $G >> 0$ or $G << 0$. Then $|G|$ is a large number. Here the expressions of the formulae of the Local Truncation Error are different for the numerical methods of the same family.

The asymptotic expressions of the Local Truncation Errors (based on the methodology presented above) are given by :

### 5.3 Classical method

$$LTE_{CL} = h^8\left(\frac{31349\,q\left(x\right)}{13440000}\,G^4+\cdots\right)+O\left(h^{10}\right) \tag{23}$$

### 5.4 The predictor–corrector explicit four-step method with vanished phase-lag and its first and second derivatives developed in Sect. 4

$$\begin{aligned} LTE_{PCMeth} = h^8 \Bigg[ \Bigg( & \frac{31349\left(\frac{d^4}{dx^4}g\left(x\right)\right)q\left(x\right)}{1120000}+\frac{31349\left(\frac{d^3}{dx^3}g\left(x\right)\right)\frac{d}{dx}q\left(x\right)}{1680000} \\ & +\frac{31349\,g\left(x\right)q\left(x\right)\frac{d^2}{dx^2}g\left(x\right)}{840000}+\frac{31349\left(\frac{d}{dx}g\left(x\right)\right)^2q\left(x\right)}{1120000}\Bigg)G+\cdots\Bigg] \\ & +O\left(h^{10}\right) \end{aligned} \tag{24}$$

Based on the above analysis, we have the following theorem:

**Theorem 2** *The Local Truncation Error Analysis leads us to the following conclusions:*

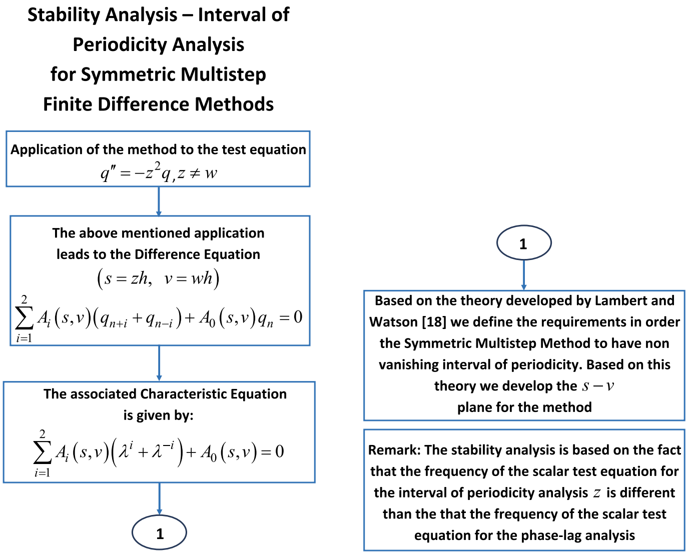



**Fig. 6** Flowchart for the stability analysis

- *For the Classical Predictor–Corrector Explicit Four-Step Method the error increases as the fourth power of $G$.*
- *For the Predictor–Corrector Explicit Four-Step Method with Vanished Phase-Lag and its First and Second Derivatives developed in Sect. 4, the error increases as the first power of $G$.*

*So, for the numerical solution of the time independent radial Schrödinger equation the New Proposed Predictor–Corrector Explicit Four-Step Method with Vanished Phase-Lag and its First and Second Derivatives developed in Sect. 4 is the most efficient, from theoretical point of view, especially for large values of $|G| = |V_c - E|$.*

## 6 Stability analysis

In order to investigate the stability of the new proposed predictor–corrector symmetric explicit four-step method we use the Flowchart mentioned in Fig. 6, in which the procedure for the the interval of periodicity analysis is described. We must mention that for this investigation we will use a scalar test equation with frequency different than the frequency of the scalar test equation used for the phase-lag analysis.

We consider the the new obtained predictor–corrector symmetric explicit four-step method (11) with the coefficients given by (12) and (18).

Application of the above described method to the scalar test equation:

$$q'' = -z^2 q \tag{25}$$

leads to the below mentioned difference equation:

$$A_2(s, v)\ (q_{n+2} + q_{n-2}) + A_1(s, v)\ (q_{n+1} + q_{n-1}) + A_0(s, v)\ q_n = 0 \tag{26}$$

where

$$A_2(s,v) = 1,\ A_1(s,v) = \frac{1}{10}\,\frac{ST_0}{ST_1}\,A_0(s,v) = \frac{1}{5}\,\frac{ST_2}{ST_1} \tag{27}$$

where $s = z\,h$ and

$$\begin{aligned}
ST_0 = {} & 16424\,\sin(v)\cos(v)\,s^2v^3 - 11364\,\sin(v)\cos(v)\,s^2v - 1060\,(\cos(v))^3\,s^4v^2 \\
& + 5300\,(\cos(v))^3\,s^2v^4 + 12720\,(\cos(v))^3\,s^2v^2 - 106\,v^6 + 300\,\sin(v)\,s^2v \\
& + 1060\,\sin(v)\,s^4v^3 - 1060\,\sin(v)\,s^2v^5 - 53\,(\cos(v))^2\,s^4v^2 \\
& + 106\,(\cos(v))^2\,s^2v^4 - 424\,\sin(v)\cos(v)\,v^5 + 7420\,\cos(v)\,s^4v^2 \\
& - 18020\,\cos(v)\,s^2v^4 - 6360\,\sin(v)\,s^4v + 38060\,\sin(v)\,s^2v^3 \\
& + 24318\,(\cos(v))^2\,s^2v^2 + 636\,\sin(v)\cos(v)\,v^3 + 12420\,\cos(v)\,s^2v^2 \\
& + 6360\,(\cos(v))^2\sin(v)\,s^4v - 29680\,(\cos(v))^2\sin(v)\,s^2v^3 \\
& - 25440\,(\cos(v))^2\sin(v)\,s^2v + 2120\,(\cos(v))^2\sin(v)\,s^4v^3 \\
& - 2120\,(\cos(v))^2\sin(v)\,s^2v^5 - 300\,\cos(v)\,v^4 + 300\,v^3\sin(v) \\
& + 100\,v^5\sin(v) - 1749\,v^4 + 159\,s^4 - 106\,s^4v^2 + 212\,s^2v^4 \\
& - 53\,(\cos(v))^2\,v^6 - 159\,(\cos(v))^2\,s^4 + 1113\,(\cos(v))^2\,v^4 \\
& - 6360\,\cos(v)\,s^4 - 12954\,s^2v^2 + 6360\,(\cos(v))^3\,s^4 \\
ST_1 = {} & \Big(53\,(\cos(v))^2\,v^3 + 424\,\sin(v)\cos(v)\,v^2 \\
& - 1113\,(\cos(v))^2\,v - 100\,v^2\sin(v) + 106\,v^3 \\
& - 636\,\sin(v)\cos(v) + 300\,\cos(v)\,v - 300\,\sin(v) + 1749\,v\Big)\,v^3 \\
ST_2 = {} & 12520\,\sin(v)\cos(v)\,s^2v^3 - 300\,\sin(v)\cos(v)\,s^2v - 500\,(\cos(v))^3\,s^4v^2 \\
& - 5000\,(\cos(v))^3\,s^2v^4 - 18636\,(\cos(v))^3\,s^2v^2 - 14890\,v^6 \\
& + 500\,\sin(v)\,s^4v^3 - 1000\,\sin(v)\,s^2v^5 - 25\,(\cos(v))^2\,s^4v^2 \\
& - 15850\,(\cos(v))^2\,s^2v^4 - 40080\,\sin(v)\cos(v)\,v^5 + 3500\,\cos(v)\,s^4v^2 \\
& - 1000\,\cos(v)\,s^2v^4 - 3000\,\sin(v)\,s^4v - 1272\,\sin(v)\,s^2v^3 \\
& - 25290\,(\cos(v))^2\,s^2v^2 - 6660\,\sin(v)\cos(v)\,v^3 + 7272\,\cos(v)\,s^2v^2 \\
& + 3000\,(\cos(v))^2\sin(v)\,s^4v - 3788\,(\cos(v))^2\sin(v)\,s^2v^3 \\
& + 11364\,(\cos(v))^2\sin(v)\,s^2v + 1000\,(\cos(v))^2\sin(v)\,s^4v^3 \\
& - 2000\,(\cos(v))^2\sin(v)\,s^2v^5 + 13272\,\cos(v)\,v^4 - 3000\,v^3\sin(v) \\
& + 3272\,v^5\sin(v) + 17265\,v^4 + 75\,s^4 - 50\,s^4v^2 + 16000\,s^2v^4 \\
& + 24885\,(\cos(v))^2\,v^6 - 75\,(\cos(v))^2\,s^4 - 26505\,(\cos(v))^2\,v^4 \\
& - 3000\,\cos(v)\,s^4 + 150\,s^2v^2 + 5500\,(\cos(v))^3\,v^6 - 15636\,(\cos(v))^3\,v^4 \\
& - 5300\,(\cos(v))^4\,v^6 + 3180\,(\cos(v))^4\,v^4 + 3000\,(\cos(v))^3\,s^4 \\
& + 500\,\sin(v)\,v^7 - 2500\,\cos(v)\,v^6 + 1060\,(\cos(v))^3\sin(v)\,s^2v^5 \\
& + 4240\,(\cos(v))^3\sin(v)\,s^2v^3 - 4240\,\cos(v)\sin(v)\,s^2v^5 \\
& + 25440\,(\cos(v))^3\sin(v)\,s^2v - 1060\,\sin(v)\,(\cos(v))^3\,v^7
\end{aligned}$$

$$+1000\,\sin(v)\,(\cos(v))^2\,v^7 + 10600\,\sin(v)\,(\cos(v))^3\,v^5$$
$$+4240\,\sin(v)\cos(v)\,v^7 - 13212\,\sin(v)\,(\cos(v))^2\,v^5$$
$$+12720\,\sin(v)\,(\cos(v))^3\,v^3 + 5364\,\sin(v)\,(\cos(v))^2\,v^3$$

*Remark 6* The frequency of the scalar test equation (6) for the phase-lag analysis, $w$, is not equal with the frequency of the scalar test equation (25) for the stability analysis, $z$, i.e. $z \neq w$.

The associated characteristic equation of the difference equation (26) is equal to:

$$A_2(s,v)\left(\lambda^4+1\right) + A_1(s,v)\left(\lambda^3+\lambda\right) + A_0(s,v)\,\lambda^2 = 0 \tag{28}$$

**Definition 1** (see [19]) A symmetric $2\,k$-step method with the characteristic equation given by (8) is said to have an *interval of periodicity* $\left(0, v_0^2\right)$ if, for all $s \in \left(0, s_0^2\right)$, the roots $\lambda_i,\ i = 1(1)4$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)},\ |\lambda_i| \leq 1,\ i = 3, 4, \ldots \tag{29}$$

where $\zeta(s)$ is a real function of $z\,h$ and $s = z\,h$.

**Definition 2** (see [19]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

**Definition 3** A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $s = v$.

In Fig. 7, we present the $s{-}v$ plane for the first block layer (stages 1 and 2) of the Hybrid type method developed in this paper. The stable area of the the $s - v$ region of the first block layer (stages 1 and 2) is the shadowed area, while the unstable area is the white area.

*Remark 7* Investigating the stability for these methods we can divide this study into two categories of problems:

- Problems where the frequency of the scalar test equation for the phase-lag analysis is not equal to the frequency of the scalar test equation for the stability analysis (i.e. $z \neq w$)
- Problems where the frequency of the scalar test equation for the phase-lag analysis is equal to the frequency of the scalar test equation for the stability analysis (i.e. $z = w$)

In the second case study, we can include problems, as for example the Schrödinger equation and related problems.

For the first case study the investigation consists the development of the $s{-}v$ plane of the method (see Fig. 7 for our new produced predictor–corrector symmetric explicit

[1] Where $S$ is a set of distinct points.

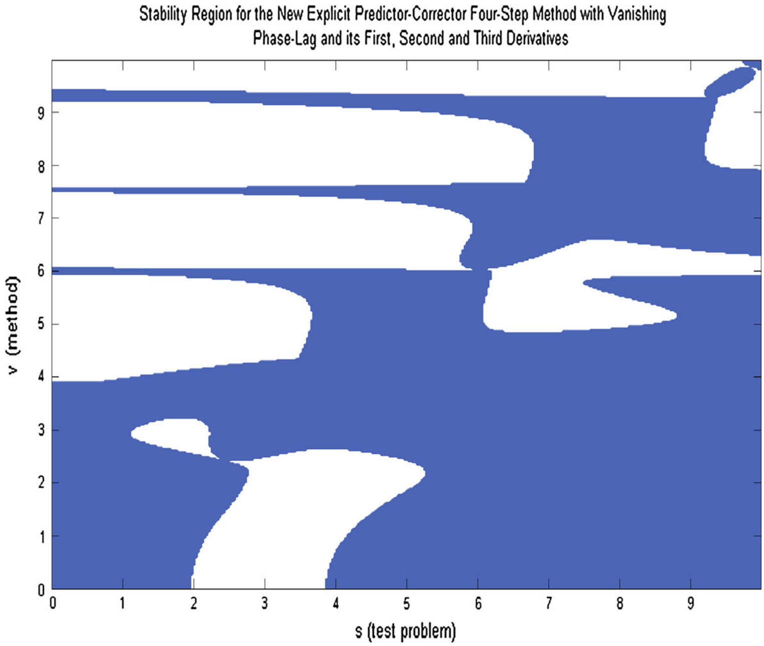



**Fig. 7** $s-v$ plane of the predictor–corrector symmetric explicit four-step method (11) with the coefficients given by (12) and (18)

four-step method). For the second case study it is necessary to observe *the surroundings of the first diagonal of the* $s - v$ *plane.*

Investigating the second case study, i.e. investigating the case where $z = w$ or $s = v$ (i.e. seeing the surroundings of the first diagonal of the $s - v$ plane), we extract the result that the interval of periodicity of the new obtained predictor–corrector symmetric explicit four-step method developed in Sect. 4 is equal to: (0, 16).

From the above analysis we have the following theorem:

**Theorem 3** *The method produced in Sect. 4:*

- *is of predictor–corrector type*
- *is of sixth algebraic order,*
- *has the phase-lag and its first, second and third derivatives equal to zero*
- *has an interval of periodicity equals to:* (0, 16) *in the case where the frequency of the scalar test equation for the phase-lag analysis is equal to the frequency of the scalar test equation for the stability analysis*

## 7 Numerical results

Our numerical tests are based on the numerical solution of the radial time-independent Schrödinger equation (1).

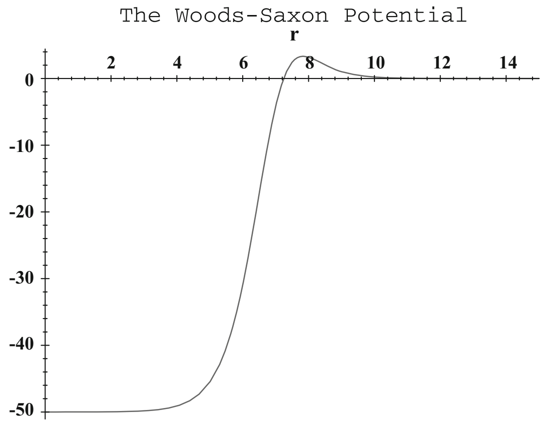



**Fig. 8** The Woods–Saxon potential

The new developed predictor–corrector symmetric explicit four-step method belonged to the category of the frequency dependent methods. Due to this, it is necessary the definition of the value of parameter $w$, in order to be possible to be applied to the numerical solution of the radial Schrödinger equation. The parameter $w$, based on the mathematical model given by (1), is given by (for the case $l = 0$):

$$w = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{30}$$

where $V(r)$ is the potential and $E$ is the energy.

## 7.1 Woods–Saxon potential

In order to be possible the numerical solution of the time-independent radial Schrödinger equation (1), it is necessary the determination of the function of the potential. For our numerical experiments, the well known Woods-Saxon potential is used. This potential can be written as

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{31}$$

with $y = \exp\left[\frac{r-X_0}{a}\right]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

The behavior of Woods-Saxon potential is shown in Fig. 8.

Several methodologies for the determination of the frequency $w$, of the frequency dependent methods, have been investigated (see [26] and references therein). For our numerical experiments we used the below described methodology (see for details [108]): In order to define the frequency $w$, we use the values of the potential on some critical points, which are determined from the study of the specific potential.

*Remark 8* The above mentioned methodology is well known applied to some potentials, such as the Woods-Saxon potential.

For the purpose of obtaining our numerical results, it is appropriate to choose $v$ as follows (see for details [1] and [82]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for} \quad r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for} \quad r = 6.5-h \\ \sqrt{-25+E}, & \text{for} \quad r = 6.5 \\ \sqrt{-12.5+E}, & \text{for} \quad r = 6.5+h \\ \sqrt{E}, & \text{for} \quad r \in [6.5+2h, 15] \end{cases} \tag{32}$$

For example, in the point of the integration region $r = 6.5 - h$, the value of $w$ is equal to: $\sqrt{-37.5+E}$. So, $v = w\,h = \sqrt{-37.5+E}\,h$. In the point of the integration region $r = 6.5 - 3\,h$, the value of $w$ is equal to: $\sqrt{-50+E}$, etc.

### 7.2 Radial Schrödinger equation: the resonance problem

The numerical example which we will use in this paper is the numerical solution of the radial time independent Schrödinger equation (1) using Woods-Saxon potential (31).

This is a boundary value problem which has an infinite interval of integration. For the approximation of the solution it is necessary the infinite interval of integration to be approximated by a finite one. For our numerical tests we consider the integration interval $r \in [0, 15]$. For our numerical experiments we consider a large domain of energies, i.e., $E \in [1, 1000]$.

*Remark 9* In the case of positive energies, $E = k^2$ the potential decays faster than the term $\frac{l(l+1)}{r^2}$.

Based on the above remark and studying this case, the Schrödinger equation effectively reduces to:

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{33}$$

for $r$ greater than some value $R$.

The above equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus, the solution of equation (1) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{34}$$

where $\delta_l$ is the phase shift that may be calculated from the formula

$$\tan \delta_l = \frac{p(r_2)\,S(r_1) - p(r_1)\,S(r_2)}{p(r_1)\,C(r_1) - p(r_2)\,C(r_2)} \tag{35}$$

for $r_1$ and $r_2$ distinct points in the asymptotic region (we choose $r_1$ as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = kr j_l(kr)$ and $C(r) = -kr n_l(kr)$. For the initial-value problems (the radial Schrödinger equation is treated as an initial-value problem) we need $q_j, \ j = 0(1)3$ before starting a four-step method. The initial condition defines the first value of $q$ i.e. $q_0$. Using high order Runge-Kutta-Nyström methods (see [115] and [116]) we determine the values $q_i, \ i = 1(1)3$. Now we have all the necessary initial values and we can compute at $r_2$ of the asymptotic region the phase shift $\delta_l$.

For positive energies, we have the so-called resonance problem. This problem consists either

– of finding the phase-shift $\delta_l$ or
– of finding those $E$, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$.

We solved the latter problem, known as *the resonance problem*.

The boundary conditions for this problem are:

$$q(0) = 0, \ q(r) = \cos\left(\sqrt{E} r\right) \text{ for large } r. \tag{36}$$

The positive eigen energies of the Woods–Saxon potential resonance problem are computed using:

– The eighth order multi-step method developed by Quinlan and Tremaine [20], which is indicated as *Method QT8*.
– The tenth order multi-step method developed by Quinlan and Tremaine [20], which is indicated as *Method QT10*.
– The twelfth order multi-step method developed by Quinlan and Tremaine [20], which is indicated as *Method QT12*.
– The fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as *Method MCR4*
– The exponentially-fitted method of Raptis and Allison [83], which is indicated as *Method RA*
– The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [24], which is indicated as *Method MCR6*
– The classical form of the fourth algebraic order four-step method developed in Sect. 4, which is indicated as *Method NMCL*. [2]
– The Phase-Fitted Method (Case 1) developed in [45], which is indicated as *Method NMPF1*
– The Phase-Fitted Method (Case 2) developed in [45], which is indicated as *Method NMPF2*
– The Method developed in [49] (Case 2), which is indicated as *Method NMC2*
– The Method developed in [49] (Case 1), which is indicated as *Method NMC1*
– The New Obtained Method developed in Sect. 4, which is indicated as *Method NMPCPL2DV*

[2] With the term classical we mean the method of Sect. 4 with constant coefficients.

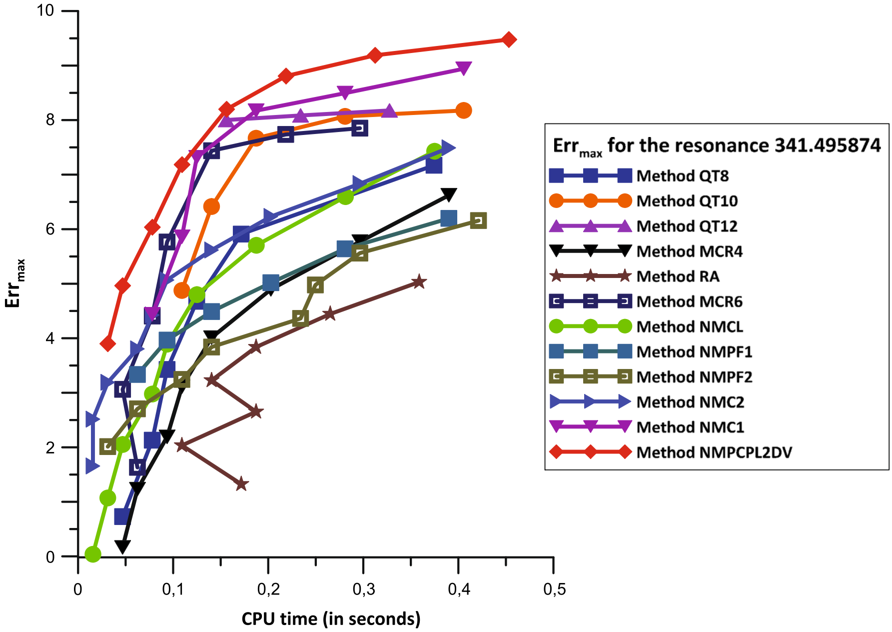



**Fig. 9** Accuracy (digits) for several values of $CPU$ Time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

We compare the computed eigenenergies via the above mentioned methods with reference values. [3] In Figs. 9 and 10, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{37}$$

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds). We note that the CPU time (in seconds) counts the computational cost for each method.

## 8 Conclusions

A predictor–corrector explicit four-step method of sixth algebraic order was studied in this paper. More specifically, we developed a method with vanishing the phase-lag and its first, second and third derivatives. We studied the specific method as one block. We investigated how this eliminations effects on the computational efficiency of the proposed method.

[3] The reference values are computed using the well known two-step method of Chawla and Rao [24] with small step size for the integration.

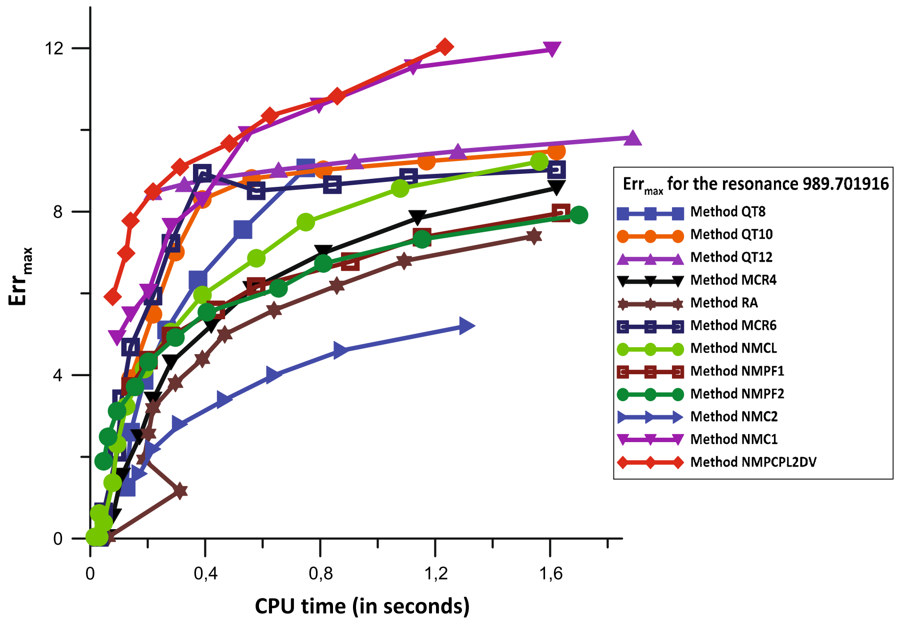



**Fig. 10** Accuracy (digits) for several values of $CPU$ Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

We studied the obtained method via the comparative local truncation error analysis and via the stability analysis (using scalar test equation with frequency different than the frequency of the phase-lag analysis)

Finally, we examined the computational efficiency of the proposed method via numerical experiments which was based on the numerical solution of the resonance problem of the radial time independent Schrödinger equation.

The proposed method is very effective on any problem with oscillating and/or periodical solutions or problems with solutions contain the functions cos and sin or any combination of them.

From the numerical experiments described above, we can make the following remarks:

1. The classical form of the sixth algebraic order four-step method developed in Sect. 4, which is indicated as *Method NMCL* is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as *Method MCR4*. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [83], which is indicated as *Method RA*. The method *Method NMCL* is more efficient than the eighth algebraic order multistep method developed by Quinlan and Tremaine [20], which is indicated as *Method QT8*, the Phase-Fitted Method (Case 1) developed in [45], which is indicated as *Method NMPF1* and the Phase-Fitted Method (Case 2) developed in [45], which is indicated as *Method NMPF1*.

2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [20], which is indicated as *Method QT10* is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as *Method MCR4*. The *Method QT10* is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [20], which is indicated as *Method QT8*. Finally, the *Method QT10* is more efficient than the classical form of the sixth algebraic order four-step method developed in Sect. 4, which is indicated as *Method NMCL*.
3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [20], which is indicated as *Method QT12* is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [20], which is indicated as *Method QT10*
4. The Method developed in [49] (Case 1), which is indicated as *Method NMC1* is more efficient than the twelfth algebraic order multistep method developed by Quinlan and Tremaine [20], which is indicated as *Method QT12*
5. Finally, the predictor–corrector explicit four-step method of sixth algebraic order with vanished phase-lag and its first, second and third derivatives (obtained in Sect. 4), which is indicated as *Method NMPCPL2DV*, is the most efficient one.

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

## References

1. L.G. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
2. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
3. I. Prigogine, Stuart Rice (eds.), *Advances in Chemical Physics. Vol. 93: New Methods in Computational Quantum Mechanics* (Wiley, London, 1997)
4. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
5. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
6. K. Tselios, T.E. Simos, Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
7. Z.A. Anastassi, T.E. Simos, An optimized Runge–Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
8. D.F. Papadopoulos, T.E. Simos, A new methodology for the construction of optimized Runge–Kutta-Nyström methods. Int. J. Mod. Phys. C **22**(6), 623–634 (2011)
9. Dimitris F. Papadopoulos, T.E. Simos, A modified Runge–Kutta-Nyström method by using phase lag properties for the numerical solution of orbital problems. Appl. Math. Inf. Sci. **7**(2), 433–437 (2013)
10. Th Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic Runge–Kutta-Nyström methods. Appl. Math. Inf. Sci. **7**(1), 81–85 (2013)
11. A.A. Kosti, Z.A. Anastassi, T.E. Simos, Construction of an optimized explicit Runge–Kutta-Nyström method for the numerical solution of oscillatory initial value problems. Comput. Math. Appl. **61**(11), 3381–3390 (2011)
12. A.A. Kosti, Z.A. Anastassi, T.E. Simos, An optimized explicit Runge–Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems. J. Math. Chem. **47**(1), 315–330 (2010)
13. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge–Kutta-Nyström methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem **31**(2), 211–232 (2002)
14. T.E. Simos, A fourth algebraic order exponentially-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. IMA J. Numer. Anal. **21**(4), 919–931 (2001)

15. T.E. Simos, Exponentially-fitted Runge–Kutta-Nyström method for the numerical solution of initial-value problems with oscillating solutions. Appl. Math. Lett. **15**(2), 217–225 (2002)
16. Ch. Tsitouras, T.E. Simos, Optimized Runge–Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
17. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge–Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
18. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge–Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. J. Math. Chem. **41**(1), 79–100 (2007)
19. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
20. G.D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits. Astron. J. **100**, 1694–1700 (1990)
21. Ch. Tsitouras, ITh Famelis, T.E. Simos, On modified Runge–Kutta trees and methods. Comput. Math. Appl. **62**(4), 2101–2111 (2011)
22. http://burtleburtle.net/bob/math/multistep.html
23. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)
24. M.M. Chawla, P.S. Rao, An explicit sixth-order method with phase-lag of order eight for $y'' = f(t, y)$. J. Comput. Appl. Math. **17**, 363–368 (1987)
25. M.M. Chawla, P.S. Rao, An Noumerov-typ method with minimal phase-lag for the integration of second order periodic initial-value problems II Explicit Method. J. Comput. Appl. Math. **15**, 329–337 (1986)
26. T.E. Simos, P.S. Williams, A finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**, 189–205 (1997)
27. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
28. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. J. Math. Chem. **31**(2), 135–144 (2002)
29. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 93–106 (2003)
30. T.E. Simos, I.T. Famelis, C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions. Numer. Algorithms **34**(1), 27–40 (2003)
31. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. J. Comput. Appl. Math. **175**(1), 161–172 (2005)
32. Theodore E. Simos, Optimizing a class of linear multi-step methods for the approximate solution of the radial Schrödinger equation and related problems with respect to phase-lag. Central Eur. J. Phys. **9**(6), 1518–1535 (2011)
33. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 317–331 (2005)
34. Hans Van de Vyver, Phase-fitted and amplification-fitted two-step hybrid methods for $y'' = f(x, y)$. J. Comput. Appl. Math. **209**(1), 33–53 (2007)
35. Hans Van de Vyver, An explicit Numerov-type method for second-order differential equations with oscillating solutions. Comput. Math. Appl. **53**, 1339–1348 (2007)
36. T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation. J. Math. Chem. **46**(3), 981–1007 (2009)
37. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A new symmetric eight-step predictor–corrector method for the numerical solution of the radial Schrödinger equation and related orbital problems. Int. J. Mod. Phys. C **22**(2), 133–153 (2011)
38. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A symmetric eight-step predictor–corrector method for the numerical solution of the radial Schrödinger equation and related IVPs with oscillating solutions. Comput. Phys. Commun. **182**(8), 1626–1637 (2011)
39. T.E. Simos, Optimizing a hybrid two-step method for the numerical solution of the Schrödinger equation and related problems with respect to phase-lag. J. Appl. Math. Article ID 420387 (2012)

40. T.E. Simos, A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation. J. Math. Chem. **49**(10), 2486–2518 (2011)
41. Ibraheem Alolyan, T.E. Simos, A family of high-order multistep methods with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **62**(10), 3756–3774 (2011)
42. Ibraheem Alolyan, T.E. Simos, A new four-step hybrid type method with vanished phase-lag and its first derivatives for each level for the approximate integration of the Schrödinger equation. J. Math. Chem. **51**, 2542–2571 (2013)
43. Ibraheem Alolyan, T.E. Simos, A Runge–Kutta type four-step method with vanished phase-lag and its first and second derivatives for each level for the numerical integration of the Schrödinger equation. J. Math. Chem. **52**, 917–947 (2014)
44. I. Alolyan, Z.A. Anastassi, T.E. Simos, A new family of symmetric linear four-step methods for the efficient integration of the Schrödinger equation and related oscillatory problems. Appl. Math. Comput. **218**(9), 5370–5382 (2012). Z. A.
45. Z.A. Anastassi, T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems. J. Comput. Appl. Math. **236**(16), 3880–3889 (2012)
46. G.A. Panopoulos, T.E. Simos, An optimized symmetric 8-step semi-embedded predictor–corrector method for IVPs with oscillating solutions. Appl. Math. Inf. Sci. **7**(1), 73–80 (2013)
47. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A new eight-step symmetric embedded predictor–corrector method (EPCM) for orbital problems and related IVPs with oscillatory solutions. Astron. J. **145**(3). Article Number: 75 2013. doi:10.1088/0004-6256/145/3/75
48. T.E. Simos, New high order multiderivative explicit four-step methods with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. Construction and theoretical analysis. J. Math. Chem. **51**(1), 194–226 (2013)
49. T.E. Simos, On the explicit four-step methods with vanished phase-lag and its first derivative. Appl. Math. Inf. Sci. **8**(2), 447–458 (2014)
50. G.A. Panopoulos, T.E. Simos, A new optimized symmetric embedded predictor–corrector method (EPCM) for initial-value problems with oscillatory solutions. Appl. Math. Inf. Sci. **8**(2), 703–713 (2014)
51. A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation. J. Math. Chem. **47**(2), 871–890 (2010)
52. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34**(1–2), 83–94 (2003)
53. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation. J. Math. Chem. **35**(1), 55–63 (2004)
54. T. Monovasilis, T.E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation. J. Math. Chem. **42**(3), 535–545 (2007)
55. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
56. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **40**(3), 257–267 (2006)
57. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
58. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae of high-order for long-time integration of orbital problems. Appl. Math. Lett. **22**(10), 1616–1621 (2009)
59. Z. Kalogiratou, T.E. Simos, Newton–Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
60. T.E. Simos, High order closed Newton–Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. Appl. Math. Comput. **209**(1), 137–151 (2009)
61. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for the solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 787–801 (2008)
62. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. J. Math. Chem. **44**(2), 483–499 (2008)

63. T.E. Simos, High-order closed Newton–Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. Comput. Phys. Commun. **178**(3), 199–207 (2008)
64. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for numerical integration of the Schrödinger equation. Comput. Lett. **3**(1), 45–57 (2007)
65. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. RevMexAA **42**(2), 167–177 (2006)
66. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for long-time integration. Int. J. Mod. Phys. C **14**(8), 1061–1074 (2003)
67. T.E. Simos, New closed Newton–Cotes type formulae as multilayer symplectic integrators. J. Chem. Phys. *133*(10). Article Number: 104108 (2010)
68. T.E. Simos, New stable closed Newton–Cotes trigonometrically fitted formulae for long-time integration. Abstr. Appl. Anal. (2012). Article Number: 182536. doi:10.1155/2012/182536
69. T.E. Simos, High order closed Newton–Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation. J. Math. Chem. **50**(5), 1224–1261 (2012)
70. T.E. Simos, Accurately closed Newton–Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. Int. J. Mod. Phys. C **24**(3) (2013). doi:10.1142/S0129183113500149
71. T.E. Simos, New open modified Newton Cotes type formulae as multilayer symplectic integrators. Appl. Math. Model. **37**(4), 1983–1991 (2013)
72. G.Vanden Berghe, M. Van Daele, Exponentially fitted open Newton–Cotes differential methods as multilayer symplectic integrators. J. Chem. Phys. **132**, 204107 (2010)
73. Z. Kalogiratou, T. Monovasilis, T.E. Simos, A fifth-order symplectic trigonometrically fitted partitioned Runge–Kutta method. in *International Conference on Numerical Analysis and Applied Mathematics*, SEP 16–20, 2007 Corfu, Greece, *Numerical Analysis and Applied Mathematics, AIP Conference Proceedings* vol. 936, pp. 313–317 (2007)
74. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Families of third and fourth algebraic order trigonometrically fitted symplectic methods for the numerical integration of Hamiltonian systems. Comput. Phys. Commun. **177**(10), 757–763 (2007)
75. T. Monovasilis, T.E. Simos, Symplectic methods for the numerical integration of the Schrödinger equation. Comput. Mater. Sci. **38**(3), 526–532 (2007)
76. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Computation of the eigenvalues of the Schrödinger equation by symplectic and trigonometrically fitted symplectic partitioned Runge-Kutta methods. Phys. Lett. A **372**(5), 569–573 (2008)
77. Z. Kalogiratou, Th Monovasilis, T.E. Simos, New modified Runge–Kutta-Nyström methods for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **60**(6), 1639–1647 (2010)
78. Th Monovasilis, Z. Kalogiratou, T.E. Simos, A family of trigonometrically fitted partitioned Runge–Kutta symplectic methods. Appl. Math. Comput. **209**(1), 91–96 (2009)
79. Th Monovasilis, Z. Kalogiratou, T.E. Simos, Two new phase-fitted symplectic partitioned Runge–Kutta methods. Int. J. Mod. Phys. C **22**(12), 1343–1355 (2011)
80. Kostas Tselios, T.E. Simos, Optimized fifth order symplectic integrators for orbital problems. Rev. Mex. Astron. Astrofis. **49**(1), 11–24 (2013)
81. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Symplectic partitioned Runge–Kutta methods with minimal phase-lag. Comput. Phys. Commun. **181**(7), 1251–1254 (2010)
82. LGr Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. Comput. Phys. Commun. **19**, 23–27 (1980)
83. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
84. J. Vigo-Aguiar, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem **32**(3), 257–270 (2002). J
85. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor–corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
86. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor–corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
87. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. Appl. Math. Lett. **17**(5), 601–607 (2004)

88. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. Acta Appl. Math. **110**(3), 1331–1352 (2010)
89. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
90. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. J. Math. Chem. **34**(1–2), 39–58 (2003)
91. T.E. Simos, Exponentially—fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
92. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
93. Hans Van de Vyver, A trigonometrically fitted explicit hybrid method for the numerical integration of orbital problems. Appl. Math. Comput. **189**(1), 178–185 (2007)
94. T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrodinger equation. J. Math. Chem. **44**(2), 447–466 (2009)
95. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. **45**(4), 1102–1129 (2009)
96. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor–corrector methods for the numerical solution of the radial Schrödinger equation. J. Math. Chem. **37**(3), 295–316 (2005)
97. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order predictor–corrector methods. J. Math. Chem. **40**(3), 269–293 (2006)
98. Zhongcheng Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**(3), 162–174 (2005)
99. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)
100. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. **45**(4), 1102–1129 (2009)
101. Chen Tang, Wenping Wang, Haiqing Yan, Zhanqing Chen, High-order predictorcorrector of exponential fitting for the N-body problems. J. Comput. Phys. **214**(2), 505–520 (2006)
102. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions. J. Math. Chem. **46**(2), 604–620 (2009)
103. S. Stavroyiannis, T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs. Appl. Numer. Math. **59**(10), 2467–2474 (2009)
104. S. Stavroyiannis, T.E. Simos, A nonlinear explicit two-step fourth algebraic order method of order infinity for linear periodic initial value problems. Comput. Phys. Commun. **181**(8), 1362–1368 (2010)
105. Z.A. Anastassi, T.E. Simos, Numerical multistep methods for the efficient solution of quantum mechanics and related problems. Phys. Rep. **482**, 1–240 (2009)
106. R. Vujasin, M. Sencanski, J. Radic-Peric, M. Peric, A comparison of various variational approaches for solving the one-dimensional vibrational Schrödinger equation. MATCH Commun. Math. Comput. Chem. **63**(2), 363–378 (2010)
107. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
108. LGr Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **38**(3), 329–337 (1985)
109. J. Vigo-Aguiar, T.E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation. Int. J. Quantum Chem. **103**(3), 278–290 (2005)
110. T.E. Simos, G. Psihoyios, Special issue: the international conference on computational methods in sciences and engineering 2004—preface. J. Comput. Appl. Math. **191**(2), 165 (2006). 165
111. T.E. Simos, G. Psihoyios, Special issue—Selected papers of the *International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)* Kastoria, Greece, 12–16 September 2003—Preface, J. Comput. Appl. Math. **175**(1) (2005)
112. T.E. Simos, J. Vigo-Aguiar, *Special Issue—Selected Papers from the Conference on Computational and Mathematical Methods for Science and Engineering (CMMSE-2002) - Alicante University, Spain*, 20–25 September 2002 - Preface, J. Comput. Appl. Math. **158**(1) (2003)

113. T.E. Simos, Ch. Tsitouras, I. Gutman, Preface for the special issue numerical methods in chemistry. MATCH Commun. Math. Comput. Chem. **60**(3) (2008)
114. T.E. Simos, I. Gutman, *Papers presented on the International Conference on Computational Methods in Sciences and Engineering* (Castoria, Greece, September 12–16, 2003). MATCH Commun. Math. Comput. Chem. **53**(2), A3–A4 (2005)
115. J.R. Dormand, M.E.A. El-Mikkawy, P.J. Prince, Families of Runge-Kutta-Nyström formulae. IMA J. Numer. Anal. **7**, 235–250 (1987)
116. J.R. Dormand, P.J. Prince, A family of embedded Runge–Kutta formulae. J. Comput. Appl. Math. **6**, 19–26 (1980)