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ORIGINAL PAPER

A high algebraic order predictor–corrector explicit method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the Schrödinger equation and related problems

Ibraheem Alolyan[1] · **T. E. Simos**[1,2,3]

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Abstract In this paper an eighth algebraic order predictor–corrector explicit four-step method is studied. The main scope of this paper is to study the consequences of (1) the vanishing of the phase-lag and its first, second, third and fourth derivatives and (2) the high algebraic order on the efficiency of the new developed method. A theoretical and computational study of the obtained method is also presented. More specifically, the theoretical study of the new predictor–corrector method consists of:

– The development of the new predictor–corrector method, i.e. the definition of the coefficients of the method in order its phase-lag and phase-lag's first, second, third and fourth derivatives to be vanished
– The computation of the local truncation error
– The comparative local truncation error analysis

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Highly Cited Researcher (http://isihighlycited.com/), Active Member of the European Academy of Sciences and Arts. Active Member of the European Academy of Sciences. Corresponding Member of European Academy of Arts, Sciences and Humanities.

✉ T. E. Simos
tsimos.conf@gmail.com

1 Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia

2 Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, 221 00 Tripoli, Greece

3 10 Konitsis Street, Amfithea - Paleon Faliron, 175 64 Athens, Greece

– The stability (interval of periodicity) analysis, using scalar test equation with frequency different than the frequency of the scalar test equation for the phase-lag analysis.

Finally, the computational study of the new predictor–corrector method consists of the application of the new produced predictor–corrector explicit four-step method to the numerical solution of the resonance problem of the radial time independent Schrödinger equation.

Keywords Schrödinger equation · Multistep methods · Predictor–corrector methods · Explicit methods · Interval of periodicity · P-stability · Phase-lag · Phase-fitted · Derivatives of the phase-lag

Mathematics Subject Classfication 65L05

1 Introduction

A new predictor–corrector explicit four-step method of eighth algebraic order with vanished phase-lag and its first, second, third and fourth derivatives will be studied in the present paper. The novelties of the new method are:

1. The new proposed method is of high algebraic order (eight algebraic order)
2. Optimal explicit four-step method is the basis of the predictor and the corrector of the new scheme
3. The new method has vanished the phase-lag and its first, second, third and fourth derivatives
4. 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.

As we have described above, we will develop a new predictor–corrector high algebraic order method for the efficient numerical solution of problems with mathematical models of the form of the one-dimensional time independent Schrödinger equation:

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

The mathematical model described above, includes the following functions and parameters:

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

The problem described in formula (1) is a boundary value one. Therefore, we need two boundary conditions. The initial point (first boundary condition) is given by the definition of the problem:

$$y(0) = 0. \tag{2}$$

The final point (second boundary condition), for large values of x, is defined using the physical considerations.

The radial time independent Schrödinger equation and all the similar problems belong to the category of the special second-order initial or boundary value problems of the form:

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

with periodical and/or oscillating solutions.

Remark 1 The main characteristic of the models of the above problems is that they represented by a system of second order ordinary differential equations of the form (3) in which the first derivative y' does not appear explicitly. We present below the applied sciences which have problems with mathematical models which satisfy the above characteristics:

- astronomy,
- astrophysics,
- quantum mechanics,
- quantum chemistry,
- celestial mechanics,
- electronics,
- physical chemistry,
- chemical physics, ..., etc

One case for more details in [1–4].

Remark 2 The aim and scope of the research which has done on the subject of the efficient numerical solution of the above described problems is the construction of :

1. effective,
2. fast and,
3. reliable

algorithms. We note here that an extensive research has been done on this research subject (see for example [5–108]).

The research on the above described subject which was done during the last decades had as result the main classes of finite difference methods presented in Fig. 1.

In the present paper, we will study 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 (corresponding: the implicit method with the same coefficients in the left hand side of the formula).

It is easy to see that this form facilitate the application of embedded schemes to real problems.

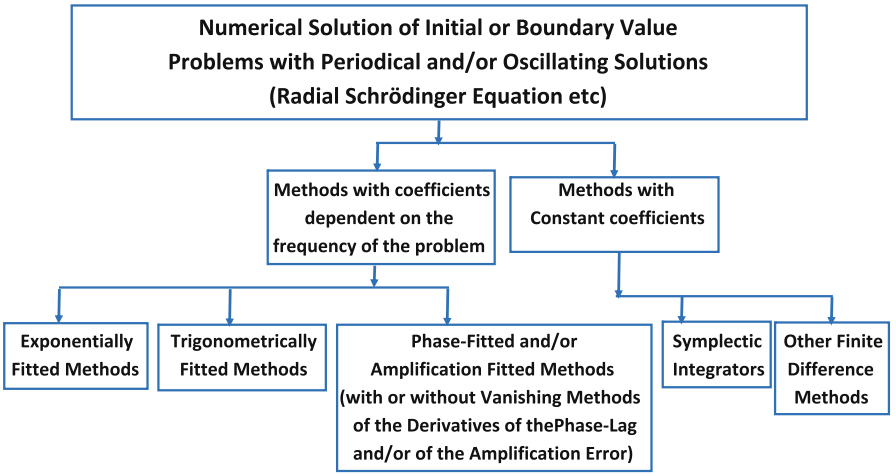

Fig. 1 Main classes of the finite difference methods developed in the last decades

The main idea is the elimination of the phase-lag and its derivatives in the whole method (when the whole method is applied to the specific scalar test equation). The study will examine how this procedure of vanishing of the phase-lag and its derivatives of the predictor–corrector method affects the effectiveness of the final proposed method.

The finally developed method will be compared with other well known methods of the literature in order its efficiency to be studied.

Remark 3 The methods developed with the above mentioned methodology can be applied efficiently to the following 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

The subjects of the research of the present paper are:

1. The computation of the coefficients of the new predictor and the new corrector method in order to have
   - the highest possible algebraic order ,
   - vanished phase-lag ,
   - vanished first derivative of the phase-lag ,
   - vanished second derivative of the phase-lag ,
   - vanished third derivative of the phase-lag ,
   - vanished fourth derivative of the phase-lag ,
2. The investigation of the local truncation error (LTE). We will present the comparative LTE analysis of the new produced predictor–corrector four-step method with other methods of the same form.

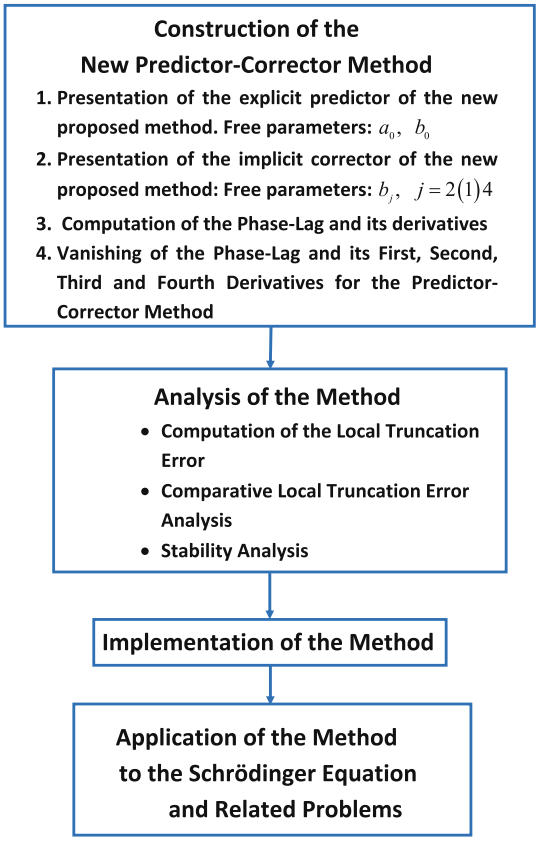

Fig. 2 Flowchart of the presentation of the analysis of the new proposed predictor–corrector high algebraic order method

3. The investigation of the stability with scalar test equation using frequency different than the frequency of the scalar test equation for the phase-lag analysis.
4. The investigation of the efficiency of the new obtained predictor–corrector four-step method using the approximate solution of the resonance problem of the radial time independent Schrödinger equation.

Using the direct formula for the computation of the phase-lag for any $2m$ symmetric multistep method which was developed by Simos et al. in [26] and [29], we will compute the phase-lag and its derivatives.

The flowchart of the analysis for the new predictor–corrector method is presented in Fig. 2.

A description of the bibliography on the research subject of the present paper is presented in Sect. 2. In Sect. 3 we present the phase-lag analysis of symmetric $2m$ symmetric methods. The construction of the new proposed explicit high algebraic order predictor–corrector method is presented in Sect. 4. The LTE of the obtained predictor–corrector method is computed in Sect. 5. In the same section we present a comparative LTE analysis with other similar methods. In Sect. 6 we present the stability analysis of the new obtained predictor–corrector method. We use scalar test

equation with frequency different than the frequency of the scalar test equation for the phase-lag analysis. Numerical results are presented in Sect. 7. Some remarks and conclusions are finally presented in Sect. 8.

2 Description of the bibliography

A recent bibliography on the subject of this paper is presented in the present section:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta–Nyström type have been obtained in [5–12].
- 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 [82–101].
- Nonlinear methods have been studied in [102,103]
- Review papers have been presented in [104–108]
- Special issues and Symposia in International Conferences have been developed on this subject (see [109–112])

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

The research area of this paper is the study of the approximate solution of the initial or boundary value problem of the form:

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

We will examine the special case of using a multistep method with $2m$ steps for the numerical solution of the problem (4):

$$\sum_{i=-m}^{m} a_i \, y_{n+i} = h^2 \sum_{i=-m}^{m} b_i \, f(x_{n+i}, y_{n+i}) \tag{5}$$

where :

- $2m$ are the number of steps over the equally spaced intervals $[x_{-i-1}, x_{i+1}]$, $i = 0(1)m-1$, where $\{x_i\}_{i=-m}^{m} \in [a, b]$
- $h = |x_{i+1} - x_i|, i = 0(1)m-1$, where h is called stepsize of integration
- $|a_0| + |b_0| \neq 0$

Remark 4 If $b_m = 0$ the method is explicit, otherwise it is implicit.

Remark 5 If the method is symmetric then

$$a_{i-m} = a_{m-i}, \; b_{i-m} = b_{m-i}, \; i = 0(1)m \tag{6}$$

If we apply a symmetric $2m$-step method [i.e. the method (5) with coefficients (6)] to the scalar test equation

$$y'' = -w^2 y, \tag{7}$$

the following difference equation is obtained

$$\begin{aligned} &A_m(v)\, y_{n+m} + \ldots + A_1(v)\, y_{n+1} \\ &+A_0(v)\, y_n + A_1(v)\, y_{n-1} + \ldots + A_m(v)\, y_{n-m} = 0, \end{aligned} \tag{8}$$

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

The associated characteristic equation is given by:

$$A_m(v)\,\lambda^m + \ldots + A_1(v)\,\lambda + A_0(v) + A_1(v)\,\lambda^{-1} + \ldots + A_m(v)\,\lambda^{-m} = 0 \tag{9}$$

Theorem 1 *[26,29] The symmetric $2m$-step method with characteristic equation given by (9) has phase-lag order k and phase-lag constant c given by:*

$$\begin{aligned} &-c\,v^{k+2} + O\left(v^{k+4}\right) \\ &= \frac{2\,A_m\,(v)\,\cos\,(m\,v) + \ldots + 2\,A_j\,(v)\,\cos\,(j\,v) + \ldots + A_0\,(v)}{2\,m^2\,A_m\,(v) + \ldots + 2\,j^2\,A_j\,(v) + \ldots + 2\,A_1\,(v)} \end{aligned} \tag{10}$$

Remark 6 A direct algorithm for the calculation of the phase-lag of any symmetric $2m$-step method is given by the formula (10).

Remark 7 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:

$$-\,c\,v^{k+2} + O\left(v^{k+4}\right) = \frac{2\,A_2(v)\,\cos(2\,v) + 2\,A_1(v)\,\cos(v) + A_0(v)}{8\,A_2(v) + 2\,A_1(v)} \tag{11}$$

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

4 The new proposed method

Let us consider the family of predictor–corrector explicit symmetric four-step methods for the approximate solution of initial or boundary value problems of the form $y'' = f\,(x, y)$:

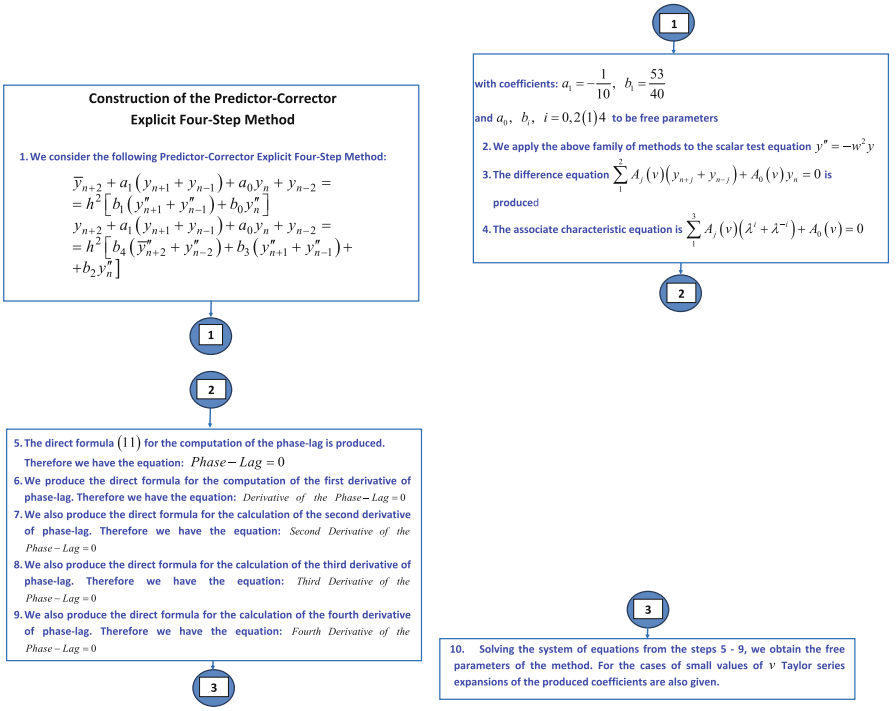

Fig. 3 Flowchart of the construction of any method of the family

$$\begin{aligned}\bar{q}_{n+2} &= -a_1 q_{n+1} - a_0 q_n - a_1 q_{n-1} - q_{n-2} \\ &\quad + h^2\left(b_1 q''_{n+1} + b_0 q''_n + b_1 q''_{n-1}\right) \\ &\quad q_{n+2} + a_1 q_{n+1} + a_0 q_n + a_1 q_{n-1} + q_{n-2} \\ &= h^2\left[b_4\ (\bar{q}''_{n+2} + q''_{n-2}) + b_3\ (q''_{n+1} + q''_{n-1}) + b_2 q''_n\right],\end{aligned} \tag{12}$$

where

$$a_1 = -\frac{1}{10},\ b_1 = \frac{53}{40} \tag{13}$$

and the coefficient a_0 and b_i, $i = 0,\ 2(1)4$ 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.

The development of the new proposed method is presented in the flowchart of the Fig. 3.

Our investigation for the method (12) is based on the above flowchart. Based on this, we apply the new method (12) to the scalar test Eq. (7). This leads to the difference Eq. (8) with $m = 2$ and $A_j\,(v)$, $j = 0,\ 1,\ 2$ given by:

$$A_2(v) = 1,\ A_1(v) = -\frac{1}{10} + v^2\left(b_4\left(\frac{1}{10} - \frac{53\,v^2}{40}\right) + b_3\right)$$
$$A_0(v) = a_0 + v^2\left(b_4\left(-v^2\,b_0 - a_0\right) + b_2\right) \tag{14}$$

Since our method (12) requests vanishing of the phase-lag and its first, second, third and fourth derivatives, we obtain the following system of equations [using the formulae (11) and (14)]:

$$\text{Phase-lag} = -\frac{T_0}{T_{denom}} = 0 \tag{15}$$
$$\text{First derivative of the phase-lag} = \frac{T_1}{T_{denom}^2} = 0 \tag{16}$$
$$\text{Second derivative of the phase-lag} = \frac{T_2}{T_{denom}^3} = 0 \tag{17}$$
$$\text{Third derivative of the phase-lag} = \frac{T_3}{T_{denom}^4} = 0 \tag{18}$$
$$\text{Fourth derivative of the phase-lag} = \frac{T_4}{T_{denom}^5} = 0 \tag{19}$$

where $T_j,\ j = 0(1)4$ and T_{denom} are given in Supplement Material A.

Solving the above system of Eqs. (15)-(19) we obtain the coefficients of the new predictor–corrector explicit four-step method:

$$a_0 = -\frac{1}{5}\frac{T_5}{T_6},\ b_0 = \frac{T_7}{T_8},\ b_2 = -\frac{T_9}{T_{10}},$$
$$b_3 = -\frac{T_{11}}{T_{12}},\ b_4 = -\frac{T_{13}}{T_{14}} \tag{20}$$

where $T_i,\ i = 5(1)14$ are given in Supplement Material B.

In order to avoid cancellations for small values of $|w|$, the following Taylor series expansions should be used:

$$a_0 = -\frac{9}{5} + \frac{13789\,v^{10}}{84672000} - \frac{70241\,v^{12}}{4694215680} + \frac{43110959\,v^{14}}{59147117568000} - \frac{44855753\,v^{16}}{1761508701388800} + \frac{3432896953273\,v^{18}}{11413783706083799040000} + \ldots$$
$$b_0 = \frac{3551}{660} - \frac{5115719\,v^2}{5410152} + \frac{341628194735\,v^4}{3104366858208} - \frac{3075605356003601\,v^6}{636177900252565440} + \frac{1431158902436299327\,v^8}{17256503674162908278323 2}$$

$$
\begin{aligned}
&- \frac{1736998190244626825946750241\, v^{10}}{16532554517898507409503915532 8000} \\
&- \frac{28836866390691743745197156275 5427\, v^{12}}{36048494467835293553291342043854530 5600} \\
&- \frac{17775440665017013917869720111237 4767\, v^{14}}{29549671885173946831503978900188435790643 20} \\
&- \frac{63872422799496347933985200682501394961 9917\, v^{16}}{16955719926400351387704309108843725210414230732 8000} \\
&- \frac{75475200576084668663148941263265569413903971 17\, v^{18}}{41065058089749011025881066230708618087102225411768320000} + \ldots \\
b_2 = &\frac{50247}{18550} - \frac{68945\, v^2}{186984} + \frac{671268581\, v^4}{12957991200} - \frac{2129375747\, v^6}{1632706891200} \\
&- \frac{21023761746067\, v^8}{26743738877856000} + \frac{1018146723119670539\, v^{10}}{12602719508800861440000} \\
&- \frac{77576393072619648371\, v^{12}}{12068364201627704914944000} + \frac{6384411063739344974171\, v^{14}}{1520613889405090819282944 0000} \\
&- \frac{24598793308305158114524473 7\, v^{16}}{12603273687278426135646439096320000} \\
&+ \frac{79223517315967090365823 33\, v^{18}}{93965235774975248111920196812800 00} + \ldots \\
b_3 = &\frac{18303}{37100} + \frac{13789\, v^2}{70119} - \frac{2046768223\, v^4}{77747947200} + \frac{12865930787\, v^6}{19592482694400} \\
&- \frac{287691169643\, v^8}{20057804158392000} + \frac{21259380677673491\, v^{10}}{75616317052805168640000} \\
&+ \frac{330519481480474067\, v^{12}}{14482037041953245897932800} + \frac{114569746298038501\, v^{14}}{60024232476516742866432000} \\
&+ \frac{85786937643965751281993 81\, v^{16}}{75619642123670556813878634577920000} \\
&+ \frac{47527185775708042888600 4347\, v^{18}}{95280749075824901585487079568179200000} + \ldots \\
b_4 = &\frac{759}{7420} - \frac{13789\, v^2}{1121904} + \frac{412031\, v^4}{971849340} - \frac{17935261\, v^6}{3918496538880} \\
&+ \frac{17506267081\, v^8}{64184973306854400} + \frac{11067156017123\, v^{10}}{945203963160064608000} \\
&+ \frac{8115873985421119\, v^{12}}{14482037041953245897932800} + \frac{52046960272748797\, v^{14}}{364947333457221796627906 5600} \\
&- \frac{96932302266564934061\, v^{16}}{18904910530917639203469658644 4800} \\
&- \frac{19917553711707874573513 01\, v^{18}}{19056149815164980317097415913635840000} + \ldots
\end{aligned} \tag{21}
$$

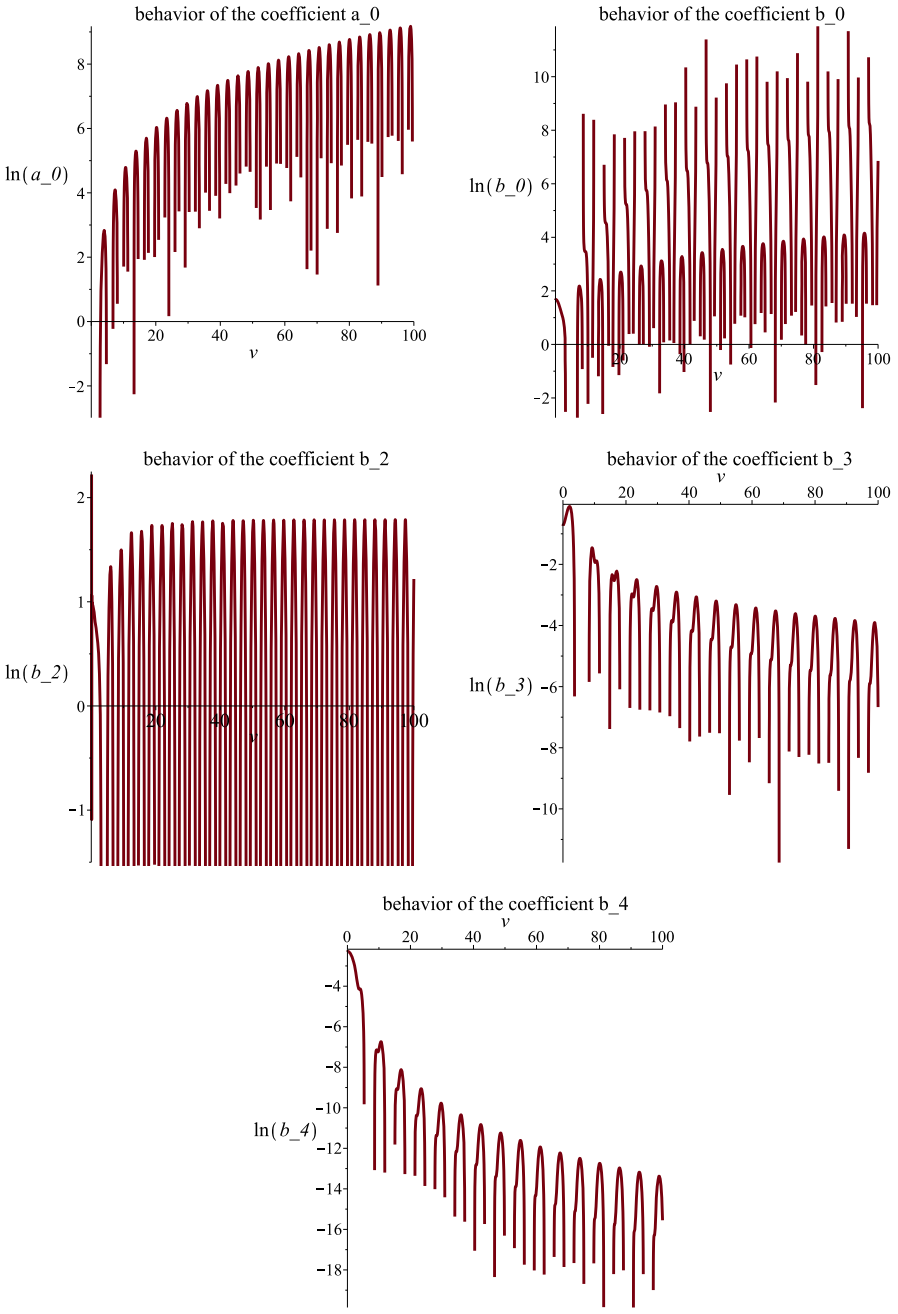

Fig. 4 Behavior of the coefficients of the new proposed method given by [20] for several values of $v = w\,h$

In Fig. 4 the behavior of the coefficients $a_0,\ b_j,\ j = 0, 2(1)4$ is presented

The finally proposed method is the predictor–corrector method (12) with the coefficients given by (20)–(21).

The LTE of this new proposed method (mentioned as $PCMeth8$) is given by:

$$LTE_{PCMeth8} = \frac{13789\,h^{10}}{84672000}\left(y_n^{(10)} + 5\,w^2\,y_n^{(8)} + 10\,w^4\,y_n^{(6)} + 10\,w^6\,y_n^{(4)} + 5w^8\,y_n^{(2)} + w^{10}\,y_n\right) + O\left(h^{12}\right) \tag{22}$$

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

5 Comparative error analysis

In this section the following methods will be investigated :

5.1 Classical predictor–corrector explicit four-step method, i.e. the method [12] with constant coefficients

$$LTE_{CL} = \frac{13789\,h^{10}}{84672000}\,y_n^{(10)} + O\left(h^{12}\right) \tag{23}$$

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

$$LTE_{PCMeth8} = \frac{13789\,h^{10}}{84672000}\left(y_n^{(10)} + 5\,w^2\,y_n^{(8)} + 10\,w^4\,y_n^{(6)} + 10\,w^6\,y_n^{(4)} + 5w^8\,y_n^{(2)} + w^{10}\,y_n\right) + O\left(h^{12}\right) \tag{24}$$

In the Fig. 5 we present the Flowchart of the algorithm on which we base our comparative LTE Analysis.

The formulae which are presented in the algorithm which is described in flowchart of the Fig. 5 and on which the computation of the new formulae of the LTE is based are given by:

$$y_n^{(2)} = (V(x) - V_c + G)\ y(x)$$
$$y_n^{(3)} = \left(\frac{d}{dx}g\,(x)\right)y\,(x) + (g\,(x) + G)\,\frac{d}{dx}y\,(x)$$

$$
\begin{aligned}
y_n^{(4)} &= \left(\frac{d^2}{dx^2}g\left(x\right)\right) y\left(x\right) + 2\left(\frac{d}{dx}g\left(x\right)\right)\frac{d}{dx}y\left(x\right) \\
&\quad + \left(g\left(x\right)+G\right)^2 y\left(x\right) \\
y_n^{(5)} &= \left(\frac{d^3}{dx^3}g\left(x\right)\right) y\left(x\right) + 3\left(\frac{d^2}{dx^2}g\left(x\right)\right)\frac{d}{dx}y\left(x\right) \\
&\quad + 4\left(g\left(x\right)+G\right) y\left(x\right)\frac{d}{dx}g\left(x\right) + \left(g\left(x\right)+G\right)^2\frac{d}{dx}y\left(x\right) \\
y_n^{(6)} &= \left(\frac{d^4}{dx^4}g\left(x\right)\right) y\left(x\right) + 4\left(\frac{d^3}{dx^3}g\left(x\right)\right)\frac{d}{dx}y\left(x\right) \\
&\quad + 7\left(g\left(x\right)+G\right) y\left(x\right)\frac{d^2}{dx^2}g\left(x\right) + 4\left(\frac{d}{dx}g\left(x\right)\right)^2 y\left(x\right) \\
&\quad + 6\left(g\left(x\right)+G\right)\left(\frac{d}{dx}y\left(x\right)\right)\frac{d}{dx}g\left(x\right) + \left(g\left(x\right)+G\right)^3 y\left(x\right) \\
y_n^{(7)} &= \left(\frac{d^5}{dx^5}g\left(x\right)\right) y\left(x\right) + 5\left(\frac{d^4}{dx^4}g\left(x\right)\right)\frac{d}{dx}y\left(x\right) \\
&\quad + 11\left(g\left(x\right)+G\right) y\left(x\right)\frac{d^3}{dx^3}g\left(x\right) + 15\left(\frac{d}{dx}g\left(x\right)\right) y\left(x\right)\frac{d^2}{dx^2}g\left(x\right) \\
&\quad + 13\left(g\left(x\right)+G\right)\left(\frac{d}{dx}y\left(x\right)\right)\frac{d^2}{dx^2}g\left(x\right) + 10\left(\frac{d}{dx}g\left(x\right)\right)^2\frac{d}{dx}y\left(x\right) \\
&\quad + 9\left(g\left(x\right)+G\right)^2 y\left(x\right)\frac{d}{dx}g\left(x\right) + \left(g\left(x\right)+G\right)^3\frac{d}{dx}y\left(x\right)
\end{aligned}
$$

$$
\begin{aligned}
y_n^{(8)} &= \left(\frac{d^6}{dx^6}g\left(x\right)\right) y\left(x\right) + 6\left(\frac{d^5}{dx^5}g\left(x\right)\right)\frac{d}{dx}y\left(x\right) \\
&\quad + 16\left(g\left(x\right)+G\right) y\left(x\right)\frac{d^4}{dx^4}g\left(x\right) + 26\left(\frac{d}{dx}g\left(x\right)\right) y\left(x\right)\frac{d^3}{dx^3}g\left(x\right) \\
&\quad + 24\left(g\left(x\right)+G\right)\left(\frac{d}{dx}y\left(x\right)\right)\frac{d^3}{dx^3}g\left(x\right) + 15\left(\frac{d^2}{dx^2}g\left(x\right)\right)^2 y\left(x\right) \\
&\quad + 48\left(\frac{d}{dx}g\left(x\right)\right)\left(\frac{d}{dx}y\left(x\right)\right)\frac{d^2}{dx^2}g\left(x\right) + 22\left(g\left(x\right)+G\right)^2 y\left(x\right)\frac{d^2}{dx^2}g\left(x\right) \\
&\quad + 28\left(g\left(x\right)+G\right) y\left(x\right)\left(\frac{d}{dx}g\left(x\right)\right)^2 \\
&\quad + 12\left(g\left(x\right)+G\right)^2\left(\frac{d}{dx}y\left(x\right)\right)\frac{d}{dx}g\left(x\right) + \left(g\left(x\right)+G\right)^4 y\left(x\right)
\end{aligned}
$$

...

We will study two cases for the value of E:

– The Energy (E) bf is closed to the potential, i.e., $G = V_c - E \approx 0$. Consequently, there aren't terms of the LTE which have non zero powers of G (i.e. G^j,

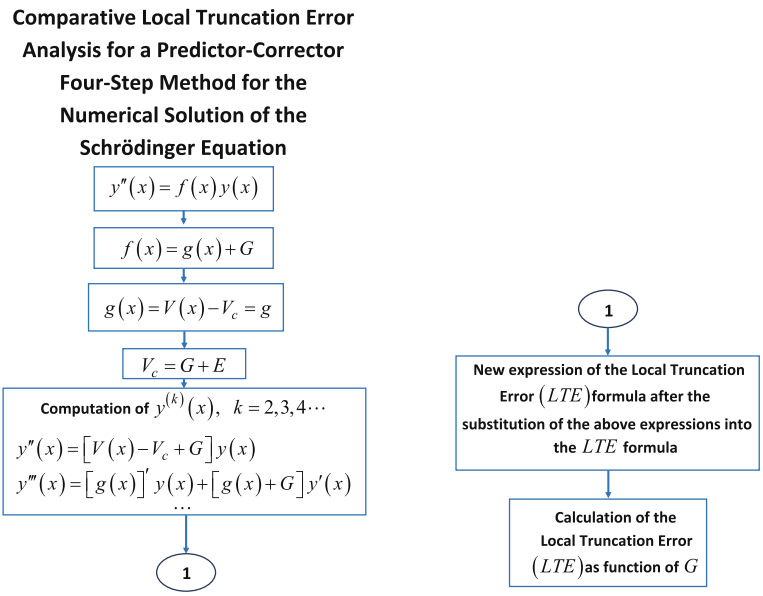

Fig. 5 Flowchart of the algorithm for the computations on the comparative error analysis

$j \neq 0$). Therefore, only the free of G terms of the formulae of the LTE exist. Since the evaluated methods are of the same form it is easy for one to see that the free of G terms of the methods are the same in both cases (of the classical methods (methods with constant coefficients) and of the methods with vanished the phase-lag and its derivatives). Consequently, the error for the two kind of methods: (1) classical methods (methods with constant coefficients) and (2) methods with vanished the phase-lag and its derivatives, will be approximately the same.

– For the quantity G we have: $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number. Here the expressions of the formulae of the LTE are different for the numerical methods of the same family [classical methods (methods with constant coefficients) and (2) methods with vanished the phase-lag and its derivatives].

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

5.3 Classical method

$$LTE_{CL} = h^{10}\left(\frac{13789\, y\,(x)}{84672000}\right) G^5 + \cdots + O\left(h^{12}\right) \tag{25}$$

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

$$LTE_{PCMeth8} = h^{10}\left(\frac{13789\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}g\left(x\right)\right)y\left(x\right)}{5292000}\right)G^2 + \cdots + O\left(h^{12}\right) \quad (26)$$

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

Theorem 2 *The analysis presented above gives us the following conclusions:*

- *For the classical predictor–corrector explicit four-step method the error increases as the fifth power of G.*
- *For the predictor–corrector explicit four-step method with vanished phase-lag and its first, second, third and fourth derivatives developed in Sect. 4, the error increases as the second 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, second, third and fourth 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 Fig. 6 we present the flowchart of the algorithm which describes the procedure for the sability analysis of the new proposed predictor–corrector high algebraic order symmetric explicit four-step method.

We will investigate the new proposed predictor–corrector symmetric explicit four-step method (12) with the coefficients given by (13) and (20).

If we apply the above described method to the scalar test equation:

$$y'' = -z^2\, y \quad (27)$$

we have the following difference equation:

$$A_2\left(s,v\right)\,\left(q_{n+2}+q_{n-2}\right) + A_1\left(s,v\right)\,\left(q_{n+1}+q_{n-1}\right) + A_0\left(s,v\right)\,q_n = 0 \quad (28)$$

where

$$A_2\left(s,v\right) = 1,\; A_1\left(s,v\right) = \frac{1}{10}\,\frac{T_{15}}{T_{16}}\,A_0\left(s,v\right) = \frac{1}{5}\,\frac{T_{17}}{T_{16}} \quad (29)$$

where $s = z\,h$ and $T_k,\; k = 15(1)17$ are given in Supplement Material C.

Remark 8 The frequency of the scalar test Eq. (27) for the stability analysis, z is different than the frequency of the scalar test Eq. (7) for the phase-lag analysis, w, is different than , i.e. $z \neq w$.

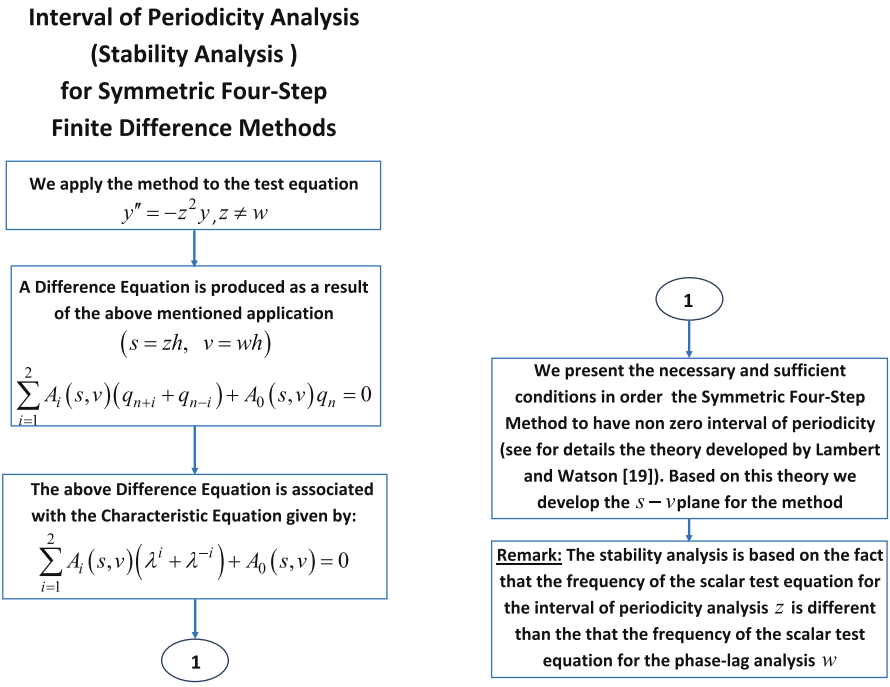

Fig. 6 Flowchart for the stability analysis of the new proposed predictor–corrector high algebraic order symmetric explicit four-step method

There is an associated characteristic equation to the difference Eq. (28) which is :

$$A_2(s, v)\left(\lambda^4 + 1\right) + A_1(s, v)\left(\lambda^3 + \lambda\right) + A_0(s, v)\ \lambda^2 = 0 \tag{30}$$

Definition 1 (see [19]) A symmetric $2k$-step method with the characteristic equation given by (9) 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 λ_i, $i = 1(1)4$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)},\ |\lambda_i| \leq 1,\ i = 3, 4, \cdots \tag{31}$$

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. $s = v$.

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

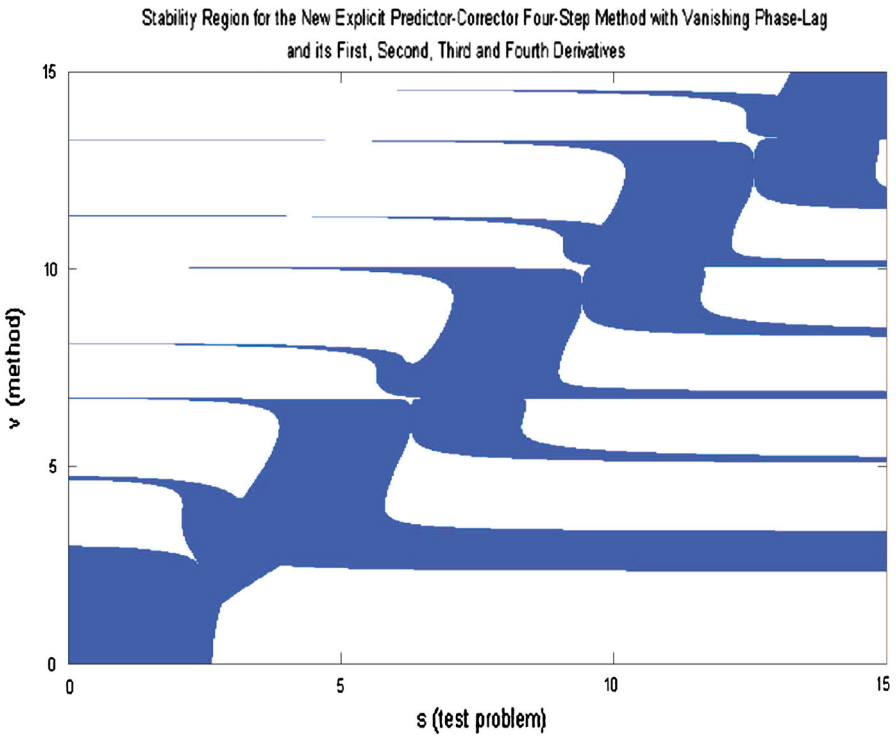

Fig. 7 $s - v$ plane of the predictor–corrector symmetric explicit four-step method [12] with the coefficients given by [13, 20]

In Fig. 7, we present the $s - v$ plane of the new proposed predictor–corrector four-step method. The shadowed area of the the $s - v$ region is the stable area, while the white area is the unstable area.

Remark 9 The study of the stability of these category of methods requires the division of the problems for which these methods can be applied into two categories:

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

The Schrödinger equation and related problems are belonged into the second category of problems described above.

For the first category of problems we have to develop the $s - v$ plane in order to investigate the stability of the proposed method (see Fig. 7 for our new produced predictor–corrector symmetric four-step method).

For the second category of problems we have to observe the surroundings of the first diagonal of the $s - v$ plane.

Studying the second category of problems, i.e. studying 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 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 eighth algebraic order,*
- *has the phase-lag and its first, second, third and fourth 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

The approximate solution of the one-dimensional time-independent Schrödinger Eq. (1) is used for our numerical experiments

Remark 10 Since the new obtained predictor–corrector symmetric four-step method is belonging to the case of frequency dependent algorithms, it is easy for one to see that the determination of the value of parameter w (frequency) is a necessity. This is because it is necessary for the application of the developed method to the approximate solution of the one-dimensional Schrödinger equation. For our problem and model given by (1) the parameter w (frequency) is given by (for the case $l = 0$):

$$w = \sqrt{|V(x) - k^2|} = \sqrt{|V(x) - E|} \tag{32}$$

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

7.1 Woods–Saxon potential

Since we use the approximate solution of the time-independent one-dimensional Schrödinger Eq. (1) for our numerical experiments and since the mathematical model of this equation uses a function, named potential, it is easy for one to see that the definition of the potential is necessary in order to proceed in the programming of the solution of this problem. For our numerical tests, we use the Woods–Saxon potential. This potential can be written as

$$V(x) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{33}$$

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

In Fig. 8 we present the Woods–Saxon potential.

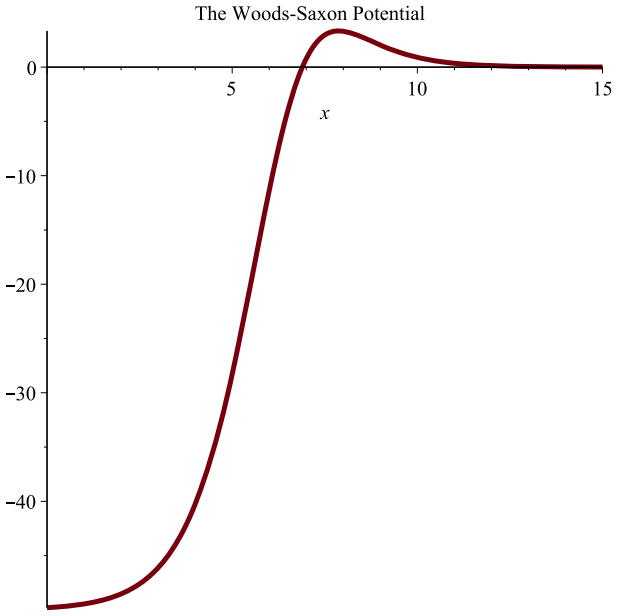

Fig. 8 The Woods–Saxon potential

In the literature several methodologies has been introduced for the determination of the frequency w, which is necessary for the frequency dependent methods—see begin of this section—(see [26] and references therein). The below described method is used for our numerical tests (see for details [107]).

More specifically, in order to determine the frequency w , the values of the potential on some critical points are used. The critical points mentioned above are determined from the study of the specific potential.

Remark 11 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 w as follows (see for details [1] and [82]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5-h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5+h \\ \sqrt{E}, & \text{for } x \in [6.5+2h, 15] \end{cases} \tag{34}$$

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

7.2 One-dimensional (radial) Schrödinger equation: the resonance problem

Our numerical experiments are based on the approximation solution of the one-dimensional (radial) time independent Schrödinger Eq. (1) with Woods–Saxon potential (33).

The above mentioned problem is belonged to the second order boundary value problems and has an infinite interval of integration. It is well known that in these cases we have to approximate the infinite interval of integration by a finite one. For our numerical experiments the integration interval $x \in [0, 15]$ is considered. Additionally for our numerical tests we use a large domain of energies, i.e., $E \in [1, 1000]$.

Remark 12 In the case of positive energies, $E = k^2$ the term $\frac{l(l+1)}{r^2}$ decays much slower that the potential.

Based on the above remark the radial Schrödinger equation effectively reduces to:

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(r) = 0 \tag{35}$$

for x greater than some value X.

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

$$\begin{aligned} y(x) &\approx Akxj_l(kx) - Bkrn_l(kx) \\ &\approx AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{36}$$

where δ_l is the phase shift that may be calculated from the formula

$$\tan\delta_l = \frac{p(r_2)S(r_1) - p(r_1)S(r_2)}{p(r_1)C(r_1) - p(r_2)C(r_2)} \tag{37}$$

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 $S(r) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. For the initial-value problems (the radial Schrödinger equation is treated as an initial-value problem) we need $y_j,\ j = 0(1)3$ before starting a four-step method. The initial condition defines the first value of y i.e. y_0. Using high order Runge–Kutta–Nyström methods(see [113,114]) we determine the values $y_i,\ i = 1(1)3$. Now we have all the necessary initial values and we can compute at r_2 of the asymptotic region the phase shift δ_l.

For positive energies, we have the so-called resonance problem. This problem consists either : (1) of finding the phase-shift δ_l or (2) 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:

$$y(0) = 0, \;\; y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{38}$$

The positive eigenenergies 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 [25] with minimal phase-lag, 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 [24] with minimal phase-lag, 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 NMPCPL4DV.

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

$$Err = |E_{calculated} - E_{accurate}| \tag{39}$$

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.

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

[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.

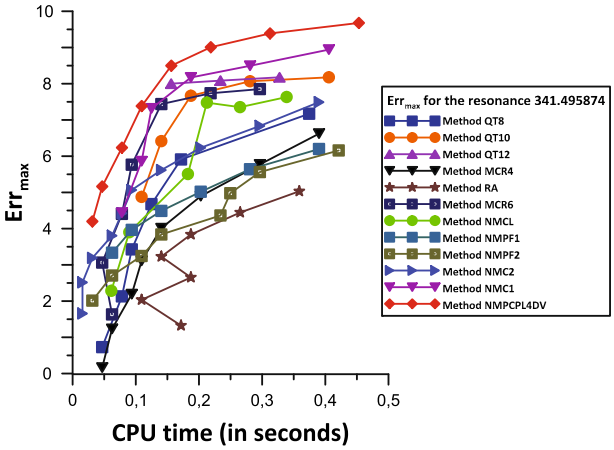

Fig. 9 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

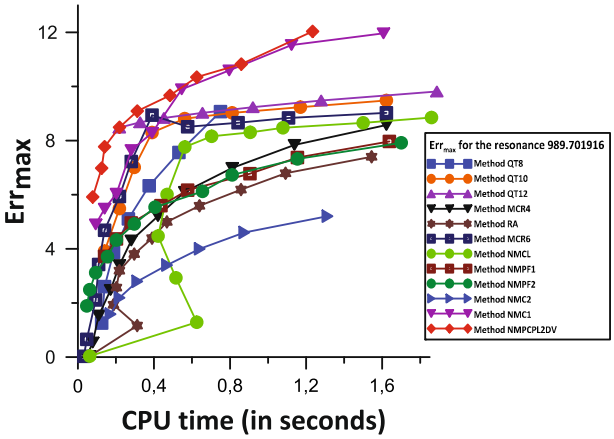

Fig. 10 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

8 Conclusions

In this paper we investigated a predictor–corrector four-step method of eighth algebraic order. We obtained the above method together with with vanishing the phase-lag and its first, second, third and fourth derivatives. We mention here that the investigation of the method was done as one block method. We studied the effect of the vanishing of the phase-lag and its derivatives on the computational effectiveness of the produced method.

Additionally we investigated

– the comparative LTE analysis and

– the stability analysis (using scalar test equation with frequency different than the frequency of the phase-lag analysis)

Finally, the computational effectiveness of the obtained method was studied via numerical tests on the approximate 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 [25] with minimal phase-lag, 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 [25] with minimal phase-lag, 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, third and fourth derivatives (obtained in Sect. 4), which is indicated as Method NMPCPL4DV, 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).

Conflict of interest The authors declare that they have no conflict of interest.

Ethical Standard Consent to submit has been received explicitly from all co-authors, as well as from the responsible authorities—tacitly or explicitly—at the institute/organization where the work has been carried out, before the work is submitted.

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