J Math Chem (2013) 51:2542–2571
DOI 10.1007/s10910-013-0227-7

ORIGINAL PAPER

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

Ibraheem Alolyan · T. E. Simos

Received: 28 June 2013 / Accepted: 8 July 2013 / Published online: 25 July 2013

Abstract In this paper we present a new methodology for the development of four-step hybrid type methods of sixth algebraic order with vanished phase-lag and its derivatives. The methodology is based on the vanishing of the phase-lag and its derivatives on its level of the hybrid method. We present a comparative error and stability analysis for the produced new method. The efficiency of the new obtained methods is examined by application to the resonance problem of the Schrödinger equation.

Keywords Numerical solution · Schrödinger equation · Multistep methods · Hybrid methods · Runge–Kutta type methods · Interval of periodicity · P-stability · Phase-lag · Phase-fitted · Derivatives of the phase-lag

---

T. E. Simos: 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 European Academy of Arts, Sciences and Humanities.

I. Alolyan
Chair of Actuarial and Applied Mathematics, Department of Mathematics, College of Sciences, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

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

T. E. Simos
Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, 221 00 Tripoli, Greece

T. E. Simos (✉)
10 Konitsis Street, Amfithea—Paleon Faliron, 175 64 Athens, Greece
e-mail: tsimos.conf@gmail.com

1 Introduction

1.1 Description of the problem and of the new proposed method

The numerical solution of second order initial or boundary value problems of the form:

$$q''(r) = f(r, q(r)) \tag{1}$$

with periodical and/or oscillating solutions is investigated in this paper. We note that there are many real problems in physics and chemistry with mathematical models which are expressed as initial or boundary value problems if the above mentioned category (for example the Schrödinger's equation).

More specifically in this paper we study a new methodology for the construction of efficient four-step hybrid type methods. The subjects of the study are:

- The development of numerical hybrid methods (i.e. methods with more that one stage) with vanished of the phase-lag and its derivatives on each level of the hybrid method
- The vanishing of the phase-lag and its derivatives on each level of the method
- How the above vanishing affects the efficiency of the obtained numerical scheme and finally
- If the above methodology produces more efficient methods than the vanishing of the phase-lag and its derivatives in the whole of the method (and not on each stage).

The methods constructed with the methodology presented in this paper are very effective not only to problems with oscillatory and / or periodic behavior of the solution but also to problems with solution which contains the functions cos and sin or to problems with solution that is a combination of the functions cos and sin.

The main objective of the research presented here is to determine, following the new presented methodology mentioned above, a hybrid type two-stage four-step method with the following properties:

- the highest possible algebraic order
- the phase-lag vanished on each stage of the method
- the first derivative of the phase-lag vanished on each stage of the method as well

The satisfaction of the above objectives requires the determination of the phase-lag and its first derivative. Using the literature of [1] and [2], Simos and co-authors has determined a direct formula for the computation of the phase-lag for a $2m$-method. Based on this formula we will calculate also the first derivative of the phase-lag.

The efficiency of the algorithm which will be developed using the new methodology presented above, will be investigated with the following studies:

- the comparative study of the local truncation error of the new produced method with other methods of the same form (comparative error analysis),
- the study of the stability analysis of the new obtained method and
- the results obtained by the application of the new produced method to the resonance problem of the one-dimensional time independent Schrödinger equation (see for more details [3]).

The format of the paper is given below:

- In Sect. 2 we present the phase-lag analysis of symmetric $2k$-methods.
- The new hybrid two-stage four-step method is developed in Sect. 3.
- In Sect. 4 we develop the comparative error analysis.
- The stability properties of the new obtained method are studied in Sect. 5.
- In Sect. 6, the numerical results are presented.
- Finally, remarks and conclusions are presented in Sect. 7.

1.2 Bibliography of the research subject

The aim and scope of the research subject is the development of efficient and credible numerical methods for the numerical solution of the second order initial or boundary value problems of the form (1) (see for example [1,3–100]). Examples of the problems which are faced are: the radial Schrödinger equation, the N-body problem etc.

The main research areas during the last decades on the above presented research subject was:

- Phase-fitted methods and numerical methods with minimal phase-lag
- Exponentially and trigonometrically fitted Runge–Kutta and Runge–Kutta Nyström methods
- Multistep phase-fitted methods and multistep methods with minimal phase-lag
- Symplectic integrators
- Exponentially and trigonometrically fitted multistep methods
- Nonlinear methods

In the following we present some bibliography on these areas:

1. Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta Nyström type have been obtained in [4–10].
2. In [11–16] exponentially and trigonometrically fitted Runge–Kutta and Runge–Kutta Nyström methods are constructed.
3. Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [1,3,21–43].
4. Symplectic integrators are investigated in [44–72].
5. Exponentially and trigonometrically fitted multistep methods have been produced in [73–93].
6. Nonlinear methods have been studied in [94] and [95]
7. Review papers have been presented in [96–100]
8. Special issues and Symposia in International Conferences have been developed on this subject (see [101–104])

2 Study of the phase-lag for finite difference symmetric 2 p-step methods

We consider the numerical solution of the initial or boundary value problem of the form (1).

In order to study the approximate solution of the above mentioned problem we divide the interval of integration $[a, b]$ into $p + 1$ equally spaced intervals $\{x_i\}_{i=0}^{p}$.

For the numerical solution of the above mentioned problem we consider a p-step method which is applied over the above mentioned intervals using the step-size $h = |x_{i+1} - x_i|$, $i = 0(1)p - 1$. We will study the case of symmetric 2 p-step methods i.e. the case for which: $a_i = a_{p-i}$, $b_i = b_{p-i}$, $i = 0(1)\frac{p}{2}$.

In order to investigate the phase-lag for the above mentioned symmetric 2 p-step method, the following algorithm must be followed:

1. Application of the symmetric 2 p-step method to the scalar test equation

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

2. The above application leads to the following difference equation

$$A_p(v)\, q_{n+p} + \cdots + A_1(v)\, q_{n+1} + A_0(v)\, q_n + A_1(v)\, q_{n-1} + \cdots + A_p(v)\, q_{n-p} = 0 \tag{3}$$

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

3. The above difference equation (3) corresponds to the following characteristic equation The equation given by:

$$A_p(v)\, \lambda^p + \cdots + A_1(v)\, \lambda + A_0(v) + A_1(v)\, \lambda^{-1} + \cdots + A_p(v)\, \lambda^{-p} = 0 \tag{4}$$

4. Based on the above mentioned polynomials $A_0(v)$, $A_1(v)$, …, $A_p(v)$ the following theorem has been proved (see [24] and [26])

Theorem 1 [24] *and* [26] *The symmetric* $2m$*-step method with characteristic equation given by* (4) *has phase-lag order* q *and phase-lag constant* c *given by:*

$$-c\, v^{q+2} + O\left(v^{q+4}\right) = \frac{2\, A_p\,(v)\, \cos\,(p\, v) + \cdots + 2\, A_j\,(v)\, \cos\,(j\, v) + \cdots + A_0\,(v)}{2\, p^2\, A_p\,(v) + \cdots + 2\, j^2\, A_j\,(v) + \cdots + 2\, A_1\,(v)} \tag{5}$$

Remark 1 The formula (5) is a direct method for the calculation of the phase-lag of any symmetric 2 p-step method.

3 Development of the new method

Let us consider the family of hybrid type symmetric four-step methods for the numerical solution of problems of the form $q'' = f\,(x, q)$:

$$\hat{q}_{n+2} = 2\, q_{n+1} - 2\, q_n + 2\, q_{n-1} - q_{n-2} + h^2 \left(b_0\, q''_{n+1} + b_1\, q''_n + b_0\, q''_{n-1}\right) q_{n+2} - 2\, q_{n+1}$$
$$+ 2\, q_n - 2\, q_{n-1} + q_{n-2} = h^2 \left[b_4\, \left(\hat{q}''_{n+2} + q''_{n-2}\right) + b_3\, \left(q''_{n+1} + q''_{n-1}\right) + b_2\, q''_n\right] \tag{6}$$

Notations for the above mentioned general family of methods:

1. the coefficient $b_i, i = 0(1)4$ are free parameters,
2. h is the step size of the integration,
3. n is the number of steps,
4. q_n is the approximation of the solution on the point x_n
5. $x_n = x_0 + n\,h$ and
6. x_0 is the initial value point.

3.1 First level of the hybrid method

Let us now consider the first level of the above mentioned method:

$$q_{n+2} - 2\,q_{n+1} + 2\,q_n - 2\,q_{n-1} + q_{n-2} = h^2\left(b_0\,q''_{n+1} + b_1\,q''_n + b_0\,q''_{n-1}\right) \quad (7)$$

Applying the above part of the method (7) to the scalar test equation (2), this leads to the difference equation (3) with $p = 2$ and $A_j(v),\ j = 0,\ 1,\ 2$ given by:

$$\begin{aligned} A_2\,(v) = 1,\ A_1\,(v)\ &=\ -2 + v^2\,b_0 \\ A_0\,(v) = 2 + v^2\,b_1 & \end{aligned} \quad (8)$$

Requiring the above method to have the phase-lag and its first derivative vanished, the following system of equations is obtained (using the formulae (5) (for $p = 2$) and (8)):

$$\text{Phase-Lag} = \frac{1}{2}\,\frac{4\ (\cos(v))^2 - 4\ \cos(v) + 2\ \cos(v)\,v^2 b_0 + v^2 b_1}{2 + v^2 b_0} = 0 \quad (9)$$

$$\text{First Derivative of the Phase-Lag} = -\frac{T_0}{\left(2 + v^2 b_0\right)^2} = 0 \quad (10)$$

where

$$\begin{aligned} T_0 = {} & 8\ \cos(v)\sin(v) + 4\ \cos(v)\sin(v)\,v^2 b_0 - 4\ \sin(v) \\ & + \sin(v)\,v^4 {b_0}^2 - 8\ \cos(v)\,v\,b_0 - 2\,v\,b_1 + 4\,v\,b_0\,(\cos(v))^2 \end{aligned}$$

The coefficients of the first level of the proposed hybrid four-step methods are defined by the solution of the above system of Eqs. (9)–(10):

$$\begin{aligned} b_0 &= \frac{-2\,v\sin(2\,v) + 2\ \sin(v)\,v + 4\ \cos(v) - 2 - 2\ \cos(2\,v)}{\sin(v)\,v^3} \\ b_1 &= \frac{6\ \cos(v) + 2\ \cos(3\,v) + v\sin(3\,v) + \sin(v)\,v - 4 - 4\ \cos(2\,v)}{\sin(v)\,v^3} \end{aligned} \quad (11)$$

The formulae given by (11) are subject to heavy cancellations for some values of $|w|$. In this case the following Taylor series expansions should be used:

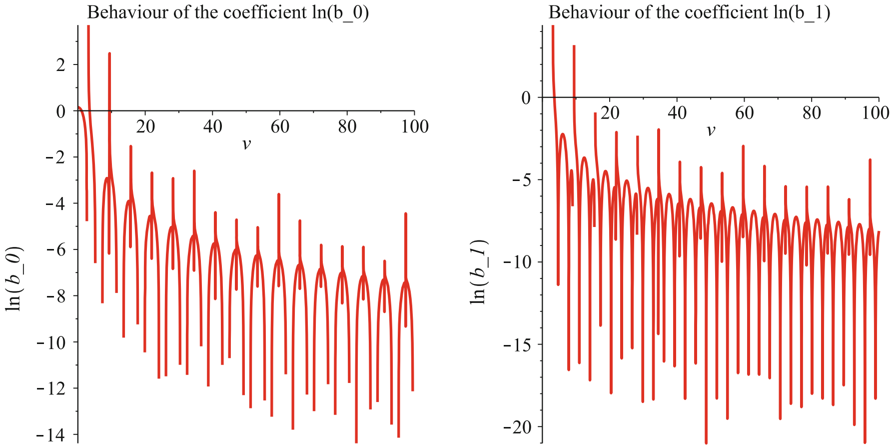

Fig. 1 Behavior of the coefficients of the new proposed method given by (11) for several values of $v = w\,h$

$$
\begin{aligned}
b_0 = {} & \frac{7}{6} - \frac{3}{20}\,v^2 + \frac{31}{10080}\,v^4 - \frac{47}{181440}\,v^6 - \frac{31}{1900800}\,v^8 - \frac{1097}{622702080}\,v^{10} \\
& - \frac{185869}{1046139494400}\,v^{12} - \frac{1067441}{59281238016000}\,v^{14} - \frac{221930509}{121645100408832000}\,v^{16} \\
& - \frac{4722116561}{2554547108585472000}\,v^{18} + \cdots \; b_1 = -\frac{1}{3} + \frac{3}{10}\,v^2 - \frac{409}{5040}\,v^4 + \frac{611}{90720}\,v^6 \\
& - \frac{2621}{6652800}\,v^8 + \frac{12973}{1556755200}\,v^{10} - \frac{235783}{373621248000}\,v^{12} - \frac{26441}{846874828800}\,v^{14} \\
& - \frac{45172549}{12164510040883200}\,v^{16} - \frac{4713203623}{1277273554292736000}\,v^{18} + \cdots
\end{aligned}
\tag{12}
$$

The behavior of the coefficients is given in the following Fig. 1.

3.2 Second level of the hybrid method

We consider now the second level of the proposed method (6):

$$
\begin{aligned}
& q_{n+2} - 2\,q_{n+1} + 2\,q_n - 2\,q_{n-1} + q_{n-2} \\
& \quad = h^2 \left(b_4\, q''_{n+2} + b_3\, q''_{n+1} + b_2\, q''_n + b_3\, q''_{n-1} + b_4\, q''_{n-2} \right)
\end{aligned}
\tag{13}
$$

where $b_2 = 2 - 2\,b_4 - 2\,b_3$ (Fig. 2).

If we apply the second level (13) to the scalar test equation (2), the difference equation (3) with $p = 2$ and $A_j(v), \;\; j = 0, \; 1, \; 2$ given by:

$$
\begin{aligned}
A_2\,(v) &= 1 + v^2\, b_4, \;\; A_1\,(v) \; = \; -2 + v^2\, b_3 \\
A_0\,(v) &= 2 + 2\,v^2 \left(1 - b_4 - b_3 \right)
\end{aligned}
\tag{14}
$$

is produced.

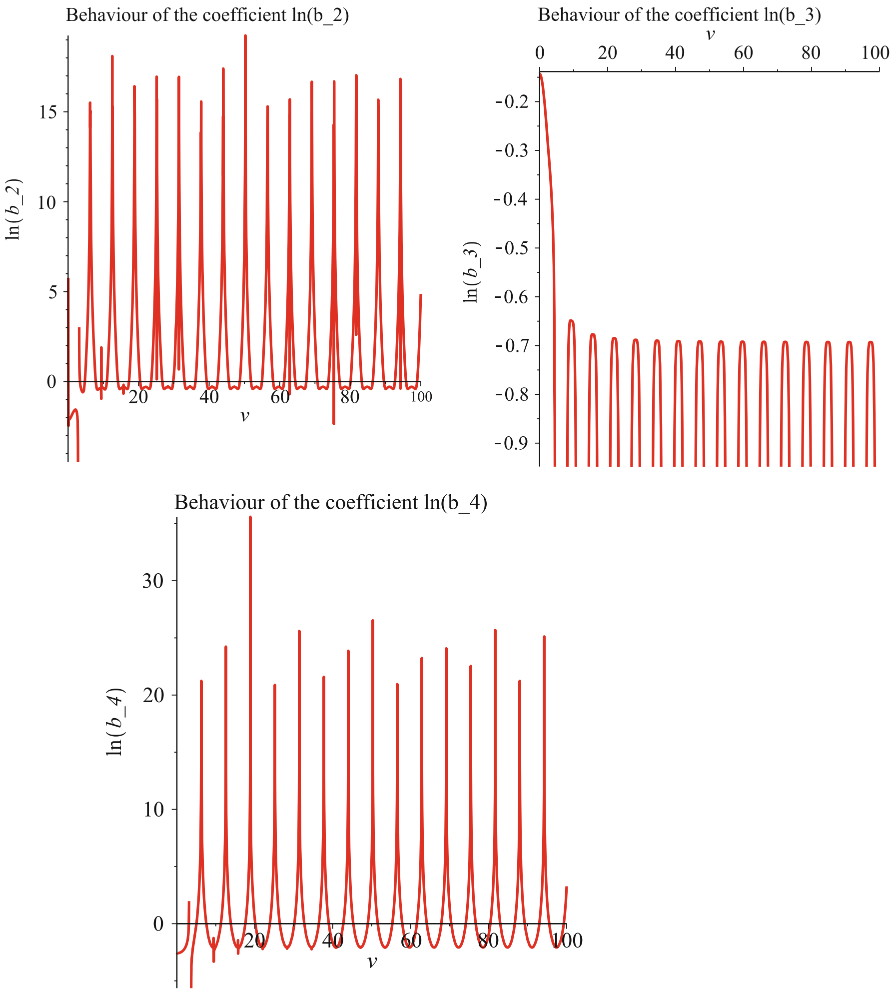

Fig. 2 Behavior of the coefficients of the new proposed method given by (17) for several values of $v = w\,h$

If now we require the above second level of the method (6) to have the phase-lag and its first derivative vanished, the following system of equations is obtained (using the formulae (5) (for $p = 2$) and (14)):

$$\text{Phase-Lag} = \frac{2\,(\cos(v))^2 + 2\,(\cos(v))^2\,v^2 b_4 + \cos(v)\,v^2 b_3 - 2\,\cos(v) - 2\,v^2 b_4 - v^2 b_3 + v^2}{2 + 4\,v^2 b_4 + v^2 b_3} = 0 \tag{15}$$

$$\text{First Derivative of the Phase-Lag} = -\frac{T_1}{\left(2 + 4\,v^2 b_4 + v^2 b_3\right)^2} = 0 \tag{16}$$

where

$$
\begin{aligned}
T_1 = & -4\,v - 4\,\sin(v) + 8\,\cos(v)\sin(v) + 24\,\cos(v)\,v^2 b_4 \sin(v) \\
& +4\,\cos(v)\sin(v)\,v^2 b_3 + 16\,\cos(v)\,v^4 {b_4}^2 \sin(v) + 4\,\sin(v)\,v^4 b_3 b_4 + 8\,v b_4 \\
& +4\,v b_3 + 8\,(\cos(v))^2\,v b_4 - 8\,\cos(v)\,v b_3 + \sin(v)\,v^4 {b_3}^2 - 8\,\sin(v)\,v^2 b_4 \\
& +4\,v\,(\cos(v))^2\,b_3 - 16\,v b_4 \cos(v) + 4\,\cos(v)\,v^4 b_4 \sin(v)\,b_3
\end{aligned}
$$

The coefficients of the second level of the proposed hybrid four-step methods are defined by the solution of the above system of Eqs. (15)–(16):

$$
\begin{aligned}
b_3 &= \frac{T_2}{-4\,v^3\cos(v) + 3\,v^3 + v^3\cos(2\,v)} \\
b_4 &= \frac{T_3}{4\,v^3\sin(2\,v) - 5\,\sin(v)\,v^3 - v^3\sin(3\,v)}
\end{aligned}
\tag{17}
$$

where

$$
\begin{aligned}
T_2 = & -4\,v^3\cos(v) + 6\,v + 2\,v\cos(2\,v) - 8\,v\cos(v) \\
& -2\,\sin(v) + 4\,\sin(2\,v) - 2\,\sin(3\,v) \\
T_3 = & \; v\sin(3\,v) + 5\,\sin(v)\,v + 14\,\cos(v) + 2\,\cos(3\,v) \\
& -2\,\sin(v)\,v^3 - 4\,v\sin(2\,v) - 8 - 8\,\cos(2\,v)
\end{aligned}
$$

The formulae given by (17) are subject to heavy cancellations for some values of $|w|$. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_3 = & \frac{13}{15} - \frac{19}{756}\,v^2 + \frac{113}{113400}\,v^4 - \frac{293}{29937600}\,v^6 - \frac{8213}{81729648000}\,v^8 \\
& - \frac{15563}{980755776000}\,v^{10} - \frac{128309}{166728481920000}\,v^{12} - \frac{7073837}{212878925715456000}\,v^{14} \\
& - \frac{273644387}{210750136458301440000}\,v^{16} - \frac{1539507169}{32315020923606220800000}\,v^{18} + \cdots \\
b_4 = & \frac{3}{40} + \frac{19}{3024}\,v^2 + \frac{139}{259200}\,v^4 + \frac{5771}{119750400}\,v^6 + \frac{271391}{59439744000}\,v^8 \\
& + \frac{135227}{301771008000}\,v^{10} + \frac{238998847}{5335311421440000}\,v^{12} + \frac{226149607}{50089158991872000}\,v^{14} \\
& + \frac{40514887351}{88736899561390080000}\,v^{16} + \frac{221316705139}{4787410507200921600000}\,v^{18} + \cdots
\end{aligned}
\tag{18}
$$

The behavior of the coefficients is given in the following Fig. 1.

The construction of this method is based on Flowchart mentioned in the Fig. 3.

The combination of the above two mentioned levels leads to the proposed method (6) with the coefficients given by (11)–(12) and (17)–(18). The local truncation error of this new proposed method (mentioned as $HybMethI$) is given by:

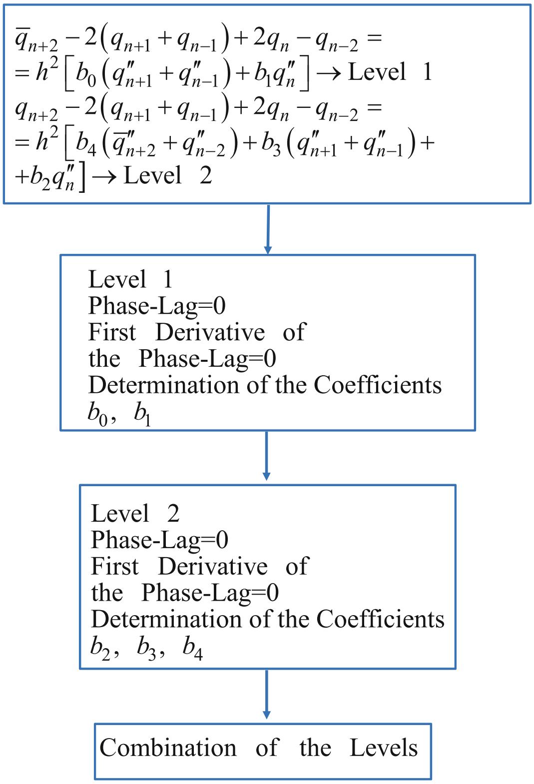

Fig. 3 Flowchart for the construction of the method

$$LTE_{HybMethI} = \frac{751\, h^8}{302400} \left(q_n^{(8)} + 2\, w^2\, q_n^{(6)} + w^4\, q_n^{(4)} \right) + O\left(h^{10}\right) \tag{19}$$

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

4 Comparative error analysis

We will study the following methods:

4.1 Classical method (i.e. the method (6) with constant coefficients)

$$LTE_{CL} = -\frac{751\, h^8}{302400}\, p_n^{(8)} + O\left(h^{10}\right) \tag{20}$$

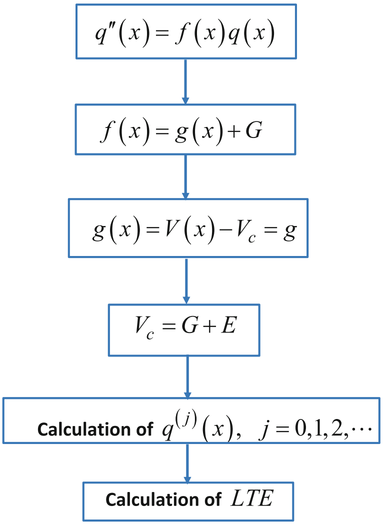

Fig. 4 Flowchart for the error analysis

4.2 The method with vanished phase-lag and its first and second derivatives developed in [3]

$$LTE_{MethI}=-\frac{751\,h^8}{302400}\left(p_n^{(8)}+3\,w^2\,p_n^{(6)}+3\,w^4\,p_n^{(4)}+w^6\,p_n^{(2)}\right)+O\left(h^{10}\right) \tag{21}$$

4.3 The new proposed hybrid method with vanished phase-lag and its first derivative in each level developed in Sect. 3

$$LTE_{MethII}=\frac{751\,h^8}{302400}\left(q_n^{(8)}+2\,w^2\,q_n^{(6)}+w^4\,q_n^{(4)}\right)+O\left(h^{10}\right) \tag{22}$$

Following the Flowchart mentioned in the Fig. 4, we develop the error analysis. Using the procedure described on the flowchart and the formulae:

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

$$
\begin{aligned}
q_n^{(6)} = & \left(\frac{d^4}{dx^4} g(x)\right) q(x) + 4 \left(\frac{d^3}{dx^3} g(x)\right) \frac{d}{dx} q(x) \\
& +7 \, (g(x) + G)\, q(x) \frac{d^2}{dx^2} g(x) + 4 \left(\frac{d}{dx} g(x)\right)^2 q(x) \\
& +6 \, (g(x) + G) \left(\frac{d}{dx} q(x)\right) \frac{d}{dx} g(x) + (g(x) + G)^3 q(x) \\
q_n^{(7)} = & \left(\frac{d^5}{dx^5} g(x)\right) q(x) + 5 \left(\frac{d^4}{dx^4} g(x)\right) \frac{d}{dx} q(x) \\
& +11 \, (g(x) + G)\, q(x) \frac{d^3}{dx^3} g(x) + 15 \left(\frac{d}{dx} g(x)\right) q(x) \frac{d^2}{dx^2} g(x) \\
& +13 \, (g(x) + G) \left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x) + 10 \left(\frac{d}{dx} g(x)\right)^2 \frac{d}{dx} q(x) \\
& +9 \, (g(x) + G)^2 q(x) \frac{d}{dx} g(x) + (g(x) + G)^3 \frac{d}{dx} q(x) \\
q_n^{(8)} = & \left(\frac{d^6}{dx^6} g(x)\right) q(x) + 6 \left(\frac{d^5}{dx^5} g(x)\right) \frac{d}{dx} q(x) \\
& +16 \, (g(x) + G)\, q(x) \frac{d^4}{dx^4} g(x) + 26 \left(\frac{d}{dx} g(x)\right) q(x) \frac{d^3}{dx^3} g(x) \\
& +24 \, (g(x) + G) \left(\frac{d}{dx} q(x)\right) \frac{d^3}{dx^3} g(x) + 15 \left(\frac{d^2}{dx^2} g(x)\right)^2 q(x) \\
& +48 \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x) + 22 \, (g(x) + G)^2 q(x) \frac{d^2}{dx^2} g(x) \\
& +28 \, (g(x) + G)\, q(x) \left(\frac{d}{dx} g(x)\right)^2 \\
& +12 \, (g(x) + G)^2 \left(\frac{d}{dx} q(x)\right) \frac{d}{dx} g(x) + (g(x) + G)^4 q(x) \ldots
\end{aligned}
$$

we produce the expressions of the Local Truncation Errors. For the methods mentioned above the expression can be found in the “Appendix 8”.

Two cases in terms of the value of E are studied during the investigation of the Local Truncation Errors:

- The Energy is close to the potential, i.e., $G = V_c - E \approx 0$. Consequently, the free terms of the polynomials in G are considered only. Thus, for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G are the same for the cases of the classical method and of the methods with vanished the phase-lag and its derivatives.
- $G >> 0$ or $G << 0$. Then $|G|$ is a large number.

Based on the analysis presented above, we have the following asymptotic expansions of the Local Truncation Errors:

4.4 Classical method

$$LTE_{CL} = h^8 \left(\frac{751}{302400} q(x)\ G^4 + \cdots \right) + O\left(h^{10}\right) \tag{23}$$

4.5 The method with vanished phase-lag and its first and second derivatives developed in [3]

$$LTE_{MethI} = h^8 \left[\left(\frac{751}{75600} \left(\frac{d^2}{dx^2} g(x) \right) q(x) \right) G^2 + \cdots \right] + O\left(h^{10}\right) \tag{24}$$

4.6 The new proposed method with vanished phase-lag and its first, second and third derivatives developed in Sect. 4

$$\begin{aligned} LTE_{MethII} = h^8 \Bigg[\Bigg(& \frac{751}{33600} \left(\frac{d^2}{dx^2} g(x) \right) q(x) + \frac{751}{151200} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) \\ & + \frac{751}{302400} \left(g(x)\right)^2 q(x) \Bigg) G^2 + \cdots \Bigg] + O\left(h^{10}\right) \end{aligned} \tag{25}$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Hybrid Four-Step Method the error increases as the fourth power of G. For the the method with vanished phase-lag and its first and second derivatives developed in* [3], *the error increases as the second power of G. For the new obtained method with vanished phase-lag and its first derivative in each level which developed in this paper, the error increases as the second power of G. So, for the numerical solution of the time independent radial Schrödinger equation the Method with Vanished Phase-Lag and its First, Second and Third Derivatives and the New Proposed Method with Vanished Phase-Lag and its First Derivative in each level are the most efficient and they have the same approximately behavior, from theoretical point of view, especially for large values of $|G| = |V_c - E|$.*

5 Stability analysis

Let us apply the new obtained method (6) with the coefficients given by (11)–(12) and (17)–(18) to the scalar test equation:

$$q'' = -z^2 q. \tag{26}$$

This leads to the following difference equation:

$$A_2(s, v)\ (q_{n+2} + q_{n-2}) + A_1(s, v)\ (q_{n+1} + q_{n-1}) + A_0(s, v)\ q_n = 0 \tag{27}$$

where

$$
\begin{aligned}
A_2(s, v) &= 1, \\
A_1(s, v) &= \frac{T_4}{\left((\cos(v))^3 - (\cos(v))^2 - \cos(v) + 1\right) v^6} \\
A_0(s, v) &= -2 \frac{T_5}{\left((\cos(v))^3 - (\cos(v))^2 - \cos(v) + 1\right) v^6}
\end{aligned} \tag{28}
$$

where

$$
\begin{aligned}
T_4 = &-4\,(\cos(v))^4 s^4 v^2 + 8 s^4 (\cos(v))^4 + 12 s^4 (\cos(v))^3 v \sin(v) \\
&-4\,\sin(v)\, v^3 s^2 (\cos(v))^3 - 2\,(\cos(v))^3 v^6 \\
&-16 s^4 (\cos(v))^3 + 6 s^4 v^2 (\cos(v))^3 \\
&+8 s^4 (\cos(v))^2 + 4\,\sin(v)\, v^3 s^2 (\cos(v))^2 + 2 s^4 v^4 (\cos(v))^2 \\
&-2 s^2 v^6 (\cos(v))^2 - 20 s^4 \sin(v)\, v\, (\cos(v))^2 \\
&+2 s^4 v^2 (\cos(v))^2 + 2 v^6 (\cos(v))^2 \\
&-6 s^4 v^2 \cos(v) - 2 s^4 \sin(v)\, v^3 \cos(v) + 8 s^4 \sin(v)\, v \cos(v) \\
&+s^4 v^4 \cos(v) - s^2 v^6 \cos(v) + 2 v^6 \cos(v) + 2 s^4 v^2 - 2 v^6 - s^4 v^4 + s^2 v^6 \\
T_5 = &-2 s^4 v^2 (\cos(v))^5 + 8 s^4 (\cos(v))^5 \\
&+8\,\sin(v)\, v s^4 (\cos(v))^4 + 2\,(\cos(v))^4 s^4 v^2 \\
&-16 s^4 (\cos(v))^4 + 8 s^4 (\cos(v))^3 - (\cos(v))^3 s^2 v^6 \\
&-(\cos(v))^3 v^6 - 4\,\sin(v)\, v^3 s^2 (\cos(v))^3 \\
&+(\cos(v))^3 s^4 v^4 - 12 s^4 (\cos(v))^3 v \sin(v) \\
&+2 s^4 v^2 (\cos(v))^3 + 4\,\sin(v)\, v^3 s^2 (\cos(v))^2 \\
&+4 s^4 \sin(v)\, v\, (\cos(v))^2 - 2 s^4 v^2 (\cos(v))^2 - 2 s^4 \sin(v)\, v^3 (\cos(v))^2 \\
&+v^6 (\cos(v))^2 - s^2 v^6 (\cos(v))^2 \\
&+s^4 v^4 (\cos(v))^2 + v^6 \cos(v) - v^6
\end{aligned}
$$

and $s = z\,h$.

Remark 2 The frequency of the scalar test equation (26), z, is not equal with the frequency of the scalar test equation (2), w, i.e. $z \neq w$.

The corresponding characteristic equation is given by:

$$
A_2(s, v)\left(\lambda^4 + 1\right) + A_1(s, v)\left(\lambda^3 + \lambda\right) + A_0(s, v)\,\lambda^2 = 0 \tag{29}
$$

Definition 1 (see [17]) A symmetric $2k$-step method with the characteristic equation given by (4) is said to have an *interval of periodicity* $\left(0, \mathrm{v}_0^2\right)$ if, for all $s \in \left(0, s_0^2\right)$, the roots $\lambda_i,\ i = 1(1)4$ satisfy

$$
\lambda_{1,2} = e^{\pm i\,\zeta(s)},\ |\lambda_i| \leq 1,\ i = 3, 4, \ldots \tag{30}
$$

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

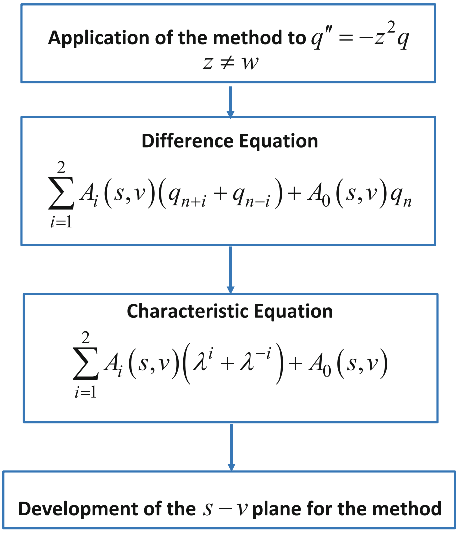

Fig. 5 Flowchart for the stability analysis

The Flowchart mentioned in the Fig. 5 presents the stability analysis.

Definition 2 (see [17]) 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. 6 we present the s–v plane for the method developed in this paper. A shadowed area denotes the s–v region where the method is stable, while a white area denotes the region where the method is unstable.

Remark 3 For the solution of the Schrödinger equation the frequency of the phase fitting is equal to the frequency of the scalar test equation. So, for this case of problems it is necessary to observe *the surroundings of the first diagonal of the s–v plane*.

We study now the case where the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $s = v$ (i.e. see the surroundings of the first diagonal of the s–v plane). Based on this study we extract the result that the interval of periodicity of the new method developed in Sect. 3 is equal to: (0, 15).

From the above analysis we have the following theorem:

Theorem 3 *The method developed in Sect. 3:*

- *is of sixth algebraic order,*
- *has the phase-lag and its first derivative equal to zero on the first level of the hybrid method*

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

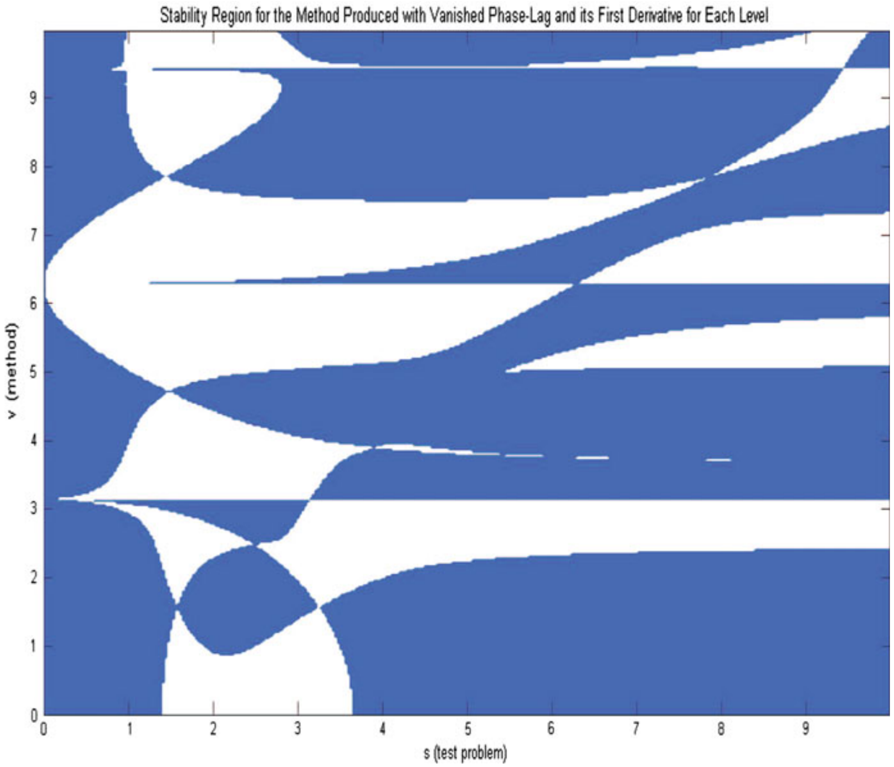

Fig. 6 s–v plane of the the new obtained method with vanished phase-lag and its first derivative in each level

- *has the phase-lag and its first derivative equal to zero on the second level of the hybrid method*
- *has an interval of periodicity equals to:* $(0, 15)$ *in the case where the frequency of the scalar test equation is equal with the frequency of phase fitting*

6 Numerical results

The approximate solution of the the one-dimensional time-independent Schrödinger equation is used in order to study the efficiency of the new proposed method.

The one dimensional time independent Schrödinger equation (see [105,106]):

$$q''(r) = [l(l+1)/r^2 + V(r) - k^2]q(r). \tag{31}$$

is a boundary value problem with one boundary condition given by:

$$q(0) = 0 \tag{32}$$

and a the other boundary condition, for large values of r, determined by physical conditions.

For completion point of view, we have to give the following definitions of the functions, quantities and parameters for the above mathematical model (31):

1. The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(x) \to 0$ as $x \to \infty$,
2. The quantity k^2 is a real number denoting *the energy*,
3. The quantity l is a given integer representing the *angular momentum*,
4. V is a given function which denotes the *potential*.

It is necessary the value of parameter w (mentioned above (see for example the notation after (3) and the formulae in Sect. 3) to be defined since the new proposed method is a frequency dependent method. The above definition is required in order the application of the new method to the radial Schrödinger equation to be possible. Based on (31), the parameter w is given by (for the case $l = 0$):

$$w = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{33}$$

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

6.1 Woods–Saxon potential

The well known Woods–Saxon potential is used for the purpose of our numerical application. We can write this potential as

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{34}$$

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. 7.

From the literature (see for details [99]) it is known that for some potentials, such as the Woods–Saxon potential, some critical points, which are defined from the investigation of the appropriate potential, are used in order parameter w to be defined.

For the purpose of obtaining our numerical results, it is appropriate to choose v as follows (see for details [73] and [107]):

$$w = \begin{cases} \sqrt{-50 + E}, & \text{for } r \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } r = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } r = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } r = 6.5 + h \\ \sqrt{E}, & \text{for } r \in [6.5 + 2h, 15] \end{cases} \tag{35}$$

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.

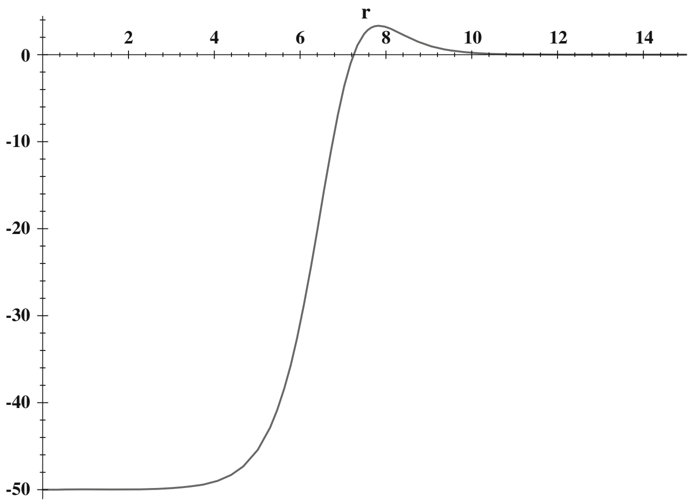

Fig. 7 The Woods–Saxon potential

6.2 Radial Schrödinger equation: the resonance problem

We consider the approximate solution of the one-dimensional time independent Schrödinger equation (31) in the known case of the Woods–Saxon potential (34) as a purpose of this application. In order to solve numerically this problem we have to approximate the true (infinite) interval of integration by a finite one. We take the integration interval $r \in [0, 15]$ for the purposes of our numerical experiments. We consider equation (31) in a rather large domain of energies, i.e., $E \in [1, 1000]$.

In the case of positive energies, $E = k^2$, the potential decays faster than the term $\frac{l(l+1)}{r^2}$ and the Schrödinger equation effectively reduces to

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{36}$$

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 Eq. (31) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{37}$$

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

$$\tan \delta_l = \frac{q(r_2)\,S(r_1) - q(r_1)\,S(r_2)}{q(r_1)\,C(r_1) - q(r_2)\,C(r_2)} \tag{38}$$

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 $C(r) = -kr n_l(kr)$. Since the problem is treated as an initial-value problem, we need $q_j,\ j = 0, (1)3$ before starting a four-step method. From the initial condition, we obtain q_0. The values $q_i,\ i = 1(1)3$ are obtained by using high order Runge–Kutta–Nyström methods(see [108] and [109]). With these starting values, we evaluate 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 of finding the phase-shift δ_l or finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$. We actually solve the latter problem, known as the resonance problem.

The boundary conditions for this problem are:

$$q(0) = 0,\ q(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{39}$$

We compute the approximate positive eigenenergies of the Woods–Saxon resonance problem using:

- The eighth order multi-step method developed by Quinlan and Tremaine [18], which is indicated as Method QT8.
- The tenth order multi-step method developed by Quinlan and Tremaine [18], which is indicated as Method QT10.
- The twelfth order multi-step method developed by Quinlan and Tremaine [18], which is indicated as Method QT12.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [23], which is indicated as Method MCR4
- The exponentially-fitted method of Raptis and Allison [74], which is indicated as Method MRA
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [22], which is indicated as Method MCR6
- The classical form of the sixth algebraic order four-step method developed in Sect. 4, which is indicated as Method NMCL.[2]
- The hybrid four-step method of sixth algebraic order with vanished phase-lag and its first and second derivatives (obtained in [3]), which is indicated as Method MPHD
- The new hybrid four-step method of sixth algebraic order with vanished phase-lag and its first derivative in each level (obtained in Sect. 3), which is indicated as Method HYBPLDEA
- The four-step method of sixth algebraic order with vanished phase-lag and its first derivative globally (obtained in "Appendix 9"), which is indicated as Method HYBPLDEAGLOB

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

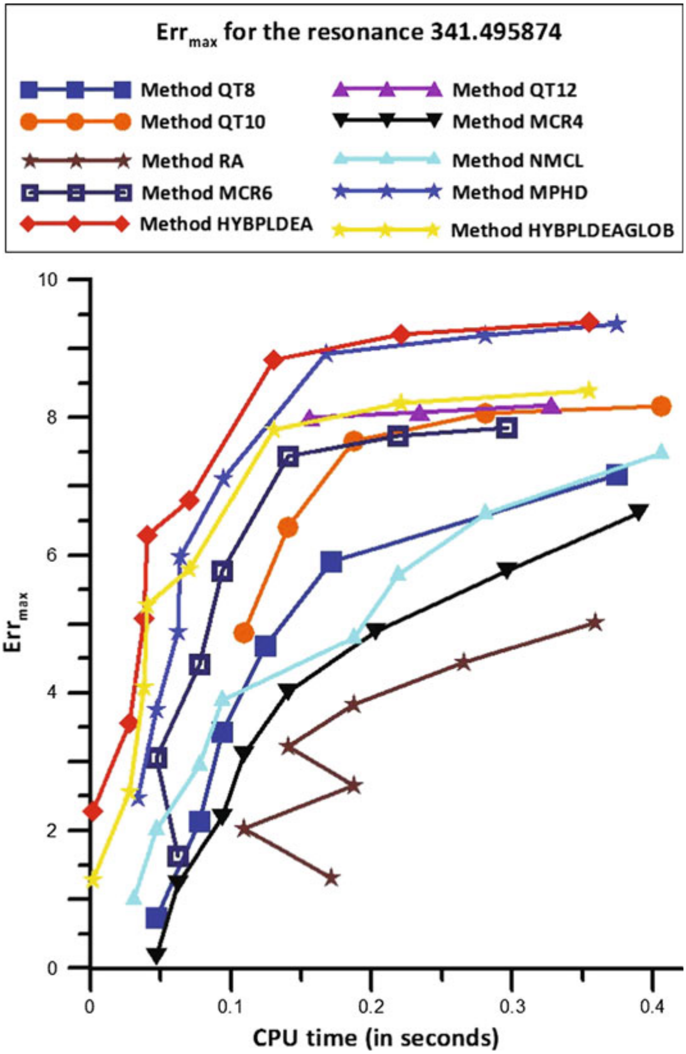

Fig. 8 Accuracy (digits) for several values of CPU Time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

The numerically calculated eigenenergies are compared with reference values.[3] In Figs. 8 and 9, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{40}$$

[3] The reference values are computed using the well known two-step method of Chawla and Rao [22] with small step size for the integration.

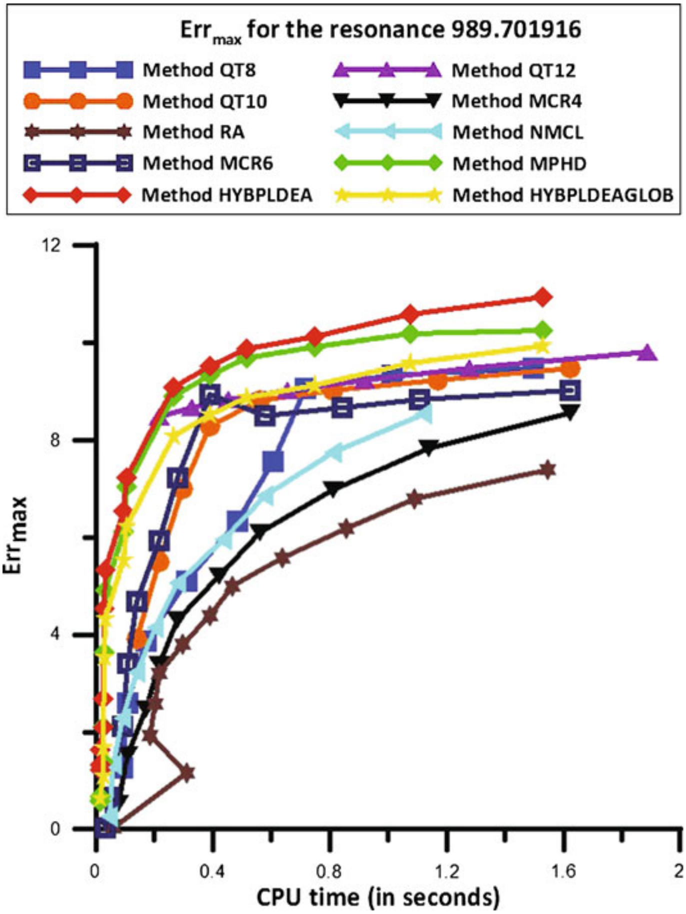

Fig. 9 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

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.

7 Conclusions

In this paper we presented a new methodology for the development of four-step hybrid type methods of sixth algebraic order with vanished phase-lag and its derivatives. This new methodology is based on the vanishing of the phase-lag and its derivatives in each level of the hybrid method. We have also investigated the influencing of the vanishing of the phase-lag and its first derivative on the efficiency of the above mentioned methods for the numerical solution of the radial Schrödinger equation and related problems. Based on the the above, a two-stage four-step sixth algebraic order methods with vanished phase-lag and its first derivative in each level was obtained. This new method is very efficient on any problem with oscillating solutions or problems with solutions contain the functions cos and sin or any combination of them.

From the results presented 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 [23], which is indicated as Method MCR4. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [74], which is indicated as Method MRA.
2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [18], which is indicated as Method QT10 is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [23], 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 [18], which is indicated as Method QT8. Finally, the Method QT10 is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [22], which is indicated as Method MCR6 for large CPU time and less efficient than the Method MCR6 for small CPU time.
3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [18], which is indicated as Method QT12 is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [18], which is indicated as Method QT10
4. The hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first and second derivatives (obtained in [3]), which is indicated as Method MPHD is more efficient than all the methods mentioned above.
5. The four-step method of sixth algebraic order with globally vanished phase-lag and its first derivative (obtained in "Appendix 9"), which is indicated as Method HYBPLDEAGLOB is more efficient than all the methods mentioned above except the hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first and second derivatives (obtained in [3]), which is indicated as Method MPHD.
6. The new hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first derivative in each level of the method (obtained in Sect. 3), which is indicated as Method HYBPLDEA 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).

8 Appendix A

8.1 New method with vanished phase-lag and its first derivative in each level (developed in Sect. 3)

$$\begin{aligned}
\mathrm{LTE}_{\mathrm{HYBPLDEA}} = h^8 \Bigg[& \Bigg(\frac{751}{33600} \left(\frac{d^2}{dx^2} g(x) \right) q(x) + \frac{751}{151200} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) \\
& + \frac{751}{302400} (g(x))^2 q(x) \Bigg) G^2 + \Bigg(\frac{751}{21600} \left(\frac{d^4}{dx^4} g(x) \right) q(x) \\
& + \frac{751}{18900} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} q(x) \\
& + \frac{751}{25200} g(x) \left(\frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) + \frac{751}{10080} g(x) q(x) \frac{d^2}{dx^2} g(x) \\
& + \frac{751}{15120} \left(\frac{d}{dx} g(x) \right)^2 q(x) + \frac{751}{151200} (g(x))^3 q(x) \Bigg) G \\
& + \frac{751}{302400} \left(\frac{d^6}{dx^6} g(x) \right) q(x) + \frac{751}{50400} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} q(x) \\
& + \frac{751}{18900} g(x) q(x) \frac{d^4}{dx^4} g(x) + \frac{751}{20160} \left(\frac{d^2}{dx^2} g(x) \right)^2 q(x) \\
& + \frac{9763}{151200} \left(\frac{d}{dx} g(x) \right) q(x) \frac{d^3}{dx^3} g(x) \\
& + \frac{751}{12600} g(x) \left(\frac{d}{dx} q(x) \right) \frac{d^3}{dx^3} g(x) \\
& + \frac{751}{25200} (g(x))^2 \left(\frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) \\
& + \frac{751}{6300} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} q(x) \right) \frac{d^2}{dx^2} g(x) \\
& + \frac{8261}{151200} (g(x))^2 q(x) \frac{d^2}{dx^2} g(x) + \frac{751}{10800} g(x) q(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{751}{302400} (g(x))^4 q(x) \Bigg]
\end{aligned} \tag{41}$$

9 Appendix B

9.1 Development of the corresponding method (6) with vanished phase-lag and its first derivative as a global method

Consider the method (6) with

$$b_2 = 2 - 2\,b_4 - 2\,b_3 \tag{42}$$

Applying this method to the scalar test equation (2), this leads to the difference equation (3) with $p = 2$ and $A_j(v),\ \ j = 0,\ 1,\ 2$ given by:

$$A_2(v) = -2 + v^2 \left(b_4 \left(2 - \frac{7}{6} v^2 \right) + b_3 \right)$$
$$A_0(v) = 2 - 4\, b_4 v^2 + \frac{1}{3} v^4 b_4 + 2\, v^2 - 2\, v^2 b_3 \tag{43}$$

Requiring the above method to have the phase-lag and its first derivative vanished, the following system of equations is produced (using the formulae (5) (for $p = 2$) and (8)):

$$\text{Phase-Lag} = -\frac{T_6}{-12 - 12\, b_4 v^2 + 7\, v^4 b_4 - 6\, v^2 b_3} = 0 \tag{44}$$

$$\text{First Derivative of the Phase-Lag} = \frac{T_7}{\left(-12 - 12\, b_4 v^2 + 7\, v^4 b_4 - 6\, v^2 b_3\right)^2} = 0 \tag{45}$$

where

$$\begin{aligned}
T_6 = {} & 12\ (\cos(v))^2 - 12\ \cos(v) + 12\ \cos(v)\, b_4 v^2 \\
& -7\ \cos(v)\, v^4 b_4 + 6\ \cos(v)\, v^2 b_3 - 12\, b_4 v^2 + v^4 b_4 + 6\, v^2 - 6\, v^2 b_3 \\
T_7 = {} & 144\, v - 288\ \cos(v)\sin(v)\, b_4 v^2 + 168\ \cos(v)\sin(v)\, v^4 b_4 \\
& -144\ \cos(v)\sin(v)\, v^2 b_3 - 144\ \sin(v)\, b_4 v^4 b_3 + 84\ \sin(v)\, v^6 b_4 b_3 \\
& -288\ \cos(v)\sin(v) - 144\, {b_4}^2 v^5 + 84\, v^5 b_4 - 288\, b_4 v + 48\, v^3 b_4 \\
& -144\, v b_3 - 288\, v\,(\cos(v))^2\, b_4 - 144\, v\,(\cos(v))^2\, b_3 + 336\ (\cos(v))^2\, b_4 v^3 \\
& +576\ \cos(v)\, b_4 v - 672\ \cos(v)\, v^3 b_4 + 288\ \cos(v)\, v b_3 - 144\ \sin(v)\, {b_4}^2 v^4 \\
& +168\ \sin(v)\, {b_4}^2 v^6 - 49\ \sin(v)\, v^8 {b_4}^2 - 36\ \sin(v)\, v^4 {b_3}^2 - 72\, v^5 b_4 b_3 \\
& +144\ \sin(v)
\end{aligned}$$

Solving the above system of Eqs. (44)–(45) we obtain the coefficients of method:

$$b_3 = \frac{T_8}{-12\, v^5 \sin(2\, v) + 14\ \cos(v)\, v^4 - 14\, v^4 \cos(3\, v) - 24\ \sin(v)\, v^5 - 4\, v^4 + 4\, v^4 \cos(2\, v)}$$
$$b_4 = \frac{T_9}{24\, v^5 \cos(v) + 18\, v^5 + 6\, v^5 \cos(2\, v) - 12\, v^4 \sin(2\, v) - 7\, v^4 \sin(3\, v) - 3\, v^4 \sin(v)} \tag{46}$$

where

$$\begin{aligned}
T_8 = {} & 24 - 28\, v^2 - 48\ \cos(v) + 20\, v^4 - 24\ \cos(4\, v) + 24\, v \sin(3\, v) \\
& -72\, v \sin(v) - 8\, v^2 \cos(3\, v) - 12\, v \sin(4\, v) \\
& +24\, v \sin(2\, v) + 28\, v^4 \cos(2\, v) + 8\ \cos(v)\, v^2 + 7\, v^3 \sin(4\, v)
\end{aligned}$$

$$
\begin{aligned}
&+34\,v^3 \sin(2\,v) + 10\,v^3 \sin(3\,v) + 28\,v^2 \cos(4\,v) \\
&-14\,v^5 \sin(2\,v) + 48\,\cos(v)\,v^4 + 66\,\sin(v)\,v^3 \\
&-28\,\sin(v)\,v^5 + 48\,\cos(3\,v) \\
T_9 =\ & 6\,\sin(4\,v) - 12\,\sin(2\,v) + 24\,\cos(v)\,v^3 \\
&+18\,v^3 + 6\,v^3 \cos(2\,v) - 9\,v - 3\,v\cos(4\,v) + 12\,v\cos(2\,v)
\end{aligned}
$$

The formulae given by (46) are subject to heavy cancellations for some values of $|w|$. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_3 =\ & \frac{13}{15} + \frac{751}{37800}\,v^2 - \frac{13183}{4536000}\,v^4 + \frac{2051099}{20956320000}\,v^6 \\
&- \frac{18538909}{8172964800000}\,v^8 - \frac{161500511}{6865290432000000}\,v^{10} \\
&- \frac{6304721869}{2334198746880000000}\,v^{12} - \frac{99206807572601}{614687898003379200000000}\,v^{14} \\
&- \frac{364118197589}{36016869023635500000000}\,v^{16} \\
&- \frac{1842607971683867}{2923958569366074240000000000}\,v^{18} + \cdots \\
b_4 =\ & \frac{3}{40} - \frac{751}{151200}\,v^2 + \frac{137}{1296000}\,v^4 - \frac{17819}{5239080000}\,v^6 \\
&- \frac{159571}{2043241200000}\,v^8 - \frac{83869147}{13730580864000000}\,v^{10} \\
&- \frac{5215749839}{1400519248128000000}\,v^{12} - \frac{3570319431619}{153671974500844800000000}\,v^{14} \\
&- \frac{53380779263761}{36881273880202752000000000}\,v^{16} \\
&- \frac{37973153075648473}{421050033988714690560000000000}\,v^{18} + \cdots
\end{aligned}
\qquad (47)
$$

The behavior of the coefficients is given in the following Fig. 10.

In Fig. 11 we present the s–v plane for the method developed in the “Appendix 9”. A shadowed area denotes the s–v region where the method is stable, while a white area denotes the region where the method is unstable.

For the case where the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $s = v$ (i.e. see the surroundings of the first diagonal of the s–v plane), the interval of periodicity of the method presented in “Appendix 9” is equal to: (0, 11), i.e. the interval of periodicity of the new proposed method in Sect. 3 is larger ((0, 15)) than the the interval of periodicity of the method presented in “Appendix 9”.

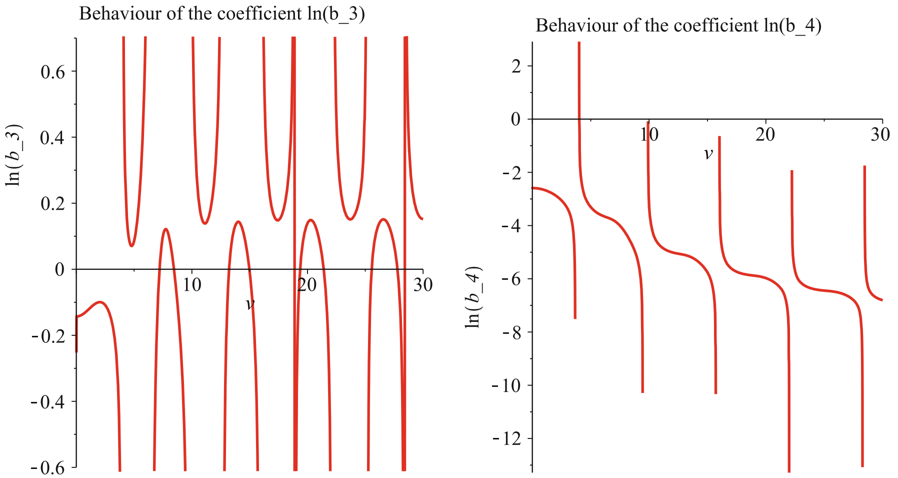

Fig. 10 Behavior of the coefficients of the new proposed method given by (46) for several values of $v = w\,h$

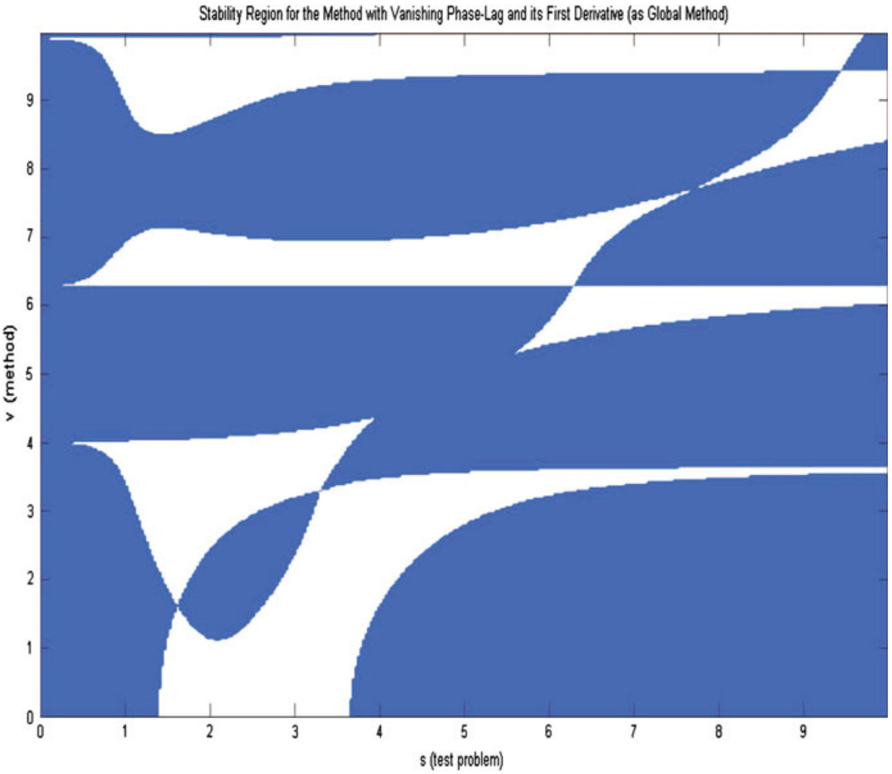

Fig. 11 s–v plane of the the method obtained in the "Appendix 9" with vanished phase-lag and its first derivative as global method

10 Appendix C: Implementation of the new proposed method

Consider the method (6). The implementation of this new method is based on the following algorithm:

$$
\begin{aligned}
M_n &= 2\,q_{n+1} - 2\,q_n + 2\,q_{n-1} - q_{n-2} \\
\hat{q}_{n+2} &= M_n + h^2 \Big(b_0\, q''_{n+1} + b_1\, q''_n + b_0\, q''_{n-1} \Big) \\
q_{n+2} &= M_n + h^2 \left[b_4\, \left(\hat{q}''_{n+2} + q_{n-2}\right) + b_3\, \left(q_{n+1} + q_{n-1}\right) + b_2\, q_n \right]
\end{aligned}
\tag{48}
$$

References

1. 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)
2. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
3. I. Alolyan, T.E. Simos, A new four-step Runge–Kutta type method with vanished phase-lag and its first, second and third derivatives for the numerical solution of the Schrödinger equation. J. Math. Chem. **51**(5), 1418–1445 (2013)
4. 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)
5. 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)
6. 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)
7. 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)
8. D.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)
9. Th Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic Runge–Kutta–Nyström methods. Appl. Math. Inf. Sci. **7**(1), 81–85 (2013)
10. 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)
11. 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)
12. 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)
13. 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)
14. Ch. Tsitouras, T.E. Simos, Optimized Runge–Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
15. 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)
16. 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)
17. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
18. G.D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits. Astron. J. **100**, 1694–1700 (1990)

19. Ch. Tsitouras, ITh Famelis, T.E. Simos, On modified Runge–Kutta trees and methods. Comput. Math. Appl. **62**(4), 2101–2111 (2011)
20. http://burtleburtle.net/bob/math/multistep.html
21. 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)
22. 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)
23. 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)
24. 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)
25. 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)
26. 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)
27. 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)
28. 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)
29. T.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)
30. 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)
31. H. 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)
32. H. Van de Vyver, An explicit Numerov-type method for second-order differential equations with oscillating solutions. Comput. Math. Appl. **53**, 1339–1348 (2007)
33. T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation. J. Math. Chem. **46**(3), 981–1007 (2009)
34. 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)
35. 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)
36. 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)
37. 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. **2012** Article ID 420387 (2012)
38. 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)
39. 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)
40. 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)
41. 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

42. 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. Part I: construction and theoretical analysis. J. Math. Chem. **51**(1), 194–226 (2013)
43. A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation. J. Math. Chem. **47**(2), 871–890 (2010)
44. 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)
45. 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)
46. 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)
47. 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)
48. 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)
49. 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)
50. 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)
51. Z. Kalogiratou, T.E. Simos, Newton–Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
52. 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)
53. 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 (2008a)
54. 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 (2008b)
55. 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 (2008c)
56. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for numerical integration of the Schrödinger equation. Comput. Lett. **3**(1), 45–57 (2007)
57. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. RevMexAA **42**(2), 167–177 (2006)
58. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for long-time integration. Int. J. Mod. Phys. C **14**(8), 1061–1074 (2003)
59. T.E. Simos, New closed Newton–Cotes type formulae as multilayer symplectic integrators. J. Chem. Phys. **133**(10) Article Number: 104108 (2010)
60. T.E. Simos, New stable closed Newton–Cotes trigonometrically fitted formulae for long-time integration. Abstr. Appl. Anal. Article Number: 182536 (2012a). doi:10.1155/2012/182536
61. 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)
62. 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) (2013a). doi:10.1142/S0129183113500149
63. T.E. Simos, New open modified Newton Cotes type formulae as multilayer symplectic integrators. Appl. Math. Model. **37**(4), 1983–1991 (2013b)
64. G. Vanden Berghe, M. Van Daele, Exponentially fitted open Newton Cotes differential methods as multilayer symplectic integrators. J. Chem. Phys. **132**, 204107 (2010)
65. Z. Kalogiratou, T. Monovasilis, T.E. Simos, A fifth-order symplectic trigonometrically fitted partitioned Runge–Kutta method. International Conference on Numerical Analysis and Applied Mathematics, Sept. 16–20, 2007 Corfu, Greece. Numerical Analysis and Applied Mathematics. in *AIP Conference Proceedings*, vol. 936 (2007), pp. 313–317

66. 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)
67. T. Monovasilis, T.E. Simos, Symplectic methods for the numerical integration of the Schrödinger equation. Comput. Mater. Sci. **38**(3), 526–532 (2007)
68. 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), 563–573 (2008)
69. 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)
70. 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)
71. K. Tselios, T.E. Simos, Optimized fifth order symplectic integrators for orbital problems. Revista Mexicana de Astronomia y Astrofisica **49**(1), 11–24 (2013)
72. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Symplectic partitioned Runge–Kutta methods with minimal phase-lag. Comput. Phys. Commun. **181**(7), 1251–1254 (2010)
73. L.Gr 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)
74. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
75. 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)
76. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor–corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
77. 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)
78. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. Appl. Math. Lett. **17**(5), 601–607 (2004)
79. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. Acta Applicandae Mathematicae **110**(3), 1331–1352 (2010)
80. 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)
81. 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)
82. T.E. Simos, Exponentially—fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
83. 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)
84. H. Van de Vyver, A trigonometrically fitted explicit hybrid method for the numerical integration of orbital problems. Appl. Math. Comput. **189**(1), 178–185 (2007)
85. 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)
86. 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)
87. 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)
88. 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)
89. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**(3), 162–174 (2005)
90. 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)
91. 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)

92. C. Tang, W. Wang, H. Yan, Z. Chen, High-order predictorcorrector of exponential fitting for the N-body problems. J. Comput. Phys. **214**(2), 505–520 (2006)
93. 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)
94. 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)
95. 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)
96. 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)
97. 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)
98. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
99. L.Gr 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)
100. 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)
101. 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), 165–165 (2006)
102. 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), IX–IX (2005)
103. 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), IX–IX (2003)
104. 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)
105. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
106. I. Prigogine, S. Rice (eds.), *Advances in Chemical Physics Vol. 93: New Methods in Computational Quantum Mechanics* (Wiley, New York, 1997)
107. LGr Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
108. 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)
109. J.R. Dormand, P.J. Prince, A family of embedded Runge Kutta formulae. J. Comput. Appl. Math. **6**, 19–26 (1980)