J Math Chem (2009) 46:981–1007
DOI 10.1007/s10910-009-9553-1

ORIGINAL PAPER

A new Numerov-type method for the numerical solution of the Schrödinger equation

T. E. Simos

Received: 1 December 2006 / Accepted: 30 September 2008 / Published online: 22 July 2009

Abstract In the present paper we develop a new methodology for the development of efficient numerical methods for the approximate solution of the one-dimensional Schrödinger equation. The new methodology is based on the requirement that the phase-lag and its derivatives to be vanished. The efficiency of the new methodology is proved via error analysis and numerical results.

Keywords Numerical solution · Schrödinger equation · Multistep methods · Hybrid methods · P-stability · Phase-lag · Phase-fitted

1 Introduction

The one-dimensional Schrödinger equation can be written as:

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

T. E. Simos is an active member of the European Academy of Sciences and Arts, active member of the European Academy of Sciences and corresponding member of European Academy of Arts, Sciences and Humanities.

T. E. Simos
Laboratory of Computational Sciences, Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, 221 00 Tripolis, Greece

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

Many problems in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics, etc. can be express via the above boundary value problem (see for example [23,24,41,48]).

We give the definitions of some terms in (1):

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

The boundary conditions are:

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

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

The last years an extended research on the construction of numerical algorithms for the solution of the Schrödinger equation has been done. The aim of this research is the development of fast and reliable methods for the solution of the Schrödinger equation and related problems (see for example [1–12,14–22,25–40,43–47,49–59,61–114]).

We can divide the numerical methods for the approximate solution of the Schrödinger equation and related problems into two main categories:

1. Methods with constant coefficients
2. Methods with coefficients depending on the frequency of the problem.[1]

In this paper, we introduce a new methodology for the development of efficient numerical methods for the numerical solution of the radial Schrödinger equation and related problems. The new methodology is based on the requirement of vanishing of the phase-lag and its derivatives. The efficiency of the new methodology will be studied via the error analysis and the application of the new developed method to the approximate solution of the one-dimensional Schrödinger equation.

More specifically, we will develop a hybrid Numerov-type methods of eighth algebraic order. The development of the method is based on the requirement of vanishing of the phase-lag and its derivatives. We will investigate the stability and the error of the new produced method. Finally, we will apply the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The paper is organized as follows. In Sect. 2 we present the theory of the new methodology. In Sect. 3 we present the development of the new method. The error analysis is presented in Sect. 4. In Sect. 5, we will study the stability properties of the new constructed methods. In Sect. 6 the numerical results are presented. Finally, in Sect. 7 remarks and conclusions are discussed.

[1] When using a functional fitting algorithm for the solution of the radial Schrödinger equation, the fitted frequency is equal to: $\sqrt{|l(l+1)/x^2 + V(x) - k^2|}$.

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

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

consider a multistep method with m steps which can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)m - 1$.

If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

When a symmetric $2k$-step method, that is for $i = -k(1)k$, is applied to the scalar test equation

$$y'' = -\omega^2 y \tag{4}$$

a difference equation of the form

$$\begin{aligned} &A_k(H)\, y_{n+k} + \cdots + A_1(H)\, y_{n+1} + A_0(H)\, y_n \\ &\quad + A_1(H)\, y_{n-1} + \cdots + A_k(H)\, y_{n-k} = 0 \end{aligned} \tag{5}$$

is obtained, where $H = \omega h$, h is the step length and $A_0(H), A_1(H), \ldots, A_k(H)$ are polynomials of H.

The characteristic equation associated with (5) is given by:

$$A_k(H)\, \lambda^k + \cdots + A_1(H)\, \lambda + A_0(H) + A_1(H)\, \lambda^{-1} + \cdots + A_k(H)\, \lambda^{-k} = 0 \tag{6}$$

Theorem 1 [92] *The symmetric $2k$-step method with characteristic equation given by (6) has phase-lag order q and phase-lag constant c given by*

$$\begin{aligned} &-c\, H^{q+2} + O\left(H^{q+4}\right) \\ &\quad = \frac{2\, A_k(H)\, \cos(k\, H) + \cdots + 2\, A_j(H)\, \cos(j\, H) + \cdots + A_0(H)}{2\, k^2\, A_k(H) + \cdots + 2\, j^2\, A_j(H) + \cdots + 2\, A_1(H)} \end{aligned} \tag{7}$$

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric $2k$-step method.

3 The new Numerov-type hybrid method—construction of the new method

$$\begin{aligned} &\overline{y}_n = y_n - a_0\, h^2\, \left(y''_{n+1} - 2\, y''_n + y''_{n-1}\right) - 2\, a_1\, h^2\, y''_n \\ &y_{n+1} + c_1\, y_n + y_{n-1} = h^2\, \left[b_0\, \left(y''_{n+1} + y''_{n-1}\right) + b_1 \overline{y}''_n\right] \end{aligned} \tag{8}$$

Application of the above method to the scalar test Eq. 4 gives the following difference equation:

$$A_1(H)\, y_{n+1} + A_0(H)\, y_n + A_1(H)\, y_{n-1} = 0$$

where $H = \omega h$, h is the step length and $A_0(H)$ and $A_1(H)$ are polynomials of H.

The characteristic equation associated with (9) is given by:

$$A_1(H)\, \lambda + A_0(H) + A_1(H)\, \lambda^{-1} = 0 \tag{9}$$

where

$$A_1(H) = 1 + H^2\, b_0 + H^4\, b_1\, a_0$$
$$A_0(H) = c_1 + H^2\, b_1 - 2\, H^4\, b_1\, a_0 + 2\, H^4\, b_1\, a_1$$

Applying the formula (7) with $k = 1$ we have that the phase-lag is equal to:

$$\text{phl} = \frac{2A_1(H)\cos(H) + A_0(H)}{2A_1(H)} = \frac{1}{2}\frac{T_0}{T1} \tag{10}$$

where $T_0 = 2\left(1 + H^2 b_0 + H^4 b_1 a_0\right)\cos(H) + c_1 + H^2 b_1 - 2H^4 b_1 a_0 + 2H^4 b_1 a_1$ and $T_1 = 1 + H^2 b_0 + H^4 b_1 a_0$.

the first derivative of the phase-lag is given by:

$$\dot{\text{phl}} = \frac{T_2}{T_3} \tag{11}$$

where:

$$T_2 = -\Big(2c_1 b_1 a_0 H^3 + \sin(H) H^8 {b_1}^2 {a_0}^2 - 2H^5 b_1 a_1 b_0 + 2H^5 b_1 a_0 b_0 + 2\sin(H) H^4 b_1 a_0 - 4H^3 b_1 a_1 + 4H^3 b_1 a_0 - H b_1 + \sin(H) + 2\sin(H) H^2 b_0 + \sin(H) H^4 {b_0}^2 + H^5 {b_1}^2 a_0 + 2\sin(H) H^6 b_0 b_1 a_0 + H c_1 b_0\Big)$$

and

$$T_3 = \left(1 + H^2 b_0 + H^4 b_1 a_0\right)^2$$

the second derivative of the phase-lag can be written as:

$$\ddot{\text{phl}} = \frac{T_4}{T_5} \tag{12}$$

where:

$$T_4 = -\Big(3\cos(H) H^8 {b_1}^2 {a_0}^2 + 3\cos(H) H^4 b_1 a_0 + 3\cos(H) H^4 {b_0}^2 + 3\cos(H) H^2 b_0 + 6\cos(H) H^6 b_0 b_1 a_0 + H^6 {b_1}^2 a_0 b_0 - 6H^8 {b_1}^2 {a_0}^2 b_0 + 2H^6 b_1 a_0 {b_0}^2 - 2H^6 b_1 a_1 {b_0}^2 - 10 c_1 {b_1}^2 {a_0}^2 H^6 - 9 c_1 b_1 a_0 H^4 b_0 + 6H^8 {b_1}^2 a_1 b_0 a_0$$

$$- 3H^8 {b_1}^3 {a_0}^2 - 3c_1 {b_0}^2 H^2 + \cos(H) H^6 {b_0}^3 + \cos(H) H^{12} {b_1}^3 {a_0}^3 + 3\cos(H) H^{10} {b_1}^2 {a_0}^2 b_0 + 3\cos(H) H^8 {b_0}^2 b_1 a_0 - b_1 + 12 b_1 a_0 H^2 + 20 H^6 {b_1}^2 a_1 a_0 + 6 c_1 b_1 a_0 H^2 - 6 H^4 b_1 a_1 b_0 + 6 H^4 b_1 a_0 b_0 + 12 H^4 {b_1}^2 a_0 + \cos(H) - 12 H^2 b_1 a_1 + c_1 b_0 + 3 H^2 b_1 b_0 - 20 H^6 {b_1}^2 {a_0}^2 \Big)$$

and

$$T_5 = \left(1 + H^2 b_0 + H^4 b_1 a_0\right)^3 .$$

the third derivative of the phase-lag can be written as:

$$\dddot{\text{phl}} = \frac{T_6}{T_7} \tag{13}$$

where:

$$T_6 = \Big(-12 H^{11} {b_1}^4 {a_0}^3 - 12 c_1 {b_0}^3 H^3 + 12 H^9 {b_1}^3 {a_0}^2 b_0 + 24 H^9 {b_1}^2 {a_0}^2 {b_0}^2 - 24 H^{11} {b_1}^3 {a_0}^3 b_0 - 60 c_1 {b_1}^3 {a_0}^3 H^9 - 120 H^9 {b_1}^3 {a_0}^3 + 12 H^3 b_1 {b_0}^2 + \sin(H) H^8 {b_0}^4 - 24 H^9 {b_1}^2 a_1 {b_0}^2 a_0 + 4\sin(H) H^{14} {b_1}^3 {a_0}^3 b_0 + 4\sin(H) H^{10} {b_0}^3 b_1 a_0 + 6\sin(H) H^{12} {b_1}^2 {a_0}^2 {b_0}^2 + 48 H^5 {b_1}^2 a_0 b_0 + 96 H^7 {b_1}^2 {a_0}^2 b_0 + 12\sin(H) H^{10} {b_1}^2 {a_0}^2 b_0 + 24 H^3 b_1 a_0 b_0 + 6\sin(H) H^8 {b_1}^2 {a_0}^2 + 4\sin(H) H^4 b_1 a_0 + 120 c_1 {b_1}^2 {a_0}^2 H^5 + \sin(H) + \sin(H) H^{16} {b_1}^4 {a_0}^4 + 72 c_1 b_1 a_0 H^3 b_0 - 96 H^7 {b_1}^2 a_1 b_0 a_0 - 24 H^3 b_1 a_1 b_0 + 12 c_1 {b_0}^2 H - 60 H^3 {b_1}^2 a_0 + 4\sin(H) H^6 {b_0}^3 + 24 H b_1 a_1 + 120 H^7 {b_1}^3 {a_0}^2 - 12 H b_1 b_0 - 24 b_1 a_0 H + 240 H^5 {b_1}^2 {a_0}^2 + 4\sin(H) H^2 b_0 + 6\sin(H) H^4 {b_0}^2 + 12\sin(H) H^6 b_0 b_1 a_0 - 72 c_1 {b_1}^2 {a_0}^2 H^7 b_0 - 48 c_1 b_1 a_0 H^5 {b_0}^2 + 24 H^{11} {b_1}^3 a_1 b_0 {a_0}^2 + 120 H^9 {b_1}^3 a_1 {a_0}^2 + 12\sin(H) H^8 {b_0}^2 b_1 a_0 - 12 c_1 b_1 a_0 H + 4\sin(H) H^{12} {b_1}^3 {a_0}^3 - 240 H^5 {b_1}^2 a_1 a_0\Big)$$

and

$$T_7 = \left(1 + H^2 b_0 + H^4 b_1 a_0\right)^4$$

and finally the fourth derivative of the phase-lag can be written as:

$$\ddddot{\text{phl}} = \frac{T_8}{T_9} \tag{14}$$

where:

$$T_8 = \Big(10\cos(H) H^8 {b_1}^2 {a_0}^2 + 5\cos(H) H^4 b_1 a_0 + 10\cos(H) H^4 {b_0}^2 + 5\cos(H) H^2 b_0$$

$$+ 20\cos(H)H^6 b_0 b_1 a_0 - 180{b_1}^2 a_0 H^2 - 120 c_1 {b_0}^3 H^2 - 1212 H^{10} {b_1}^4 {a_0}^3$$
$$+ 10\cos(H)H^6 {b_0}^3 + 10\ \cos(H)H^{12} {b_1}^3 {a_0}^3 + 30\cos(H)H^{10} {b_1}^2 {a_0}^2 b_0$$
$$+ 30\cos(H)H^8 {b_0}^2 b_1 a_0 + 840 H^{12} {b_1}^4 {a_0}^4 + 12 c_1 {b_0}^2 - 3720 H^8 {b_1}^3 {a_0}^3$$
$$+ 120 H^2 b_1 {b_0}^2 + 1620 H^6 {b_1}^3 {a_0}^2 + 1560 {b_1}^2 {a_0}^2 H^4 - 60 H^4 b_1 {b_0}^3$$
$$- 120 H^{12} {b_1}^4 {a_0}^3 b_0 + 420 c_1 {b_1}^4 {a_0}^4 H^{12} - 840 H^{12} {b_1}^4 a_1 {a_0}^3 + 12 H^{10} {b_1}^3 {a_0}^2 {b_0}^2$$
$$+ 24 H^{10} {b_1}^2 {a_0}^2 {b_0}^3 - 240 H^{12} {b_1}^3 {a_0}^3 {b_0}^2 + 120 H^{14} {b_1}^4 {a_0}^4 b_0 + 300 c_1 {b_0}^3 H^6 b_1 a_0$$
$$+ 240 H^{12} {b_1}^3 a_1 {b_0}^2 {a_0}^2 - 120 H^{14} {b_1}^4 a_1 b_0 {a_0}^3 + 600 c_1 {b_1}^2 {a_0}^2 H^8 {b_0}^2$$
$$- 24 H^{10} {b_1}^2 a_1 {b_0}^3 a_0 + 588 c_1 {b_1}^3 {a_0}^3 H^{10} b_0 + \cos(H)H^{10} {b_0}^5 + \cos(H)H^{20} {b_1}^5 {a_0}^5$$
$$+ 10\cos(H)H^{16} {b_1}^3 {a_0}^3 {b_0}^2 + 5\cos(H)H^{18} {b_1}^4 {a_0}^4 b_0 + 5\cos(H)H^{12} {b_0}^4 b_1 a_0$$
$$+ 10\cos(H)H^{14} {b_0}^3 {b_1}^2 {a_0}^2 + 1248 H^{10} {b_1}^3 a_1 b_0 {a_0}^2 + 360 H^6 {b_1}^2 a_1 a_0 b_0$$
$$+ 300 c_1 b_1 a_0 H^2 b_0 + 780 c_1 {b_1}^2 {a_0}^2 H^4 + 120 H^4 b_1 a_1 {b_0}^2 - 120 H^4 b_1 a_0 {b_0}^2$$
$$- 360 H^6 {b_1}^2 {a_0}^2 b_0 + 720 H^4 {b_1}^2 a_0 b_0 - 240 H^2 b_1 a_1 b_0 - 1560 H^4 {b_1}^2 a_1 a_0$$
$$+ 5\cos(H)H^{16} {b_1}^4 {a_0}^4 + 5\cos(H)H^8 {b_0}^4 + 20\cos(H)H^{14} {b_1}^3 {a_0}^3 b_0$$
$$+ 20\cos(H)H^{10} {b_0}^3 b_1 a_0 + 30\cos(H)H^{12} {b_1}^2 {a_0}^2 {b_0}^2 - 780 c_1 b_1 a_0 H^4 {b_0}^2$$
$$+ \cos(H) + 60 c_1 {b_0}^4 H^4 - 24 b_1 a_0 + 60 H^{14} {b_1}^5 {a_0}^4 + 24 b_1 a_1$$
$$- 120 H^8 {b_1}^2 a_1 {b_0}^2 a_0 - 1800 c_1 {b_1}^2 {a_0}^2 H^6 b_0 - 1860 c_1 {b_1}^3 {a_0}^3 H^8$$
$$+ 240 b_1 a_0 H^2 b_0 + 3720 H^8 {b_1}^3 a_1 {a_0}^2 - 300 H^6 {b_1}^2 a_0 {b_0}^2 - 540 H^8 {b_1}^3 {a_0}^2 b_0$$
$$+ 120 H^8 {b_1}^2 {a_0}^2 {b_0}^2 - 1248 H^{10} {b_1}^3 {a_0}^3 b_0 - 12 b_1 b_0 - 12 c_1 b_1 a_0\Big)$$

and

$$T_9 = \left(1 + H^2 b_0 + H^4 b_1 a_0\right)^5$$

Demanding the phase-lag and its first, second, third and fourth derivatives to be equal to zero we find out the coefficients mentioned in the "Appendix 1".

For small values of $|H|$ the formulae given by (35) are subject to heavy cancellations. In this case the Taylor series expansions should be used (see "Appendix 1").

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

The local truncation error of the new proposed method is given by:

$$\mathrm{LTE} = \frac{59 h^{10}}{76204800}\left(y_n^{(10)} - 5\omega^2 y_n^{(8)} + 10\omega^4 y_n^{(6)} - 10\omega^6 y_n^{(4)} + 5\omega^8 y_n^{(2)} - \omega^8 y_n\right) \tag{15}$$

4 Error analysis

We will study the following methods:

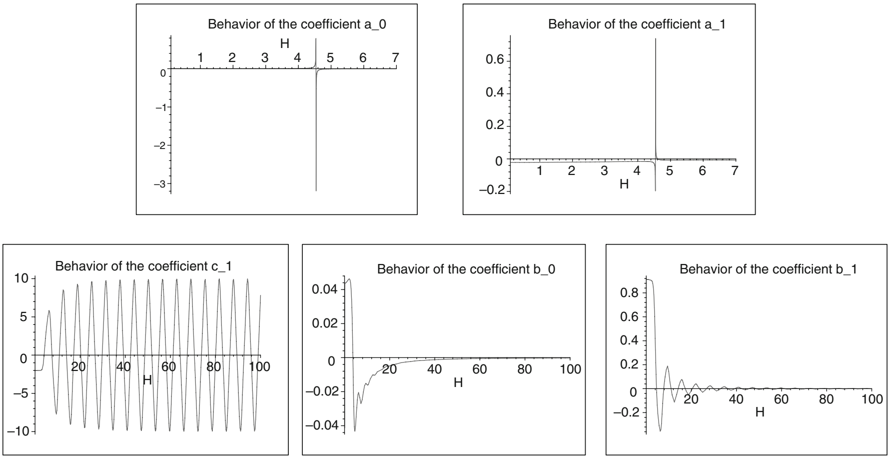

Fig. 1 Behavior of the coefficients of the new method given by (35–39) for several values of H

- The Classical Method of the Family[2] (mentioned as $PL0$)
- The New Developed Method of the Family (mentioned as $PL1$)

The error analysis is based on the following steps:

- The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)\, y(x) \tag{16}$$

- Based on the paper of Ixaru and Rizea [27], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{17}$$

where $g(x) = V(x) - V_c = g$, where V_c is the constant approximation of the potential and $G = v^2 = V_c - E$.
- We express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \ldots,$ which are terms of the local truncation error formulae, in terms of the Eq. 16. The expressions are presented as polynomials of G
- Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae

[2] We call Classical Method the method of the family with the constant coefficients.

Based on the procedure mentioned above and on the formulae:

$$
\begin{aligned}
y_n^{(2)} &= (V(x) - V_c + G)\ y(x) \\
y_n^{(4)} &= \left(\frac{d^2}{dx^2} V(x)\right) y(x) + 2\left(\frac{d}{dx} V(x)\right)\left(\frac{d}{dx} y(x)\right) \\
&\quad + (V(x) - V_c + G)\left(\frac{d^2}{dx^2} y(x)\right) \\
y_n^{(6)} &= \left(\frac{d^4}{dx^4} V(x)\right) y(x) + 4\left(\frac{d^3}{dx^3} V(x)\right)\left(\frac{d}{dx} y(x)\right) \\
&\quad + 3\left(\frac{d^2}{dx^2} V(x)\right)\left(\frac{d^2}{dx^2} y(x)\right) + 4\left(\frac{d}{dx} V(x)\right)^2 y(x) \\
&\quad + 6\ (V(x) - V_c + G)\left(\frac{d}{dx} y(x)\right)\left(\frac{d}{dx} V(x)\right) \\
&\quad + 4\ (U(x) - V_c + G)\ y(x)\left(\frac{d^2}{dx^2} V(x)\right) \\
&\quad + (V(x) - V_c + G)^2\left(\frac{d^2}{dx^2} y(x)\right) \cdots
\end{aligned}
$$

we obtain the expressions of the local truncation error mentioned in “Appendix 3”.

We consider two cases in terms of the value of E:

- The energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. 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 new developed methods.
- $G \gg 0$ or $G \ll 0$. Then $\mid G \mid$ is a large number. So, we have the following asymptotic expansions of the Eqs. 45 and 46.

4.1 The classical method of the family

$$
\mathrm{LTE}_{\mathrm{PL0}} = \frac{59\, h^{10}}{76204800}\, y(x)\, G^5 + \cdots \tag{18}
$$

4.2 The new developed method of the family

$$
\mathrm{LTE}_{\mathrm{PL1}} = \frac{59\, h^{10}}{4762800}\left(\frac{d^4}{dx^4}\, g(x)\right) y(x)\, G^2 + \cdots \tag{19}
$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Method of the New Family of Methods the error increases as the fifth power of G. For the New Method of the Family of Methods the error increases as the second power of G. So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Method of the Family of Methods is the most accurate one, especially for large values of* $\mid G \mid=\mid V_c - E \mid$.

5 Stability analysis

We apply the new family of methods to the scalar test equation:

$$y'' = -t^2 y, \tag{20}$$

where $t \neq \omega$. We obtain the following difference equation:

$$A_1(H, s)\, y_{n+1} + A_0(H, s)\, y_n + A_1(H, s)\, y_{n-1} = 0$$

where $s = t\,h$, h is the step length and $A_0(H, s)$ and $A_1(H, s)$ are polynomials of s.
The characteristic equation associated with (21) is given by:

$$A_1(H, s)\, s + A_0(H, s) + A_1(H, s)\, s^{-1} = 0 \tag{21}$$

where

$$\begin{aligned} A_1(H, s) &= 1 + s^2\, b_0 + s^4\, b_1\, a_0 \\ A_0(H, s) &= c_1 + s^2\, b_1 - 2\, s^4\, b_1\, a_0 + 2\, s^4\, b_1\, a_1 \end{aligned} \tag{22}$$

Definition 1 (see [42]) A symmetric four-step method with the characteristic equation given by (21) is said to have an *interval of periodicity* $\left(0, w_0^2\right)$ if, for all $w \in \left(0, w_0^2\right)$, the roots $z_i,\ i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i\, \theta(t\,h)}, \quad |z_i| \leq 1, \ \ i = 3, 4 \tag{23}$$

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

Definition 2 (see [42]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Theorem 3 (see [60]) *A symmetric two-step method with the characteristic equation given by* (21) *is said to have a nonzero interval of periodicity* $\left(0, s_0^2\right)$ *if, for all* $s \in \left(0, s_0^2\right)$ *the following relations are hold*

$$P_1(H, s)\, P_2(H, s) < 0, \tag{24}$$

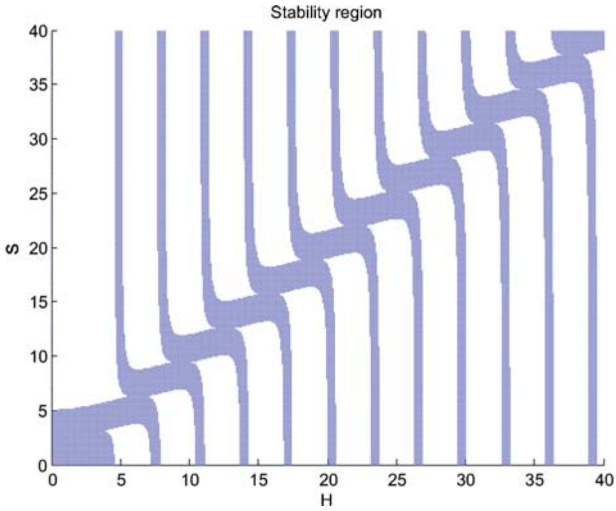

Fig. 2 $s - H$ Plane of the new method of the family of method developed in this paper

where $H = \omega h, s = th$ *and:*

$$\begin{aligned} P_1(H,s) &= A_0(H,s) + 2\,A_1(H,s), \\ P_2(H,s) &= A_0(H,s) - 2\,A_1(H,s) \end{aligned} \tag{25}$$

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

Based on (22) the stability polynomials (25) for the new developed methods take the form:

$$\begin{aligned} P_1(H,s) &= c_1 + s^2\,b_1 + 2\,s^4\,b_1\,a_1 + 2 + 2\,s^2\,b_0, \\ P_2(H,s) &= c_1 + s^2\,b_1 - 4\,s^4\,b_1\,a_0 + 2\,s^4\,b_1\,a_1 - 2 - 2\,s^2\,b_0 \end{aligned} \tag{26}$$

In the Fig. 2 we present the $s - H$ plane for the new method of the new family of method developed in this paper (Sect. 3).

In the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $H = s$, we have the Fig. 3 for the stability polynomials of the new developed methods. A method is P-stable if the $s - H$ plane is completely shadowed. From the above diagrams it is easy for one to see that the interval of periodicity of all the new methods is equal to: $\left(0, \pi^2\right)$.

Remark 1 For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the $w - H$ plane.

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

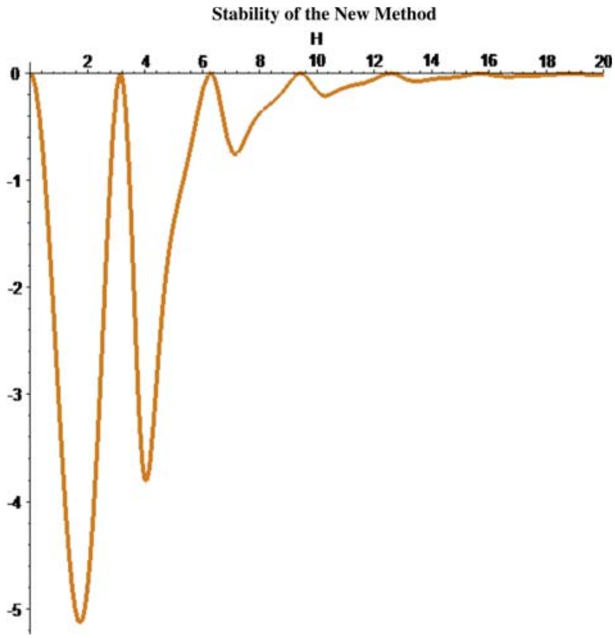

Fig. 3 Stability polynomial of the new developed method in the case that $H = s$

6 Numerical results: conclusion

In order to illustrate the efficiency of the new methods obtained Sect. 3 we apply them to the radial time independent Schrödinger equation.

In order to apply the new methods to the radial Schrödinger equation the value of parameter v is needed. For every problem of the one-dimensional Schrödinger equation given by (1) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{27}$$

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

6.1 Woods–Saxon potential

We use as potential the well known Woods–Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a(1+z)^2} \tag{28}$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

The behavior of Woods–Saxon potential is shown in the Fig. 4.

It is well known that for some potentials, such as the Woods–Saxon potential, the definition of parameter v is not given as a function of x but based on some critical points which have been defined from the investigation of the appropriate potential (see for details [26]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [26]):

$$v = \begin{cases} \sqrt{-50+E}, & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5-h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5+h \\ \sqrt{E}, & \text{for } x \in [6.5+2h, 15] \end{cases} \tag{29}$$

6.2 Radial schrödinger equation: the resonance problem

Consider the numerical solution of the radial time independent Schrödinger equation (1) in the well-known case of the Woods–Saxon potential (28). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$. We consider Eq. 1 in a rather large domain of energies, i.e. $E \in [1, 1000]$.

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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{30}$$

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 has (when $x \to \infty$) the asymptotic form

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{31}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{32}$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need y_0 before starting a one-step method. From the initial condition we obtain

y_0. With these starting values we evaluate at x_1 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" when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0, \quad y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{33}$$

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

- the Numerov's method which is indicated as "Method I"
- the exponentially fitted four-step method developed by Raptis [58] which is indicated as "Method II"
- the two-step Numerov-type method with minimum phase-lag produced by Chawla and Rao [13] which is indicated as "Method III"
- Exponentially fitted two-step method developed by Raptis and Allison [56] which is indicated as "Method IV"
- Exponentially fitted four-step method developed by Raptis [59] which is indicated as "Method V"
- the classical form (see Foot note 2) of the new proposed Numerov-type method which is indicated as "Method VI".
- the new two-step Numerov-type method with phase-lag and its first, second, third and fourth derivatives equal to zero obtained in Sect. 3 which is indicated as "Method VII".

The computed eigenenergies are compared with exact ones.

In Figs. 5, 6, and 7, we present the maximum absolute error $\log_{10}$ (Err) where

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}| \tag{34}$$

of the eigenenergies E_2, E_3 and E_4, for several values of NFE = number of function evaluations.

7 Conclusions

In the present paper we have developed a family of methods of sixth algebraic order for the numerical solution of the radial Schrödinger equation.

More specifically we have developed a two-step Numerov-type method with phase-lag and its first, second, third and fourth derivatives equal to zero.

We have applied the new method to the resonance problem of the radial Schrödinger equation.

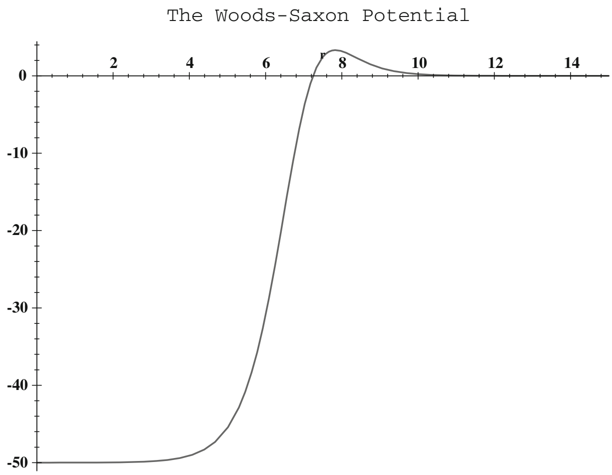

Fig. 4 The Woods–Saxon potential

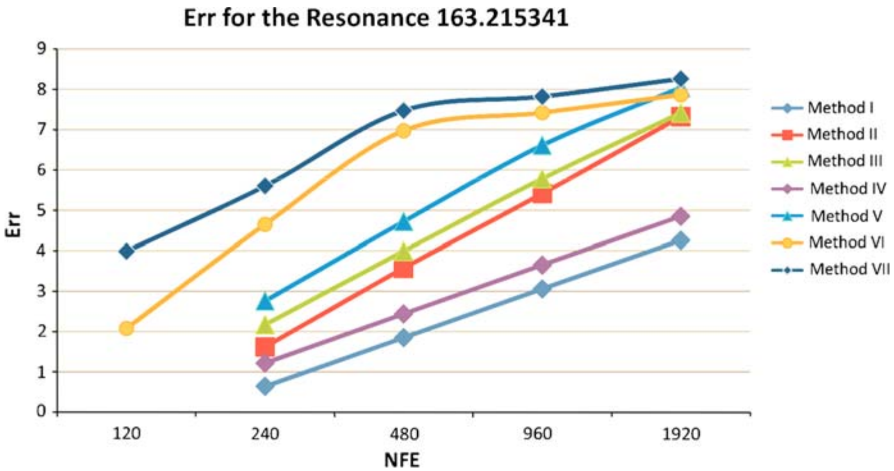

Fig. 5 Error Errmax for several values of n for the eigenvalue $E_1 = 163.215341$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

Based on the results presented above we have the following conclusions:

- The exponentially fitted four-step method developed by Raptis [58] (Method II) is more efficient than the Numerov's method (Method I).
- The two-step Numerov-type method with minimum phase-lag produced by Chawla and Rao [13] (Method III) is more efficient than the exponentially fitted four-step method developed by Raptis [58] (Method II) for the energy 163.215341, less efficient for the energy 989.701916 and of the same efficiency for the energy 341.495874.

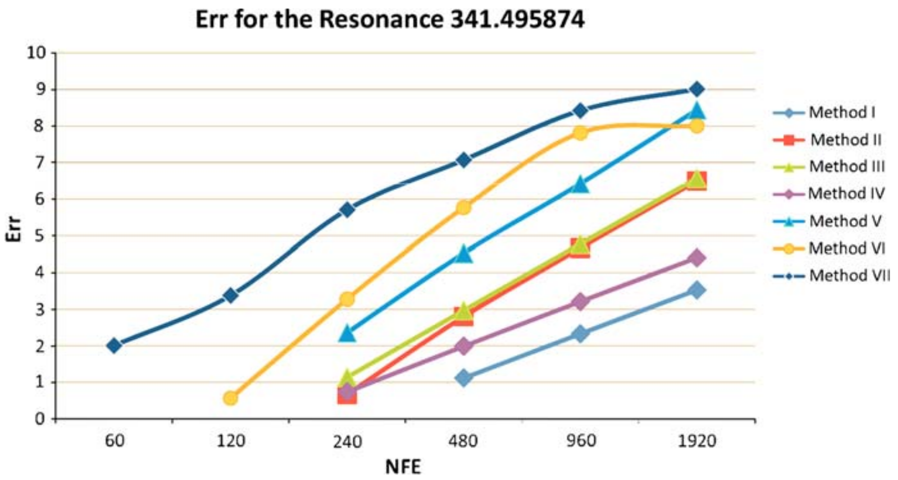

Fig. 6 Error Errmax for several values of n for the eigenvalue $E_3 = 341.495874$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

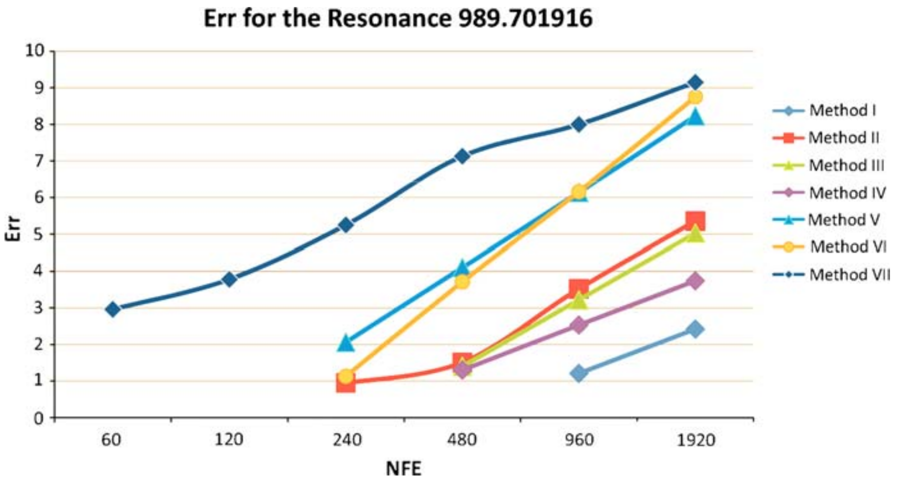

Fig. 7 Error Errmax for several values of n for the eigenvalue $E_4 = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

- The two-step method developed by Raptis and Allison [56] (Method IV) is more efficient than Numerov's method (Method I) but less efficient than all the other methods.
- The exponentially fitted four-step method developed by Raptis [59] (Method V) is better than the Numerov's method (Method I), the exponentially fitted four-step method developed by Raptis [58] (Method II), the two-step Numerov-type method with minimum phase-lag produced by Chawla and Rao [13] (Method III) and the two-step method developed by Raptis and Allison [56] (Method IV)

- The classical form of the new proposed Numerov-type method (Method VI) is better than the Numerov's method (Method I), the exponentially fitted four-step method developed by Raptis [58] (Method II), the two-step Numerov-type method with minimum phase-lag produced by Chawla and Rao [13] (Method III), the two-step method developed by Raptis and Allison [56] (Method IV). For the energies 163.215341 and 341.495874 is better than the exponentially fitted four-step method developed by Raptis [59] (Method V) but for the energy for the 989.701916 has approximately the same behavior than the exponentially fitted four-step method developed by Raptis [59] (Method V)
- Finally the new developed two-step Numerov-type method with phase-lag and its first, second, third and fourth derivatives equal to zero (Method VII) is more efficient than all the other methods.

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

Appendix 1

$$a_1 = \Big(-H^4\cos(3H) + 2H^4\cos(2H) + 18 - 18H\sin(3H) - 36H\sin(2H) - 6H^3\sin(2H) - 18\cos(2H) + 126\sin(H)H + 6H^2\cos(2H) - 51\sin(H)H^3 - 3H^3\sin(3H) - 59\cos(H)H^4 - 33\cos(H)H^2 - 3H^2\cos(3H) + 9\cos(3H) + 30H^2 - 9\cos(H) - 14H^4\Big)\Big/ \Big(-12H^5\sin(3H) - 204H^5\sin(H) + 4H^6\cos(3H) + 236\cos(H)H^6 + 60H^4\cos(3H) + 660\cos(H)H^4 + 180H^2\cos(3H) - 180\cos(H)H^2\Big) \tag{35}$$

$$a_0 = \Big(-900\cos(H)H^3 - 270\cos(H)H - 135H\cos(4H) - 90H^3\cos(4H) + 1044H^2\sin(H) + 132\cos(H)H^5 - 346H^6\sin(H) - 36H^2\sin(5H) + 27\sin(3H) + 54\sin(4H) - 27\sin(5H) + 37H^6\sin(3H) + 12H^5\cos(3H) + 144H^2\sin(3H) - 576H^2\sin(2H) - 108H\cos(2H) + 468H^3\cos(3H) + 45H^4\sin(3H) + 243H\cos(3H) - 4H^7\cos(2H) - 270H^4\sin(2H) + 26H^6\sin(2H) + 72H^3\cos(2H) + 36H^5\cos(2H) - 36H^2\sin(4H) + 27H\cos(5H) - 9H^4\sin(5H) - 45H^4\sin(4H) + 630\sin(H)H^4 - H^6\sin(5H) + H^7\cos(4H) - 6H^5\cos(4H) - 7H^6\sin(4H) + 243H + 54\sin(H) + 450H^3 - 108\sin(2H) + 42H^5 - 69H^7\Big)\Big/\Big(-42H^6\sin(6H) - 1620\cos(H)H^3 - 1620H^3\cos(4H) - 72H^8\sin(4H) + 2550H^8\sin(2H) + 1080H^2\sin(H) + 6768\cos(H)H^5 - 3444H^6\sin(H) - 2H^8\sin(6H) - 540H^2\sin(5H) + 144H^5\cos(5H) + 270H^2\sin(6H) + 270H^3\cos(6H) - 14H^8\sin(5H)$$

$$+108H^5\cos(6H)+2H^9\cos(5H)-2442H^6\sin(3H)+1728H^5\cos(3H)$$
$$+540H^2\sin(3H)-810H^2\sin(2H)+1350H^3\cos(3H)-1620H^4\sin(3H)$$
$$+864H^7\cos(2H)-2160H^4\sin(2H)+9198H^6\sin(2H)-270H^3\cos(2H)$$
$$-4428H^5\cos(2H)+612H^7\cos(3H)+6576\cos(H)H^7+138H^9\cos(3H)$$
$$-1388H^8\sin(H)-634H^8\sin(3H)+1300H^9\cos(H)+12H^7\cos(5H)$$
$$-540H^4\sin(5H)+3240H^4\sin(4H)-1080\sin(H)H^4-150H^6\sin(5H)$$
$$+360H^7\cos(4H)+864H^5\cos(4H)+504H^6\sin(4H)+1620H^3$$
$$+270H^3\cos(5H)-5184H^5-4104H^7\Big) \tag{36}$$

$$b_0=\Big(4824\cos(H)H^3-1620\cos(H)H-270H\cos(4H)-216H^3\cos(4H)$$
$$+5400H^2\sin(H)-528\cos(H)H^5+692H^6\sin(H)-12H^5\cos(5H)$$
$$+270\sin(3H)+540\sin(4H)-270\sin(5H)-74H^6\sin(3H)+252H^5\cos(3H)$$
$$-3240H^2\sin(3H)+1080H^2\sin(2H)-1080H\cos(2H)-432H^3\cos(3H)$$
$$-222H^4\sin(3H)+1890H\cos(3H)+8H^7\cos(2H)+924H^4\sin(2H)$$
$$-172H^6\sin(2H)-2160H^3\cos(2H)-552H^5\cos(2H)+540H^2\sin(4H)$$
$$-270H\cos(5H)+6H^4\sin(5H)+114H^4\sin(4H)-5988\sin(H)H^4$$
$$+2H^6\sin(5H)-2H^7\cos(4H)-60H^5\cos(4H)+2H^6\sin(4H)+1350H$$
$$+540\sin(H)-1944H^3-72H^3\cos(5H)-1080\sin(2H)-1260H^5+138H^7\Big)/$$
$$\Big(-702\cos(H)H^3-27H^3\cos(4H)+5H^8\sin(4H)+146H^8\sin(2H)$$
$$+270H^2\sin(H)+3852\cos(H)H^5-4530H^6\sin(H)-135H^2\sin(5H)$$
$$-72H^5\cos(5H)-H^8\sin(5H)-447H^6\sin(3H)-756H^5\cos(3H)$$
$$+135H^2\sin(3H)-540H^2\sin(2H)+891H^3\cos(3H)-2088H^4\sin(3H)$$
$$-444H^7\cos(2H)+1224H^4\sin(2H)+1266H^6\sin(2H)-540H^3\cos(2H)$$
$$-1368H^5\cos(2H)-264H^7\cos(3H)+396\cos(H)H^7-346H^8\sin(H)$$
$$+37H^8\sin(3H)+270H^2\sin(4H)-69H^9+H^9\cos(4H)-4H^9\cos(2H)$$
$$+12H^7\cos(5H)+36H^4\sin(5H)+360H^4\sin(4H)+2196\sin(H)H^4$$
$$+51H^6\sin(5H)+18H^7\cos(4H)+18H^5\cos(4H)+123H^6\sin(4H)+567H^3$$
$$-189H^3\cos(5H)-1674H^5-1230H^7\Big) \tag{37}$$

$$b_1=\Big(2H^6\sin(6H)-6768\cos(H)H^3+1620\cos(H)H+1620H\cos(4H)$$
$$-864H^3\cos(4H)-270\sin(6H)+1080H^2\sin(H)-6576\cos(H)H^5$$
$$+1388H^6\sin(H)-270H\cos(6H)+540H^2\sin(5H)-12H^5\cos(5H)$$
$$-108H^3\cos(6H)-540\sin(3H)+540\sin(5H)+634H^6\sin(3H)$$
$$-612H^5\cos(3H)+1620H^2\sin(3H)+2160H^2\sin(2H)$$
$$+270H\cos(2H)-1728H^3\cos(3H)+2442H^4\sin(3H)$$

$$
\begin{aligned}
&- 1350\, H \cos(3\, H) - 9198\, H^4 \sin(2\, H) - 2550\, H^6 \sin(2\, H)\\
&+ 4428\, H^3 \cos(2\, H) - 864\, H^5 \cos(2\, H) - 138\, H^7 \cos(3\, H)\\
&-1300 \cos(H)\, H^7 - 3240\, H^2 \sin(4\, H) - 270\, H \cos(5\, H) - 2\, H^7 \cos(5\, H)\\
&+ 150\, H^4 \sin(5\, H) - 504\, H^4 \sin(4\, H) + 3444 \sin(H)\, H^4 + 14\, H^6 \sin(5\, H)\\
&- 360\, H^5 \cos(4\, H) + 72\, H^6 \sin(4\, H) - 1620\, H - 1080 \sin(H) + 5184\, H^3\\
&-144\, H^3 \cos(5\, H) + 810 \sin(2\, H) + 42\, H^4 \sin(6\, H) + 4104\, H^5\Big) \Big/\\
&\Big(702 \cos(H)\, H^3 + 27\, H^3 \cos(4\, H) - 5\, H^8 \sin(4\, H) - 146\, H^8 \sin(2\, H)\\
&- 270\, H^2 \sin(H) - 3852 \cos(H)\, H^5 + 4530\, H^6 \sin(H) + 135\, H^2 \sin(5\, H)\\
&+ 72\, H^5 \cos(5\, H) + H^8 \sin(5\, H) + 447\, H^6 \sin(3\, H) + 756\, H^5 \cos(3\, H)\\
&-135\, H^2 \sin(3\, H) + 540\, H^2 \sin(2\, H) - 891\, H^3 \cos(3\, H)\\
&+ 2088\, H^4 \sin(3\, H) + 444\, H^7 \cos(2\, H) - 1224\, H^4 \sin(2\, H) - 1266\, H^6 \sin(2\, H)\\
&+ 540\, H^3 \cos(2\, H) + 1368\, H^5 \cos(2\, H) + 264\, H^7 \cos(3\, H)\\
&-396 \cos(H)\, H^7 + 346\, H^8 \sin(H) - 37\, H^8 \sin(3\, H) - 270\, H^2 \sin(4\, H)\\
&+ 69\, H^9 - H^9 \cos(4\, H) + 4\, H^9 \cos(2\, H) - 12\, H^7 \cos(5\, H)\\
&- 36\, H^4 \sin(5\, H) - 360\, H^4 \sin(4\, H) - 2196 \sin(H)\, H^4 - 51\, H^6 \sin(5\, H)\\
&- 18\, H^7 \cos(4\, H) - 18\, H^5 \cos(4\, H) - 123\, H^6 \sin(4\, H) - 567\, H^3\\
&+189\, H^3 \cos(5\, H) + 1674\, H^5 + 1230\, H^7\Big) \qquad (38)
\end{aligned}
$$

$$
\begin{aligned}
c_1 = &\Big(H^6 \sin(6H) + 3924 \cos(H) H^3 - 162 \cos(H) H - 486 H \cos(4H)\\
&- 648 H^3 \cos(4H) + 135 \sin(6H) - 2736 H^2 \sin(H) + 672 \cos(H) H^5\\
&+ 1618 H^6 \sin(H) + 81 H \cos(6H) - 252 H^2 \sin(5H) + 54 H^5 \cos(5H)\\
&+72 H^2 \sin(6H) + 54 H^3 \cos(6H) + 270 \sin(3H) + 6 H^5 \cos(6H) - 270 \sin(5H)\\
&+ 479 H^6 \sin(3H) + 858 H^5 \cos(3H) - 1260 H^2 \sin(3H) + 1296 H^2 \sin(2H)\\
&- 81 H \cos(2H) + 1890 H^3 \cos(3H) + 105 H^4 \sin(3H) - 81 H \cos(3H)\\
&+ 1359 H^4 \sin(2H) - 1275 H^6 \sin(2H) + 378 H^3 \cos(2H) - 2742 H^5 \cos(2H)\\
&- 69 H^7 \cos(3H) - 650 \cos(H) H^7 + 1188 H^2 \sin(4H) + 243 H \cos(5H)\\
&- H^7 \cos(5H) - 33 H^4 \sin(5H) + 396 H^4 \sin(4H) + 714 \sin(H) H^4\\
&+ 13 H^6 \sin(5H) - 216 H^5 \cos(4H) + 36 H^6 \sin(4H) + 486 H + 540 \sin(H)\\
&-5832 H^3 + 234 H^3 \cos(5H) - 405 \sin(2H) + 3 H^4 \sin(6H) + 4392 H^5\Big)\\
&\Big/\Big(3852 \cos(H) H^3 - 702 \cos(H) H - 27 H \cos(4H) + 18 H^3 \cos(4H)\\
&+ 2196 H^2 \sin(H) + 396 \cos(H) H^5 - 346 H^6 \sin(H) + 36 H^2 \sin(5H)\\
&+ 12 H^5 \cos(5H) + 135 \sin(3H) + 270 \sin(4H) - 135 \sin(5H) + 37 H^6 \sin(3H)\\
&- 264 H^5 \cos(3H) - 2088 H^2 \sin(3H) + 1224 H^2 \sin(2H) - 540 H \cos(2H)\\
&- 756 H^3 \cos(3H) - 447 H^4 \sin(3H) + 891 H \cos(3H) - 4 H^7 \cos(2H)
\end{aligned}
$$

$$
+1266H^4\sin(2H)+146H^6\sin(2H)-1368H^3\cos(2H)-444H^5\cos(2H)
+360H^2\sin(4H)-189H\cos(5H)+51H^4\sin(5H)+123H^4\sin(4H)
-4530\sin(H)H^4-H^6\sin(5H)+H^7\cos(4H)+18H^5\cos(4H)+5H^6\sin(4H)
+567H+270\sin(H)-1674H^3-72H^3\cos(5H)-540\sin(2H)-1230H^5
-69H^7\Big) \tag{39}
$$

Appendix 2

$$
a_1 = -\frac{1}{46}+\frac{59}{126960}H^2-\frac{30979}{1927252800}H^4+\frac{18186977}{20168700552000}H^6
-\frac{32786131009}{3673930492552320000}H^8+\frac{18575423955577}{2154760233881935680000}H^{10}
-\frac{14007095145979224077}{377028740971444919220864000000}H^{12}
-\frac{386124432536554879}{7742554502092172448285600000000}H^{14}
-\frac{4024843359689988634592377}{4738889326419730047483808450560000000}H^{16}+\cdots \tag{40}
$$

$$
a_0 = \frac{13}{13800}+\frac{413}{4761000}H^2+\frac{5547083}{1011807720000}H^4+\frac{561691297}{2268978812100000}H^6
+\frac{842863393103}{918482623138080000000}H^8+\frac{3196599628269881}{11312491227880162320000000}H^{10}
+\frac{818605921582206570851}{84831466718575106824694400000000}H^{12}
+\frac{1292945522932218771153}{261311214445610820129639000000000}H^{14}
+\frac{848253808628743843741846619}{24879168963703582749289994365440000000000}H^{16}+\cdots \tag{41}
$$

$$
b_0 = \frac{11}{252}+\frac{59}{63504}H^2-\frac{2995}{88016544}H^4-\frac{1714889}{262129271040}H^6-\frac{403237411}{726622339322880}H^8
-\frac{587107461797}{1712067555912569856 0}H^{10}-\frac{129647872466 2139}{819737945770938447052800}H^{12}
-\frac{22443894102319891}{5370923020691188705089945 60}H^{14}
+\frac{29654232116575081591}{2252819527020969915011280076800 0}H^{16}+\cdots \tag{42}
$$

$$
b_1 = \frac{115}{126}-\frac{59}{31752}H^2+\frac{2995}{44008272}H^4+\frac{1714889}{131064635520}H^6-\frac{200638723}{72662233932288}H^8
-\frac{1230195843967}{535021111222678080 0}H^{10}-\frac{490648924648621}{315283825296514787328 00}H^{12}
$$

$$
\begin{aligned}
&- \frac{1051877512638955999}{1342730755172797176272486400}\, H^{14} \\
&- \frac{291379254608108378287}{11264097635104849575056400384000}\, H^{16} + \cdots
\end{aligned} \tag{43}
$$

$$
\begin{aligned}
c_1 = &-2 + \frac{59}{76204800}\, H^{10} + \frac{233}{4224794112}\, H^{12} + \frac{2348677}{692021275545600}\, H^{14} \\
&+ \frac{2645563}{17438936143749120}\, H^{16} + \cdots
\end{aligned} \tag{44}
$$

Appendix 3

The classical method of the family

$$
\begin{aligned}
\mathrm{LTE_{PL0}} = h^{10} \Bigg(& \frac{59}{952560} \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right)^3 \left(\frac{\mathrm{d}}{\mathrm{d}x}\, y(x)\right) + \frac{59}{1360800} \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\, g(x)\right)^2 y(x) \\
&+ \frac{59}{76204800} \left(\frac{\mathrm{d}^8}{\mathrm{d}x^8}\, g(x)\right) y(x) + \frac{59}{9525600} \left(\frac{\mathrm{d}^7}{\mathrm{d}x^7}\, g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x}\, y(x)\right) \\
&+ \frac{1711}{9525600} \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right)^2 y(x) \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\, g(x)\right) \\
&+ \frac{59}{1190700} \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right) y(x) \left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}\, g(x)\right) \\
&+ \frac{59}{272160} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\, g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x}\, y(x)\right) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\, g(x)\right) \\
&+ \frac{59}{777600} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\, g(x)\right) y(x) \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\, g(x)\right) \\
&+ \frac{59}{423360} \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x}\, y(x)\right) \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\, g(x)\right) \\
&+ \frac{9971}{38102400}\, g(x) y(x) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\, g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right) \\
&+ \frac{59}{238140}\, g(x) \left(\frac{\mathrm{d}}{\mathrm{d}x}\, y(x)\right) \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\, g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right) \\
&+ \frac{59}{76204800}\, g(x)^5\, y(x) + \frac{59}{76204800}\, y(x)\, G^5 \\
&+ \left(\frac{59}{1524096} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\, g(x)\right) y(x) + \frac{59}{3810240} \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x}\, y(x)\right) \right. \\
&\left. + \frac{59}{7620480}\, g(x)^2\, y(x) \right) G^3 + \left(\frac{59}{762048} \left(\frac{\mathrm{d}}{\mathrm{d}x}\, g(x)\right)^2 y(x) \right.
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{59}{508032}\,g(x)\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\\
&+\frac{2537}{38102400}\,\left(\frac{d^4}{dx^4}\,g(x)\right)\,y(x)+\frac{59}{952560}\,\left(\frac{d^3}{dx^3}\,g(x)\right)\,\left(\frac{d}{dx}\,y(x)\right)\\
&+\frac{59}{1270080}\,g(x)\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d}{dx}\,g(x)\right)+\frac{59}{7620480}\,g(x)^3\,y(x)\Bigg)\,G^2\\
&+\Bigg(\frac{12449}{76204800}\,\left(\frac{d^2}{dx^2}\,g(x)\right)^2\,y(x)+\frac{1829}{38102400}\,\left(\frac{d^5}{dx^5}\,g(x)\right)\,\left(\frac{d}{dx}\,y(x)\right)\\
&+\frac{2537}{19051200}\,g(x)\,y(x)\,\left(\frac{d^4}{dx^4}\,g(x)\right)+\frac{59}{381024}\,g(x)\,y(x)\,\left(\frac{d}{dx}\,g(x)\right)^2\\
&+\frac{9971}{38102400}\,\left(\frac{d}{dx}\,g(x)\right)\,y(x)\,\left(\frac{d^3}{dx^3}\,g(x)\right)\\
&+\frac{59}{508032}\,g(x)^2\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\\
&+\frac{59}{238140}\,\left(\frac{d}{dx}\,g(x)\right)\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\\
&+\frac{59}{1270080}\,g(x)^2\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d}{dx}\,g(x)\right)\\
&+\frac{1711}{76204800}\,\left(\frac{d^6}{dx^6}\,g(x)\right)\,y(x)+\frac{59}{476280}\,g(x)\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d^3}{dx^3}\,g(x)\right)\\
&+\frac{59}{15240960}\,g(x)^4\,y(x)\Bigg)\,G+\frac{59}{762048}\,g(x)^2\,y(x)\,\left(\frac{d}{dx}\,g(x)\right)^2\\
&+\frac{59}{3810240}\,g(x)^3\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d}{dx}\,g(x)\right)+\frac{59}{15240960}\,g(x)\,y(x)\,G^4\\
&+\frac{59}{1524096}\,g(x)^3\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)+\frac{12449}{76204800}\,g(x)\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)^2\\
&+\frac{1829}{38102400}\,g(x)\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d^5}{dx^5}\,g(x)\right)\\
&+\frac{2537}{38102400}\,g(x)^2\,y(x)\,\left(\frac{d^4}{dx^4}\,g(x)\right)\\
&+\frac{1711}{76204800}\,g(x)\,y(x)\,\left(\frac{d^6}{dx^6}\,g(x)\right)\\
&+\frac{59}{952560}\,g(x)^2\,\left(\frac{d}{dx}\,y(x)\right)\,\left(\frac{d^3}{dx^3}\,g(x)\right)\Bigg)\Bigg) \qquad (45)
\end{aligned}
$$

The new developed method of the family

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{PL}} = h^{10} \Bigg(& \frac{59}{4762800} \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g(x)\right) y(x)\, G^2 \\
& + \Bigg(\frac{59}{952560} \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right) \\
& + \frac{1357}{19051200} g(x)\, y(x) \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g(x)\right) + \frac{59}{1905120} g(x)^2\, y(x) \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right) \\
& + \frac{59}{1270080} g(x)\, y(x) \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right)^2 + \frac{59}{3175200} \left(\frac{\mathrm{d}^6}{\mathrm{d}x^6} g(x)\right) y(x) \\
& + \frac{59}{2381400} \left(\frac{\mathrm{d}^5}{\mathrm{d}x^5} g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) + \frac{1003}{9525600} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right)^2 y(x) \\
& + \frac{767}{4762800} \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right) y(x) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} g(x)\right) \\
& + \frac{59}{1905120} g(x) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} g(x)\right) \Bigg) G \\
& + \frac{59}{238140} g(x) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right) \\
& + \frac{59}{9525600} \left(\frac{\mathrm{d}^7}{\mathrm{d}x^7} g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \\
& + \frac{9971}{38102400} g(x)\, y(x) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right) \\
& + \frac{59}{952560} g(x)^2 \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} g(x)\right) \\
& + \frac{59}{1524096} g(x)^3\, y(x) \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right) + \frac{59}{762048} g(x)^2\, y(x) \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right)^2 \\
& + \frac{59}{1190700} \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right) y(x) \left(\frac{\mathrm{d}^5}{\mathrm{d}x^5} g(x)\right) \\
& + \frac{1829}{38102400} g(x) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \left(\frac{\mathrm{d}^5}{\mathrm{d}x^5} g(x)\right) \\
& + \frac{59}{952560} \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x)\right)^3 \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) + \frac{1711}{76204800} g(x)\, y(x) \left(\frac{\mathrm{d}^6}{\mathrm{d}x^6} g(x)\right) \\
& + \frac{2537}{38102400} g(x)^2\, y(x) \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g(x)\right) \\
& + \frac{59}{272160} \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right) \left(\frac{\mathrm{d}}{\mathrm{d}x} y(x)\right) \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} g(x)\right)
\end{aligned}
$$

$$+\frac{59}{3810240}g(x)^3\left(\frac{d}{dx}y(x)\right)\left(\frac{d}{dx}g(x)\right)+\frac{59}{76204800}\left(\frac{d^8}{dx^8}g(x)\right)y(x)$$
$$+\frac{59}{1360800}\left(\frac{d^3}{dx^3}g(x)\right)^2 y(x)+\frac{1711}{9525600}\left(\frac{d}{dx}g(x)\right)^2 y(x)\left(\frac{d^2}{dx^2}g(x)\right)$$
$$+\frac{12449}{76204800}g(x)\,y(x)\left(\frac{d^2}{dx^2}g(x)\right)^2$$
$$+\frac{59}{423360}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\left(\frac{d^4}{dx^4}g(x)\right)$$
$$+\frac{59}{76204800}g(x)^5 y(x)+\frac{59}{777600}\left(\frac{d^2}{dx^2}g(x)\right)y(x)\left(\frac{d^4}{dx^4}g(x)\right)\Bigg)\quad(46)$$

References

1. 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)
2. 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)
3. 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)
4. 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)
5. 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)
6. G. Avdelas, T.E. Simos, Embedded eighth order methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **26**(4), 327–341 (1999)
7. P. Amodio, I. Gladwell, G. Romanazzi, Numerical solution of general bordered ABD linear systems by cyclic reduction. J. Numer. Anal. Ind. Appl. Math. **1**(1), 5–12 (2006)
8. L. Aceto, R. Pandolfi, D. Trigiante, Stability analysis of linear multistep methods via polynomial type variation.
   J. Numer. Anal. Ind. Appl. Math. **2**(1–2), 1–9 (2007)
9. G. Avdelas, T.E. Simos, Block Runge-Kutta methods for periodic initial-value problems. Comput. Math. Appl. **31**, 69–83 (1996)
10. G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **31**, 85–102 (1996)
11. 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)
12. G. Avdelas, T.E. Simos, A generator of high-order embedded P-stable methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **72**(2), 345–358 (1996)
13. M.M. Chawla, P.S. Rao, A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems. J. Comput. Appl. Math. **11**(3), 277–281 (1984)
14. S.D. Capper, J.R. Cash, D.R. Moore, Lobatto-Obrechkoff formulae for 2nd order two-point boundary value problems. J. Numer. Anal. Ind. Appl. Math. **1**(1), 13–25 (2006)
15. S.D. Capper, D.R. Moore, On high order MIRK schemes and Hermite-Birkhoff interpolants. J. Numer. Anal. Ind. Appl. Math. **1**(1), 27–47 (2006)
16. J.R. Cash, N. Sumarti, T.J. Abdulla, I. Vieira, The derivation of interpolants for nonlinear two-point boundary value problems. J. Numer. Anal. Ind. Appl. Math. **1**(1), 49–58 (2006)
17. J.R. Cash, S. Girdlestone, Variable step Runge-Kutta-Nystrm methods for the numerical solution of reversible systems. J. Numer. Anal. Ind. Appl. Math. **1**(1), 59–80 (2006)

18. J.R. Cash, F. Mazzia, Hybrid mesh selection algorithms based on conditioning for two-point boundary value problems. J. Numer. Anal. Ind. Appl. Math. **1**(1), 81–90 (2006)
19. R.M. Corless, A. Shakoori, D.A. Aruliah, L. Gonzalez-Vega, Barycentric Hermite interpolants for event location in initial-value problems. J. Numer. Anal. Ind. Appl. Math. **3**, 1–16 (2008)
20. S.P. Corwin, S. Thompson, S.M. White, Solving ODEs and DDEs with impulses. J. Numer. Anal. Ind. Appl. Math. **3**, 139–149 (2008)
21. M. Dewar, Embedding a general-purpose numerical library in an interactive environment. J. Numer. Anal. Ind. Appl. Math. **3**, 17–26 (2008)
22. W.H. Enright, On the use of 'arc length' and 'defect' for mesh selection for differential equations. Comput. Lett. **1**(2), 47–52 (2005)
23. G. Herzberg, *Spectra of diatomic molecules* (Van Nostrand, Toronto, 1950)
24. L.Gr. Ixaru, M. Micu, *Topics in theoretical physics* (Central Institute of Physics, Bucharest, 1978)
25. L.Gr. Ixaru, *Numerical methods for differential equations and applications* (Reidel, Dordrecht, 1984)
26. 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)
27. L.Gr. Ixaru , M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comp. Phys. Commun. **38**(3), 329–337 (1985)
28. L.Gr. Ixaru, G. Vanden Berghe, *Exponential fitting, series on mathematics and its applications*, vol. 568 (Kluwer, The Netherlands, 2004)
29. F. Iavernaro, F. Mazzia, D. Trigiante, Stability and conditioning in numerical analysis. J. Numer. Anal. Ind. Appl. Math. **1**(1), 91–112 (2006)
30. F. Iavernaro, D. Trigiante, Discrete conservative vector fields induced by the Trapezoidal Method. J. Numer. Anal. Ind. Appl. Math. **1**(1), 113–130 (2006)
31. A. Konguetsof, T.E. Simos, On the construction of exponentially-fitted methods for the numerical solution of the Schrödinger Equation. J. Comput. Methods Sci. Eng. **1**, 143–165 (2001)
32. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation. Appl. Math. Comput. **112**, 99–112 (2000)
33. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods. J. Math. Chem. **37**(3), 271–279 (2005)
34. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nystrom 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
35. A. Konguetsof, T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems. Comput. Math. Appl. **45**, 547–554 (2003)
36. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
37. 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)
38. 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)
39. J. Kierzenka, L.F. Shampine, A BVP solver that controls residual and error. J. Numer. Anal. Ind. Appl. Math. **3**, 27–41 (2008)
40. R. Knapp, A method of lines framework in mathematica. J. Numer. Anal. Ind. Appl. Math. **3**, 43–59 (2008)
41. L.D. Landau, F.M. Lifshitz, *Quantum mechanics* (Pergamon, New York, 1965)
42. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
43. R.L. Lipsman, J.E. Osborn, J.M. Rosenberg, The SCHOL project at the University of Maryland: using mathematical software in the teaching of Sophomore differential equations. J. Numer. Anal. Ind. Appl. Math. **3**, 81–103 (2008)
44. 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)
45. 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)
46. F. Mazzia, A. Sestini, D. Trigiante, BS linear multistep methods on non-uniform meshes. J. Numer. Anal. Ind. Appl. Math. **1**(1), 131–144 (2006)

47. N.S. Nedialkov, J.D. Pryce, Solving differential algebraic equations by Taylor series (III): the DAETS code. J. Numer. Anal. Ind. Appl. Math. **3**, 61–80 (2008)
48. I. Prigogine, R. Stuart (eds.), *Advances in chemical physics: new methods in computational quantum mechanics*, vol. 93 (Wiley, London, 1997)
49. 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)
50. 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)
51. G. Psihoyios, A block implicit advanced step-point (BIAS) algorithm for stiff differential systems. Comput. Lett. **2**(1–2), 51–58 (2006)
52. G. Papakaliatakis, T.E. Simos, A new method for the numerical solution of fourth order BVP with oscillating solutions. Comput. Math. Appl. **32**, 1–6 (1996)
53. 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)
54. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
55. C.D. Papageorgiou, A.D. Raptis, T.E. Simos, A method for computing phase-shifts for scattering. J. Comput. Appl. Math. **29**(1), 61–67 (1990)
56. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
57. A.D. Raptis, Exponential multistep methods for ordinary differential equations. Bull. Greek Math. Soc. **25**, 113–126 (1984)
58. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Shrödinger equation with automatic error control. Comput. Phys. Commun. **28**, 427–431 (1983)
59. A.D. Raptis, On the numerical solution of the Schrodinger equation. Comput. Phys. Commun. **24**, 1–4 (1981)
60. A.D. Raptis, T.E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problem. BIT **31**, 160–168 (1991)
61. A.D. Raptis, Two-step methods for the numerical solution of the Schrödinger equation. Computing **28**, 373–378 (1982)
62. T.E. Simos, in *Atomic structure computations in chemical modelling: applications and theory*, ed. by A. Hinchliffe The Royal Society of Chemistry (UMIST, Manchester, 2000), pp. 38–142
63. T.E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems, chemical modelling: application and theory. R. Soc. Chem. **2**, 170–270 (2002)
64. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
65. T.E. Simos, *Numerical solution of ordinary differential equations with periodical solution*. Doctoral Dissertation, (National Technical University of Athens, Greece, 1990) (in Greek)
66. T.E. Simos, P.S. Williams, A new Runge-Kutta-Nystrom method with Phase-Lag of order infinity for the numerical solution of the Schrödinger equation. Commun. Math. Comput. Chem. **45**, 123–137 (2002)
67. T.E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation. Commun. Math. Comput. Chem. **45**, 7–26 (2004)
68. 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)
69. 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)
70. T.E. Simos, Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
71. 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)
72. 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)
73. 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)

74. 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)
75. T.E. Simos, A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **25**(1), 65–84 (1999)
76. T.E. Simos, Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. J. Math. Chem. **24**(1–3), 23–37 (1998)
77. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. J. Math. Chem. **21**(4), 359–372 (1997)
78. L.F. Shampine, P.H. Muir, H. Xu, A user-friendly Fortran BVP solver. J. Numer. Anal. Ind. Appl. Math. **1**(2), 201–217 (2006)
79. T.E. Simos, P-stable four-step exponentially-fitted method for the numerical integration of the Schrödinger equation. Comput. Lett. **1**(1), 37–45 (2005)
80. T.E. Simos, Stabilization of a four-step exponentially-fitted method and its application to the Schrödinger equation. Int. J. Mod. Phys. C **18**(3), 315–328 (2007)
81. T.E. Simos, A Runge-Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution. Comput. Math. Appl. **25**, 95–101 (1993)
82. T.E. Simos, Runge-Kutta interpolants with minimal phase-lag. Comput. Math. Appl. **26**, 43–49 (1993)
83. T.E. Simos, Runge-Kutta-Nyström interpolants for the numerical integration of special second-order periodic initial-value problems. Comput. Math. Appl. **26**, 7–15 (1993)
84. T.E. Simos, G.V. Mitsou, A family of four-step exponential fitted methods for the numerical integration of the radial Schrödinger equation. Comput. Math. Appl. **28**, 41–50 (1994)
85. T.E. Simos, G. Mousadis, A two-step method for the numerical solution of the radial Schrödinger equation. Comput. Math. Appl. **29**, 31–37 (1995)
86. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **33**, 67–78 (1997)
87. T.E. Simos, A new hybrid imbedded variable-step procedure for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **36**, 51–63 (1998)
88. T.E. Simos, Bessel and Neumann fitted methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **42**, 833–847 (2001)
89. 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)
90. T.E. Simos, An exponentially fitted eighth-order method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **108**(1–2), 177–194 (1999)
91. T.E. Simos, An accurate finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **91**(1), 47–61 (1998)
92. T.E. Simos, P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**(2), 189–205 (1997)
93. T.E. Simos, A family of 4-step exponentially fitted predictor-corrector methods for the numerical-integration of the Schrödinger-equation. J. Comput. Appl. Math. **58**(3), 337–344 (1995)
94. T.E. Simos, An explicit 4-step phase-fitted method for the numerical-integration of 2nd-order initial-value problems. J. Comput. Appl. Math. **55**(2), 125–133 (1994)
95. T.E. Simos, E. Dimas, A.B. Sideridis, A Runge-Kutta-Nystrom method for the numerical-integration of special 2nd-order periodic initial-value problems. J. Comput. Appl. Math. **51**(3), 317–326 (1994)
96. A.B. Sideridis, T.E. Simos, A low-order embedded Runge-Kutta method for periodic initial-value problems. J. Comput. Appl. Math. **44**(2), 235–244 (1992)
97. T.E. Simos, A.D. Raptis, A 4th-order Bessel fitting method for the numerical-solution of the SchrÖdinger-equation. J. Comput. Appl. Math. **43**(3), 313–322 (1992)
98. T.E. Simos, Explicit 2-step methods with minimal phase-lag for the numerical-integration of special 2nd-order initial-value problems and their application to the one-dimensional Schrödinger-equation. J. Comput. Appl. Math. **39**(1), 89–94 (1992)
99. T.E. Simos, A 4-step method for the numerical-solution of the Schrödinger-equation. J. Comput. Appl. Math. **30**(3), 251–255 (1990)
100. T.E. Simos, Two-step almost P-stable complete in phase methods for the numerical integration of second order periodic initial-value problems. Inter. J. Comput. Math. **46**, 77–85 (1992)
101. M. Sofroniou, G. Spaletta, Extrapolation methods in mathematica. J. Numer. Anal. Ind. Appl. Math. **3**, 105–121 (2008)

102. R.J. Spiteri, T.-P. Ter, pythNon: a PSE for the numerical solution of nonlinear algebraic equations. J. Numer. Anal. Ind. Appl. Math. **3**, 123–137 (2008)
103. 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)
104. 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)
105. 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)
106. C. Tsitouras, T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
107. R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **87**(2), 215–226 (1997)
108. R.M. Thomas, T.E. Simos, G.V. Mitsou, A family of Numerov-type exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **67**(2), 255–270 (1996)
109. 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)
110. J. Vigo-Aguiar, T.E. Simos, A family of P-stable eighth algebraic order methods with exponential fitting facilities. J. Math. Chem. **29**(3), 177–189 (2001)
111. G. Vanden Berghe, M. Van Daele, Exponentially-fitted Stmer/Verlet methods. J. Numer. Anal. Ind. Appl. Math. **1**(3), 241–255 (2006)
112. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**, 162–174 (2005)
113. W. Weckesser, VFGEN: a code generation tool. J. Numer. Anal. Ind. Appl. Math. **3**, 151–165 (2008)
114. A. Wittkopf, Automatic code generation and optimization in Maple. J. Numer. Anal. Ind. Appl. Math. **3**, 167–180 (2008)