Research Article

An Efficient Numerical Method for the Solution of the Schrödinger Equation

Licheng Zhang¹ and Theodore E. Simos^{2,3}

¹School of Information Engineering, Chang'an University, Xi'an 710064, China

²Department of Mathematics, College of Sciences, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

³Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, 221 00 Tripolis, Greece

Correspondence should be addressed to Theodore E. Simos; tsimos.conf@gmail.com

Received 27 May 2016; Accepted 5 July 2016

Academic Editor: Maria L. Gandarias

Copyright © 2016 L. Zhang and T. E. Simos. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The development of a new five-stage symmetric two-step fourteenth-algebraic order method with vanished phase-lag and its first, second, and third derivatives is presented in this paper for the first time in the literature. More specifically we will study (1) the development of the new method, (2) the determination of the local truncation error (LTE) of the new method, (3) the local truncation error analysis which will be based on test equation which is the radial time independent Schrödinger equation, (4) the stability and the interval of periodicity analysis of the new developed method which will be based on a scalar test equation with frequency different than the frequency of the scalar test equation used for the phase-lag analysis, and (5) the efficiency of the new obtained method based on its application to the coupled Schrödinger equations.

1. Introduction

The approximate solution of the close-coupling differential equations of the Schrödinger type is studied in this paper. The above-mentioned problem has the following form:

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i + 1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^N V_{im} y_{mj}, \quad (1)$$

where $1 \leq i \leq N$ and $m \neq i$ and the boundary conditions are as follows:

$$y_{ij} = 0 \quad \text{at } x = 0 \quad (2)$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x) \delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x), \quad (3)$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions. We will examine the case in which all channels are open (see [1]).

Defining a matrix K' and diagonal matrices M, N by (see [1])

$$\begin{aligned} K'_{ij} &= \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij}, \\ M_{ij} &= k_i x j_{l_i}(k_i x) \delta_{ij}, \\ N_{ij} &= k_i x n_{l_i}(k_i x) \delta_{ij} \end{aligned} \quad (4)$$

we obtain a new form of the asymptotic condition (3):

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N} \mathbf{K}'. \quad (5)$$

In several scientific areas (e.g., quantum chemistry, theoretical physics, material science, atomic physics, and molecular physics) there exists a real problem which is the rotational excitation of a diatomic molecule by neutral particle impact. The mathematical model of this problem can be expressed with close-coupling differential equations arising from the Schrödinger equation. Denoting, as in [1],

the entrance channel by the quantum numbers (j, l) , the exit channels by (j', l') , and the total angular momentum by $J = j + l = j' + l'$, we find that

$$\begin{aligned} & \left[\frac{d^2}{dx^2} + k_{j'l}^2 - \frac{l'(l'+1)}{x^2} \right] y_{j'l'}^{Jl}(x) \\ &= \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J | V | j''l''; J \rangle y_{j''l''}^{Jl}(x), \end{aligned} \quad (6)$$

where

$$k_{j'l}^2 = \frac{2\mu}{\hbar^2} \left[E + \frac{\hbar^2}{2I} \{ j(j+1) - j'(j'+1) \} \right]. \quad (7)$$

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

The above-described problem will be solved numerically via finite difference method of the form of special multistep method.

The multistep finite difference method has the general form

$$\sum_{i=-m}^m c_i y_{n+i} = h^2 \sum_{i=-m}^m b_i f(x_{n+i}, y_{n+i}), \quad (8)$$

where $\{x_i\}_{i=-m}^m$ are distinct points within the integration area and h given by $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$ is the step size or step length of the integration.

Remark 1. A method (8) is called symmetric multistep method or symmetric $2m$ -step method if $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)m$.

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

$$y'' = -\phi^2 y, \quad (9)$$

we obtain the difference equation

$$\begin{aligned} & A_m(v) y_{n+m} + \dots + A_1(v) y_{n+1} + A_0(v) y_n \\ & + A_1(v) y_{n-1} + \dots + A_m(v) y_{n-m} = 0 \end{aligned} \quad (10)$$

and the associated characteristic equation

$$\begin{aligned} & A_m(v) \lambda^m + \dots + A_1(v) \lambda + A_0(v) + A_1(v) \lambda^{-1} + \dots \\ & + A_m(v) \lambda^{-m} = 0, \end{aligned} \quad (11)$$

where $v = \phi h$, h is the step length, and $A_j(v)$ $j = 0(1)k$ are polynomials of v .

We give some definitions.

Definition 2 (see [2]). For a symmetric $2m$ -step method with characteristic equation given by (11) one will say that it has an

interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots λ_i , $i = 1(1)2m$, of (11) satisfy

$$\begin{aligned} \lambda_1 &= e^{i\theta(v)}, \\ \lambda_2 &= e^{-i\theta(v)}, \\ |\lambda_i| &\leq 1, \quad i = 3(1)2m, \end{aligned} \quad (12)$$

where $\theta(v)$ is a real function of v .

Definition 3 (see [2]). One calls P-stable method a multistep method if its interval of periodicity is equal to $(0, \infty)$.

Definition 4. One calls singularly P-stable method a multistep method if its interval of periodicity is equal to $(0, \infty) - S$ (where S is a set of distinct points).

Definition 5 (see [3, 4]). For a symmetric $2m$ -step method with the characteristic equation given by (11), one defines as the phase-lag the leading term in the expansion of

$$t = v - \theta(v). \quad (13)$$

Then, if the quantity $t = O(v^{q+1})$ as $v \rightarrow \infty$, the order of the phase-lag is q .

Definition 6 (see [5]). One calls symmetric $2m$ -step method phase-fitted if its phase-lag is equal to zero.

Theorem 7 (see [3]). The symmetric $2m$ -step method with characteristic equation given by (11) has phase-lag order q and phase-lag constant c given by

$$\begin{aligned} & -cv^{q+2} + O(v^{q+4}) \\ &= \frac{2A_m(v) \cos(mv) + \dots + 2A_j(v) \cos(jv) + \dots + A_0(v)}{2m^2 A_m(v) + \dots + 2j^2 A_j(v) + \dots + 2A_1(v)}. \end{aligned} \quad (14)$$

2. The New Five-Stage Fourteenth-Algebraic Order P-Stable Two-Step Method with Vanished Phase-Lag and Its First, Second, and Third Derivatives

We consider the following family of five-stage symmetric two-step methods:

$$\begin{aligned} \hat{y}_n &= y_n - a_0 h^2 (f_{n+1} - 2f_n + f_{n-1}), \\ \check{y}_n &= y_n - a_1 h^2 (f_{n+1} - 2\hat{f}_n + f_{n-1}) - 2a_2 h^2 \hat{f}_n, \\ \hat{y}_{n+1/2} &= \frac{1}{2} (y_n + y_{n+1}) - h^2 \left[a_3 \check{f}_n + \left(\frac{1}{8} - a_3 \right) f_{n+1} \right], \\ \hat{y}_{n-1/2} &= \frac{1}{2} (y_n + y_{n-1}) - h^2 \left[a_3 \check{f}_n + \left(\frac{1}{8} - a_3 \right) f_{n-1} \right], \\ y_{n+1} + a_4 y_n + y_{n-1} &= h^2 \left[b_1 (f_{n+1} + f_{n-1}) + b_0 f_n + b_2 (\hat{f}_{n+1/2} + \hat{f}_{n-1/2}) \right], \end{aligned} \quad (15)$$

where $a_0 = 45469/862066800$, $a_1 = -2793/26878564$, $a_2 = -86919/13439282$, $a_3 = 6719641/52720800$, $f_{n+i} = y''(x_{n+i}, y_{n+i})$, $i = -1(1/2)1$, $\hat{f}_n = y''(x_n, \hat{y}_n)$, $\check{f}_n = y''(x_n, \check{y}_n)$, and a_4, b_j , $j = 0(1)2$, are free parameters.

Application of the above-mentioned method (15) to the scalar test equation (9) leads to the difference equation (10) and the characteristic equation (11) with $m = 1$ and

$$\begin{aligned} A_1(v) &= 1 + v^2 \left(b_1 + \frac{1}{2} b_2 \right) - v^4 b_2 \left(a_3 - \frac{1}{8} \right) \\ &\quad + 2v^6 b_2 a_1 a_3 + 4v^8 b_2 a_0 a_3 (a_2 - a_1), \\ A_0(v) &= a_4 + v^2 (b_0 + b_2) + 2v^4 b_2 a_3 \\ &\quad + 4v^6 b_2 a_3 (a_2 - a_1) \\ &\quad - 8v^8 b_2 a_0 a_3 (a_2 - a_1). \end{aligned} \quad (16)$$

If we request the new method (15) to have vanished phase-lag and its first, second, and third derivatives, then the following system of equations is obtained:

$$\begin{aligned} \text{Phase-Lag (PL)} &= \frac{T_0}{T_{\text{denom}}} = 0, \\ \text{First Derivative of the Phase-Lag} &= \frac{T_1}{T_{\text{denom}}^2} = 0, \\ \text{Second Derivative of the Phase-Lag} &= \frac{T_2}{T_{\text{denom}}^3} = 0, \\ \text{Third Derivative of the Phase-Lag} &= \frac{T_3}{T_{\text{denom}}^4} = 0, \end{aligned} \quad (17)$$

where T_j , $j = 0(1)3$, are given in Appendix A.

Now solving the system of (17) we determine the other coefficients of the new obtained three-stage two-step method:

$$\begin{aligned} b_0 &= \frac{1}{136407} \frac{T_4}{T_{\text{denom1}}}, \\ b_1 &= \frac{1}{136407} \frac{T_5}{T_{\text{denom1}}}, \\ b_2 &= \frac{1}{45469} \frac{T_6}{T_{\text{denom1}}}, \\ a_4 &= \frac{T_7}{T_{\text{denom2}}}, \end{aligned} \quad (18)$$

where the formulae T_j , $j = 4(1)7$, T_{denom1} , and T_{denom2} are given in Appendix B.

Additionally to the above formulae for the coefficients a_4 , b_j , $j = 0(1)2$, we give also the following Taylor series expansions of these coefficients, for the case of heavy

cancellations for some values of $|v|$ in the formulae given by (18):

$$\begin{aligned} b_0 &= \frac{73205}{63882} + \frac{268231049v^{10}}{262060331977892448} \\ &\quad - \frac{473946402833v^{12}}{224533292438658249446400} \\ &\quad - \frac{841146961608850447v^{14}}{26876635104907392458734080000} \\ &\quad - \frac{34711252155550520483v^{16}}{23840650403457053406595478323200} \\ &\quad - \frac{450175574700292070703419v^{18}}{7016973932030008047188109768345600000} \\ &\quad + \dots, \\ b_1 &= \frac{51911}{383292} + \frac{268231049v^{10}}{1572361991867354688} \\ &\quad - \frac{61738277963993v^{12}}{1347199754631949496678400} \\ &\quad - \frac{559868876269811659v^{14}}{161259810629444354752404480000} \\ &\quad - \frac{602760578937670659833v^{16}}{3576097560518558010989321748480000} \\ &\quad - \frac{526438577422138492034251v^{18}}{84203687184360096566257317220147200000} \\ &\quad + \dots, \\ b_2 &= -\frac{19970}{95823} - \frac{268231049v^{10}}{393090497966838672} \\ &\quad + \frac{15790029293123v^{12}}{336799938657987374169600} \\ &\quad + \frac{181541151070183v^{14}}{40314952657361088688101120} \\ &\quad + \frac{21664254981643052111v^{16}}{89402439012963950274733043712000} \\ &\quad + \frac{8364955394669318397937v^{18}}{842036871843600965662573172201472000} \\ &\quad + \dots, \\ a_4 &= -2 + \frac{134317v^{16}}{15752663892725760} \\ &\quad + \frac{1170023347v^{18}}{421777575727322240000} + \dots. \end{aligned} \quad (19)$$

The behavior of the coefficients is given in Figure 1.

FIGURE 1: Behavior of the coefficients of the new obtained method given by (18) for several values of $\nu = \phi h$.

The local truncation error of the new developed five-stage two-step method (15) with the coefficients given by (18)-(19), which is indicated as NM2S5S3DV, is given by

$$\begin{aligned} \text{LTE}_{\text{NM2S5S3DV}} &= \frac{134317}{551343236245401600} h^{16} (y_n^{(16)} \\ &+ 56\phi^{10} y_n^{(6)} + 140\phi^{12} y_n^{(4)} + 120\phi^{14} y_n^{(2)} + 35\phi^{16} y_n) \\ &+ O(h^{18}). \end{aligned} \quad (20)$$

3. Analysis of the Method

3.1. Error Analysis. The test equation used for the local truncation error (LTE) analysis is given by

$$y''(x) = (V(x) - V_c + G) y(x), \quad (21)$$

where $V(x)$ is a potential function, V_c is a constant value approximation of the potential for the specific x , and $G = V_c - E$ and E is the energy. This is the radial time independent Schrödinger equation.

We will study the following methods.

3.1.1. Classical Method (i.e., Method (15) with Constant Coefficients)

$$\text{LTE}_{\text{CL}} = \frac{134317}{551343236245401600} h^{16} y_n^{(16)} + O(h^{18}). \quad (22)$$

3.1.2. The Five-Stage Two-Step Method with Vanished Phase-Lag and Its First, Second, and Third Derivatives Developed in Section 3

$$\begin{aligned} \text{LTE}_{\text{NM2S5S3DV}} &= \frac{134317}{551343236245401600} h^{16} (y_n^{(16)} \\ &+ 56\phi^{10} y_n^{(6)} + 140\phi^{12} y_n^{(4)} + 120\phi^{14} y_n^{(2)} + 35\phi^{16} y_n) \\ &+ O(h^{18}). \end{aligned} \quad (23)$$

If we substitute the higher order derivatives requested in the LTE formulae, which are obtained using the test problem (21), into the LTE expressions, we produce new formulae of LTE which have the general form

$$\text{LTE} = h^p \sum_{i=0}^m a_i G^i, \quad (24)$$

where a_i are constant numbers (classical methods) or formulae of ϕ (fitted methods) and p is the algebraic order of the specific method.

Two cases of the parameter G are studied:

- (i) *The Energy and the Potential Are Closed to Each Other.* Consequently, $G = V_c - E \approx 0 \Rightarrow G^i = 0, i = 1, 2, \dots$

Therefore, the local truncation error for the classical method (constant coefficients) and the local truncation error for the five-stage two-step method with eliminated phase-lag and its first, second, and third derivatives developed in Section 3 are the same since the formulae of the LTE are free from G (i.e., $\text{LTE} = h^p a_0$ in (24)) and the free from G terms (i.e., the terms of the formulae which do not have the quantity G) in the local truncation errors in this case are the same and are given in Appendix C. From the above it is easy to see that, for these values of G , the methods are of comparable accuracy.

- (ii) *The Energy and the Potential Have Big Difference.* Consequently, $G \gg 0$ or $G \ll 0$ and $|G|$ is a large number. For this case the most accurate method is the method with the minimum power of G in the formulae of LTE (i.e., the method with the highest accuracy is the method with minimum i in (24)).

We give now the asymptotic expansions of the local truncation errors.

3.1.3. Classical Method

$$\begin{aligned} \text{LTE}_{\text{CL}} &= \frac{134317}{551343236245401600} h^{16} (y(x) G^8 + \dots) \\ &+ O(h^{18}). \end{aligned} \quad (25)$$

3.1.4. The Four-Stage Two-Step P-Stable Method with Vanished Phase-Lag and Its First, Second, and Third Derivatives Developed in Section 3

$$\begin{aligned} \text{LTE}_{\text{NM2S5S3DV}} &= \frac{134317}{9845414932953600} \\ &\cdot h^{16} \left[\left(20g(x) y(x) \frac{d^2}{dx^2} g(x) \right. \right. \\ &+ 15 \left(\frac{d}{dx} g(x) \right)^2 y(x) \\ &+ 10 \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) \\ &\left. \left. + 31 \left(\frac{d^4}{dx^4} g(x) \right) y(x) \right) G^5 + \dots \right] + O(h^{18}). \end{aligned} \quad (26)$$

The above leads us to the following theorem.

Theorem 8. (i) *Classical method (i.e., method (15) with constant coefficients): for this method the error increases as the eighth power of G .*

(ii) *Fourteenth-algebraic order five-stage two-step method with vanished phase-lag and its first, second, and third derivatives developed in Section 3: for this method the error increases as the fifth power of G .*

Therefore, for large values of $|G| = |V_c - E|$, the new developed fourteenth-algebraic order five-stage two-step method with vanished phase-lag and its first, second, and third derivatives developed in Section 3 is the most accurate method for the numerical solution of the radial Schrödinger equation.

3.2. Stability and Interval of Periodicity Analysis. Let us define the scalar test equation for the stability and interval of periodicity analysis:

$$y'' = -\omega^2 y. \quad (27)$$

Remark 9. Comparing the test equations (9) and (27), we have that the frequency ϕ is not equal to the frequency ω ; that is, $\omega \neq \phi$.

The difference equation which is produced after application of the new method (15) with the coefficients given by (18)-(19) to the scalar test equation (27) is given by

$$A_1(s, \nu) (y_{n+1} + y_{n-1}) + A_0(s, \nu) y_n = 0, \quad (28)$$

where

$$\begin{aligned} A_1(s, \nu) &= 1 + \frac{1}{8} (8b_1 + 4b_2) s^2 + \frac{1}{8} b_2 (-8a_3 + 1) s^4 \\ &+ 4a_3 b_2 \left(\nu^2 a_0 a_2 + \frac{1}{2} a_1 \right) s^6 \\ &- 4a_0 a_1 a_3 b_2 s^8, \\ A_0(s, \nu) &= a_4 + (b_0 + b_2) s^2 + 4a_3 b_2 \left(\nu^2 a_2 + \frac{1}{2} \right) s^4 \end{aligned}$$

FIGURE 2: s - v plane of the new obtained five-stage symmetric two-step fourteenth-algebraic order method with vanished phase-lag and its first, second, and third derivatives.

$$\begin{aligned}
 & -8a_3b_2 \left(v^2 a_0 a_2 + \frac{1}{2} a_1 \right) s^6 \\
 & + 8a_0 a_1 a_3 b_2 s^8,
 \end{aligned} \tag{29}$$

$s = \omega h$, and $v = \phi h$.

Taking into account the coefficients a_i , $i = 0, 1$, and b_i , $i = 0(1)2$, and their substitution into formulae (29), the new stability polynomials are produced:

$$\begin{aligned}
 A_1(s, v) &= \frac{T_8}{T_{\text{denom}3}}, \\
 A_0(s, v) &= \frac{T_9}{T_{\text{denom}3}},
 \end{aligned} \tag{30}$$

where the formulae T_k , $k = 8, 9$, and $T_{\text{denom}3}$ are given in Appendix D.

s - v plane of the new produced method is shown in Figure 2.

Remark 10. Observing s - v region we can define two areas:

- (i) The shadowed area which defines the area where the method is stable.
- (ii) The white area which defines the area where the method is unstable.

For problems of the form of the coupled equations arising from the Schrödinger equation and related problems (in quantum chemistry, material science, theoretical physics, atomic physics, astronomy, astrophysics, physical chemistry, and chemical physics), the area of the region which plays critical role in the stability of the numerical methods is the surroundings of the first diagonal of the s - v plane, where $s = v$. Studying this case, we found that the interval of periodicity is equal to $(0, 24)$.

The above development leads to the following theorem.

Theorem 11. *The five-stage symmetric two-step method developed in Section 3*

- (i) *is of fourteenth algebraic order,*

- (ii) *has vanished the phase-lag and its first, second, and third derivatives,*
- (iii) *has an interval of periodicity equal to $(0, 24)$ (when $s = v$).*

4. Numerical Results

We will apply the new produced method to the approximate solution for coupled differential equations of the Schrödinger type.

4.1. Error Estimation. For the numerical solution of the previously referred problem we will use variable step methods. An algorithm is called variable step when it is based on the change of the step size of the integration using a local truncation error estimation (LTEE) procedure. In the past decades several methods of constant or variable steps have been developed for the approximation of coupled differential equations of the Schrödinger type and related problems (see, e.g., [1–55]).

In our numerical tests we use local estimation procedure which is based on an embedded pair and on the fact that we have better approximation for the problems with oscillatory and/or periodical solutions having maximal algebraic order of the methods.

The local truncation error in y_{n+1}^L is estimated by

$$\text{LTE} = |y_{n+1}^H - y_{n+1}^L|, \tag{31}$$

where y_{n+1}^L gives the lower algebraic order solution which is obtained using the twelfth-algebraic order method developed in [54] and y_{n+1}^H gives the higher order solution which is obtained using the five-stage symmetric two-step method of fourteenth algebraic order with vanished phase-lag and its first, second, and third derivatives developed in Section 3.

In our numerical tests the changes of the step sizes are reduced on duplication of step sizes. We use the following procedure:

- (i) If $\text{LTE} < \text{acc}$ then the step size is duplicated; that is, $h_{n+1} = 2h_n$.
- (ii) If $\text{acc} \leq \text{LTE} \leq 100 \text{acc}$ then the step size remains stable; that is, $h_{n+1} = h_n$.
- (iii) If $100 \text{acc} < \text{LTE}$ then the step size is halved and the step is repeated; that is, $h_{n+1} = (1/2)h_n$.

In the above, h_n is the step length used for the n th step of the integration and acc is the requested accuracy of the local truncation error (LTE).

Remark 12. The local extrapolation technique is also used; that is, while for a local truncation error estimation less than acc we use the lower algebraic order solution y_{n+1}^L it is the higher algebraic order solution y_{n+1}^H which is accepted at each point as integration.

4.2. Coupled Differential Equations. We will present the numerical solution of the coupled Schrödinger equations

(1) using the boundary conditions (2) and (3). Mathematical models of this form are observed in many real problems in quantum chemistry, material science, theoretical physics, atomic physics, physical chemistry and chemical physics, and so forth. The methodology fully described in [1] will be used for the approximate solution for this problem.

Equation (1) contains the potential V which can be presented as (see for details [1])

$$V(x, \hat{\mathbf{k}}_{j'j}, \hat{\mathbf{k}}_{jj}) = V_0(x) P_0(\hat{\mathbf{k}}_{j'j}, \hat{\mathbf{k}}_{jj}) + V_2(x) P_2(\hat{\mathbf{k}}_{j'j}, \hat{\mathbf{k}}_{jj}). \quad (32)$$

Based on (32), the coupling matrix element is given by

$$\langle j'l'; J | V | j''l''; J \rangle = \delta_{j'l'} \delta_{j''l''} V_0(x) + f_2(j'l', j''l''; J) V_2(x), \quad (33)$$

where f_2 coefficients are obtained from formulas given by Bernstein et al. [56] and $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i , $i = 0, 2$, are Legendre polynomials (see for details [57]). The above leads to the new form of boundary conditions:

$$y_{j'l'}^{Jl}(x) = 0 \quad \text{at } x = 0 \quad (34)$$

$$y_{j'l'}^{Jl}(x) \sim \delta_{jj'} \delta_{ll'} \exp \left[-i \left(k_{jj} x - \frac{1}{2} l \pi \right) \right], \quad (35)$$

$$- \left(\frac{k_i}{k_j} \right)^{1/2} S^J(jl; j'l') \exp \left[i \left(k_{j'j} x - \frac{1}{2} l' \pi \right) \right],$$

where

$$\mathbf{S} = (\mathbf{I} + i\mathbf{K})(\mathbf{I} - i\mathbf{K})^{-1}. \quad (36)$$

We will use the variable step method described in Section 4.1 in order to compute the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles.

We use the following parameters in our example:

$$\begin{aligned} \frac{2\mu}{\hbar^2} &= 1000.0, \\ \frac{\mu}{I} &= 2.351, \\ E &= 1.1, \end{aligned} \quad (37)$$

$$V_0(x) = \frac{1}{x^{12}} - 2 \frac{1}{x^6},$$

$$V_2(x) = 0.2283 V_0(x).$$

For our test we take $J = 6$ and we will consider excitation of the rotator from $j = 0$ state to levels up to $j' = 2, 4$, and 6 which is equivalent to sets of *four, nine, and sixteen coupled differential equations*, respectively. Using the methodology fully described by Bernstein [57] and Allison [1], we consider

TABLE 1: Coupled differential equations. Real time of computation (in seconds) (RTC) and maximum absolute error (MErr) to calculate $|S|^2$ for the variable step methods, Method I–Method X. $\text{acc} = 10^{-6}$. We note that $h_{\max}$ is the maximum step size. N indicates the number of equations of the set of coupled differential equations.

Method	N	$h_{\max}$	RTC	MErr
Method I	4	0.014	3.25	1.2×10^{-3}
	9	0.014	23.51	5.7×10^{-2}
	16	0.014	99.15	6.8×10^{-1}
Method II	4	0.056	1.55	8.9×10^{-4}
	9	0.056	8.43	7.4×10^{-3}
	16	0.056	43.32	8.6×10^{-2}
Method III	4	0.007	45.15	9.0×10^0
	9			
	16			
Method IV	4	0.112	0.39	1.1×10^{-5}
	9	0.112	3.48	2.8×10^{-4}
	16	0.112	19.31	1.3×10^{-3}
Method V	4	0.448	0.14	3.4×10^{-7}
	9	0.448	1.37	5.8×10^{-7}
	16	0.448	9.58	8.2×10^{-7}
Method VI	4	0.448	0.09	2.9×10^{-7}
	9	0.448	1.10	4.5×10^{-7}
	16	0.448	8.57	7.4×10^{-7}
Method VII	4	0.448	0.06	1.3×10^{-7}
	9	0.448	1.04	1.7×10^{-7}
	16	0.448	7.58	2.9×10^{-7}
Method VIII	4	0.448	0.04	8.8×10^{-8}
	9	0.448	1.02	9.2×10^{-8}
	16	0.448	7.48	8.9×10^{-8}
Method IX	4	0.448	0.04	9.7×10^{-8}
	9	0.448	1.01	1.2×10^{-7}
	16	0.448	7.15	2.3×10^{-7}
Method X	4	0.896	0.02	7.0×10^{-8}
	9	0.896	0.45	5.7×10^{-8}
	16	0.896	6.11	6.5×10^{-8}

the potential infinite for $x < x_0$. The wave functions then tend to zero and then the boundary conditions (34) are given by

$$y_{j'l'}^{Jl}(x_0) = 0. \quad (38)$$

For comparison purposes the following variable step methods are used:

- (i) *Method I.* The iterative Numerov method of Allison [1].
- (ii) *Method II.* The variable step method of Raptis and Cash [47].
- (iii) *Method III.* The embedded Runge-Kutta Dormand and Prince method 5(4) [49].
- (iv) *Method IV.* The embedded Runge-Kutta method ERK4(2) developed in Simos [41].

- (v) *Method V*. The embedded symmetric two-step method developed in [50].
- (vi) *Method VI*. The embedded symmetric two-step method developed in [52].
- (vii) *Method VII*. The embedded symmetric two-step method developed in [52].
- (viii) *Method VIII*. The embedded symmetric two-step method developed in [53].
- (ix) *Method IX*. The embedded symmetric two-step method developed in [54].
- (x) *Method X*. The developed embedded symmetric two-step method developed in this paper.

The results are presented in Table 1. More specifically, we present (1) the requested real time of computation by the variable step methods mentioned above in order to calculate the square of the modulus of $\mathbf{S}$ matrix for sets of 4, 9, and 6 coupled differential equations and (2) the maximum error in the computation of the square of the modulus of $\mathbf{S}$ matrix.

5. Conclusions

In this paper we introduce, for the first time in the literature, a new five-stage symmetric two-step fourteenth-algebraic order family of methods and we produced a method of the

family with vanished phase-lag and its first, second, and third derivatives. In this paper,

- (1) we introduced the new family of methods,
- (2) we developed the new method of the new family with vanished phase-lag and its first, second, and third derivatives,
- (3) we analyzed the local truncation error,
- (4) we analyzed the interval of periodicity and the stability of the new developed method,
- (5) finally, we analyzed the efficiency of the new obtained method on the numerical solution for coupled Schrödinger equations.

From the analysis presented above, we conclude that the new developed method is much more efficient than the known ones for the numerical solution for the coupled Schrödinger equations.

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

Appendix

A. Formulae of T_j , $j = 0(1)3$, and T_{denom}

$$\begin{aligned}
 T_0 &= (45469v^8b_2 + 7038360b_2v^6 + 652886640b_2v^4 - 265712832000 \\
 &\quad + (-265712832000b_1 - 132856416000b_2)v^2) \cos(v) - 45469v^8b_2 \\
 &\quad + 431033400b_2v^6 - 33866990640b_2v^4 + (-132856416000b_0 - 132856416000b_2)v^2 \\
 &\quad - 132856416000a_4, \\
 T_1 &= -2067429961 \left(-\frac{265712832000}{45469} + v^8b_2 + \frac{7038360b_2v^6}{45469} + \frac{652886640b_2v^4}{45469} \right. \\
 &\quad \left. + \left(-\frac{265712832000b_1}{45469} - \frac{132856416000b_2}{45469} \right) v^2 \right)^2 \sin(v) - 39837369710880 \\
 &\quad \cdot \left(v^{12}b_2^2 - \frac{4393400v^{10}b_2^2}{28973} - \frac{26360400v^8b_2}{28973} \left(b_0 + 2b_1 + \frac{153226717033b_2}{4994087615} \right) \right. \\
 &\quad \left. - \frac{17669903328000b_2v^6}{188196191} \left(b_0 + \frac{45469a_4}{3519180} - \frac{16290b_1}{133} - \frac{8012b_2}{133} + \frac{45469}{1759590} \right) \right. \\
 &\quad \left. - \frac{819540618336000b_2v^4}{188196191} \left(b_0 + \frac{8379a_4}{259082} + \frac{13439282b_1}{129541} + \frac{6849182b_2}{129541} - \frac{513135}{129541} \right) \right)
 \end{aligned}$$

$$\begin{aligned}
& -\frac{1639081236672000v^2b_2}{188196191}\left(a_4 + \frac{13439282}{129541}\right) \\
& + \left(\frac{166768965158400000a_4}{188196191} - \frac{333537930316800000}{188196191}\right)b_2 \\
& + \frac{333537930316800000a_4b_1}{188196191} - \frac{333537930316800000b_0}{188196191}\Big)v, \\
T_2 = & -94003972896709\left(-\frac{265712832000}{45469} + v^8b_2 + \frac{7038360b_2v^6}{45469} + \frac{652886640b_2v^4}{45469}\right. \\
& + \left(-\frac{265712832000b_1}{45469} - \frac{132856416000b_2}{45469}\right)v^2\Big)^3 \cos(v) + 5434096090152008160v^{20}b_2^3 \\
& - 1653746424225668236800v^{18}b_2^3 - 11536196067878150592000b_2^2 \\
& \cdot \left(b_0 + 2b_1 + \frac{227930737228b_2}{4994087615}\right)v^{16} - 2295953942267723189760000b_2^2 \\
& \cdot \left(b_0 + \frac{45469a_4}{5278770} - \frac{16290b_1}{133} - \frac{7009130426558198b_2}{125536380378255} + \frac{45469}{2639385}\right)v^{14} \\
& - 194734009025384053800960000b_2^2\left(b_0 + \frac{6730730601a_4}{290822990464} + \frac{379717697333b_1}{18176436904}\right. \\
& + \left.\frac{127130652893979671b_2}{15971271578806720} - \frac{356864310411}{145411495232}\right)v^{12} \\
& - 48153927914830003875840000000b_2\left(\frac{541122054664b_2^2}{24970438075}\right. \\
& + \left(\frac{72734780969b_0}{99881752300} + \frac{12770448547a_4}{1198581027600} + \frac{2191635189987b_1}{49940876150} + \frac{63965810599}{599290513800}\right) \\
& \cdot b_2 + b_1(b_0 + 2b_1)\Big)v^{10} - 2981589039377359573155840000000b_2 \\
& \cdot \left(-\frac{1773970067669b_2^2}{73624597200} + \left(\frac{90405467881b_0}{147249194400} + \frac{58393539227a_4}{6184466164800}\right.\right. \\
& - \left.\frac{8073535624019b_1}{73624597200} + \frac{141363876421}{114527151200}\right)b_2 - \frac{16290b_1^2}{133} + \left(b_0 - \frac{45469a_4}{14076720} + \frac{591097}{7038360}\right)b_1 \\
& + \frac{45469b_0}{1005480}\Big)v^8 - 460959572442991450610073600000000b_2\left(\frac{3424591b_2^2}{129541}\right. \\
& + \left(\frac{1}{2}b_0 - \frac{12668968199a_4}{682950515280} + \frac{13568823b_1}{129541} - \frac{2869992664019}{341475257640}\right)b_2 + \frac{13439282b_1^2}{129541} \\
& + \left(b_0 - \frac{11172a_4}{129541} - \frac{2907765}{129541}\right)b_1 + \frac{69825b_0}{259082} + \frac{45469a_4}{23317380} + \frac{45469}{11658690}\Big)v^6
\end{aligned}$$

$$\begin{aligned}
& -553151486931589740732088320000000b_2 \left(\left(-\frac{3}{8}a_4 + \frac{7237805}{518164} \right) b_2 + \left(-\frac{3}{4}a_4 + \frac{6719641}{259082} \right) b_1 \right. \\
& + b_0 + \frac{13965a_4}{1036328} - \frac{855225}{518164} \Big) v^4 + ((-14070153905048863102795776000000000a_4 \\
& + 28140307810097726205591552000000000) b_2^2 + ((-56280615620195452411183104000000000a_4 \\
& + 56280615620195452411183104000000000) b_1 + 28140307810097726205591552000000000b_0 \\
& - 276575743465794870366044160000000a_4 - 28693459297029315946323640320000000) b_2 \\
& + 56280615620195452411183104000000000b_1 (-a_4b_1 + b_0)) v^2 \\
& + (9380102603365908735197184000000000a_4 - 18760205206731817470394368000000000) b_2 \\
& + 18760205206731817470394368000000000a_4b_1 - 18760205206731817470394368000000000b_0, \\
T_3 = & 4274266643640461521 \left(-\frac{265712832000}{45469} + v^8b_2 + \frac{7038360b_2v^6}{45469} + \frac{652886640b_2v^4}{45469} \right. \\
& + \left(-\frac{265712832000b_1}{45469} - \frac{132856416000b_2}{45469} \right) v^2 \Big)^4 \sin(v) - 988331660492486636108160 \\
& \cdot \left(v^{26}b_2^4 - \frac{703331165780v^{24}b_2^4}{1317373337} - \frac{17573600b_2^3v^{22}}{4139} \left(b_0 + 2b_1 + \frac{52341891953b_2}{998817523} \right) \right. \\
& - \frac{229708743264000v^{20}b_2^3}{188196191} \left(b_0 + \frac{45469a_4}{6099912} - \frac{16290b_1}{133} - \frac{20280808515977707b_2}{362660654426070} + \frac{45469}{3049956} \right) \\
& - \frac{1218751529857909344000v^{18}b_2^3}{8557092608579} \left(b_0 + \frac{8254669605a_4}{385284849578} - \frac{663166829662b_1}{192642424789} \right. \\
& - \frac{2052773129691092548765b_2}{192414629552462777647} - \frac{394861571517}{192642424789} \Big) \\
& - \frac{11673827561088000000b_2^2v^{16}}{188196191} \left(\frac{25981841558644066102303b_2^2}{997636444251855529000} \right. \\
& + \left(\frac{14436736503248b_0}{20643288160585} + \frac{672095448881a_4}{83900671932000} + \frac{61372103581289784b_1}{1135380848832175} - \frac{6194383101859}{41950335966000} \right) b_2 \\
& \left. + b_1(b_0 + 2b_1) \right) - \frac{84512160980083888128000000b_2^2v^{14}}{8557092608579} \left(-\frac{200253323882994581b_2^2}{15064365645390600} \right.
\end{aligned}$$

$$\begin{aligned}
& + \left(\frac{17737276339168999b_0}{30128731290781200} + \frac{4562567732722819a_4}{632703357106405200} - \frac{56067458474270819b_1}{792861349757400} + \frac{170062002887713063}{316351678553202600} \right) b_2 \\
& - \frac{105220b_1^2}{1197} + \left(b_0 + \frac{45469a_4}{12669048} + \frac{591097}{15836310} \right) b_1 + \frac{45469b_0}{3016440} \\
& - \frac{244441255786320657705467904000000b_2^2v^{12}}{389082443819478551} \left(-\frac{18787681229658547b_2^2}{7985635789403360} \right. \\
& + \left(\frac{8969884197456053b_0}{15971271578806720} + \frac{3422548232166571a_4}{383310517891361280} - \frac{136160476648092927b_1}{7985635789403360} - \frac{280627602486327149}{191655258945680640} \right) b_2 \\
& - \frac{222153379571b_1^2}{9088218452} + \left(b_0 + \frac{380984751a_4}{72705747616} - \frac{154401947847}{36352873808} \right) b_1 \\
& + \frac{1650933921b_0}{36352873808} + \frac{2067429961a_4}{8724689713920} + \frac{2067429961}{4362344856960} \left. \right) - \frac{443126540219477925888000000000b_2v^{10}}{8557092608579} \\
& \cdot \left(\frac{4028587739494373897b_2^3}{438820490554820000} + \left(\frac{434912403523211147b_0}{877640981109640000} + \frac{2926099586132929a_4}{1755281962219280000} \right. \right. \\
& + \frac{15313712383120673847b_1}{438820490554820000} - \frac{144221396158735377}{877640981109640000} \left. \right) b_2^2 + \left(\frac{15500862502b_1^2}{454007965} \right. \\
& + \left(\frac{7273478096b_0}{49940876150} - \frac{7528278019a_4}{1997635046000} - \frac{539180954813}{499408761500} \right) b_1 \\
& + \left. \frac{98566938253b_0}{1997635046000} + \frac{49343a_4}{87868000} - \frac{100387}{2196700} \right) b_2 + b_1^2 (b_0 + 2b_1) \left. \right) \\
& - \frac{623776823123832930890612736000000000v^8b_2}{389082443819478551} \left(-\frac{665172562469b_2^3}{73624597200} \right. \\
& + \left(\frac{53593169281b_0}{147249194400} - \frac{2554367727834151a_4}{1811388909895488000} - \frac{547986492173b_1}{8180510800} + \frac{267706836641709133}{143004387623328000} \right) b_2^2 \\
& + \left(-\frac{5855940613619b_1^2}{36812298600} + \left(\frac{90405467881b_0}{73624597200} + \frac{2390206957a_4}{309223308240} + \frac{1205462023201}{386529135300} \right) b_1 \right. \\
& + \frac{28440383893b_0}{220873791600} + \frac{12770448547a_4}{7421359397760} - \frac{109828438403}{3710679698880} \left. \right) b_2 + \left(-\frac{16290b_1^2}{133} + \left(b_0 + \frac{45469a_4}{1407672} + \frac{45469}{185220} \right) b_1 + \frac{45469b_0}{502740} \right) b_1 \left. \right) \\
& - \frac{14217419993770846548447510528000000000b_2v^6}{389082443819478551} \left(\left(\frac{23281985157a_4}{167808706810} - \frac{2683972235033}{83904353405} \right) b_2^2 \right. \\
& + \left(\left(\frac{96906582357a_4}{83904353405} - \frac{14553382412876}{83904353405} \right) b_1 + b_0 + \frac{58393539227a_4}{1761991421505} + \frac{439542930952}{251713060215} \right) b_2 \\
& + \left(\frac{29449838880a_4}{16780870681} - \frac{3607051694400}{16780870681} \right) b_1^2 + \left(-\frac{3995270092a_4}{352398284301} + \frac{51938511196}{352398284301} \right) b_1 + \frac{9988175230b_0}{117466094767} \left. \right) \\
& + \frac{231449118350975844469748269056000000000b_2v^4}{389082443819478551} \left(\left(-\frac{1}{4}a_4 + \frac{1}{2} \right) b_2^2 \right. \\
& + \left((-a_4 + 1)b_1 + \frac{1}{2}b_0 + \frac{12668968199a_4}{2731802061120} + \frac{430638152579}{1365901030560} \right) b_2 \\
& - a_4b_1^2 + \left(b_0 + \frac{2793a_4}{129541} + \frac{513135}{259082} \right) b_1 - \frac{19551b_0}{518164} - \frac{45469a_4}{186539040} - \frac{45469}{93269520} \left. \right)
\end{aligned}$$

$$\begin{aligned}
& + \left(\left(\frac{29436101984019845312296648704000000000000a_4}{389082443819478551} - \frac{5887220396803969062459329740800000000000}{389082443819478551} \right) b_2^3 \right. \\
& + \left(\left(\frac{176616611904119071873779892224000000000000a_4}{389082443819478551} - \frac{23548881587215876249837318963200000000000}{389082443819478551} \right) b_1 \right. \\
& + \frac{66150270245146553335607721984000000000}{9489815702914111} - \frac{5887220396803969062459329740800000000000b_0}{389082443819478551} \\
& + \left. \frac{1735868387632318833523112017920000000000a_4}{389082443819478551} \right) b_2^2 \\
& + \left(\left(\frac{353233223808238143747559784448000000000000a_4}{389082443819478551} - \frac{23548881587215876249837318963200000000000}{389082443819478551} \right) b_1^2 \right. \\
& + \left(\frac{6002944955979456984694203875328000000000}{389082443819478551} - \frac{23548881587215876249837318963200000000000b_0}{389082443819478551} \right. \\
& + \left. \frac{3471736775264637667046224035840000000000a_4}{389082443819478551} \right) b_1 + \frac{38200467852207663324090531840000000000}{389082443819478551} \\
& - \frac{31188841156191646544530636800000000000a_4}{389082443819478551} - \frac{289311397938719805587185336320000000000b_0}{389082443819478551} \Big) b_2 \\
& - \frac{23548881587215876249837318963200000000000b_1^2 (-a_4b_1 + b_0)}{389082443819478551} \Big) v^2 \\
& + \left(\frac{11774440793607938124918659481600000000000}{389082443819478551} - \frac{5887220396803969062459329740800000000000a_4}{389082443819478551} \right) b_2^2 \\
& + \left(\left(\frac{23548881587215876249837318963200000000000}{389082443819478551} - \frac{23548881587215876249837318963200000000000a_4}{389082443819478551} \right) b_1 \right. \\
& - \frac{6002944955979456984694203875328000000000}{389082443819478551} + \frac{11774440793607938124918659481600000000000b_0}{389082443819478551} \\
& - \frac{578622795877439611174370672640000000000a_4}{389082443819478551} \Big) b_2 + \frac{23548881587215876249837318963200000000000b_1 (-a_4b_1 + b_0)}{389082443819478551} \Big) v, \\
& T_{\text{denom}} = 45469v^8b_2 + 7038360b_2v^6 + 652886640b_2v^4 - 265712832000 + (-265712832000b_1 - 132856416000b_2)v^2.
\end{aligned} \tag{A.1}$$

B. Formulae for the Coefficients of the Produced Method T_j , $j = 4(1)7$, $T_{\text{denom}1}$, and $T_{\text{denom}2}$

$$\begin{aligned}
T_4 = & (15277584v^6 + 844603200v^4 \\
& + 15669279360v^2)(\cos(v))^3 + ((-2182512v^7 \\
& - 153643056v^5 - 4378489920v^3
\end{aligned}$$

$$\begin{aligned}
& + 15669279360v) \sin(v) + 363752v^8 \\
& - 2593839192v^6 + 148398964560v^4 \\
& + 672116719680v^2 + 797138496000)(\cos(v))^2 \\
& + ((-4365024v^7 + 20674325616v^5 \\
& - 490147842240v^3 - 812807775360v) \sin(v) \\
& - 30555168v^6 - 1689206400v^4
\end{aligned}$$

$$\begin{aligned}
& -31338558720v^2) \cos(v) + (13095072v^7 \\
& + 1013523840v^5 + 31338558720v^3) \sin(v) \\
& + 727504v^8 - 5149484424v^6 + 206280915120v^4 \\
& + 937829551680v^2 - 797138496000, \\
T_5 = & (-181876v^8 - 17295684v^6 - 1200197880v^4 \\
& + 128939096160v^2 + 398569248000) (\cos(v))^2 \\
& + ((-2182512v^7 - 176559432v^5 - 5645394720v^3 \\
& - 7834639680v) \sin(v) - 7638792v^6 \\
& + 25862004000v^4 - 406403887680v^2) \cos(v) \\
& + (-1091256v^7 + 5180039592v^5 \\
& - 161329966560v^3 + 406403887680v) \sin(v) \\
& - 363752v^8 - 38410764v^6 - 2294820360v^4 \\
& + 277464791520v^2 - 398569248000, \\
T_6 = & (-88570944000v^2 - 265712832000) (\cos(v))^2 \\
& - 177141888000v^2 + 265712832000, \\
T_{\text{denom1}} = & v^3 \left(v \left(v^6 + \frac{1191127v^4}{45469} + \frac{6478080v^2}{45469} \right. \right. \\
& \left. \left. - \frac{4570206480}{45469} \right) (\cos(v))^2 + \left(\left(16v^6 \right. \right. \right. \\
& \left. \left. + \frac{50850600v^4}{45469} + \frac{1487650080v^2}{45469} - \frac{2611546560}{45469} \right) \right. \\
& \left. \cdot \sin(v) + 8v^5 + \frac{1724133600v^3}{45469} \right. \\
& \left. - \frac{135467962560v}{45469} \right) \cos(v) + \left(8v^6 \right. \\
& \left. - \frac{1718677320v^4}{45469} + \frac{29638785120v^2}{45469} \right. \\
& \left. + \frac{135467962560}{45469} \right) \sin(v) + 2v^7 + \frac{12521841v^5}{45469}
\end{aligned}$$

$$\begin{aligned}
& + \frac{674562000v^3}{45469} + \frac{7181753040v}{45469} \Bigg), \\
T_7 = & (-727504v^5 + 56306880v^3 + 5223093120v) \\
& \cdot (\cos(v))^3 + ((727504v^6 + 67219440v^4 \\
& + 2247792960v^2 + 5223093120) \sin(v) - 90938v^7 \\
& + 581713426v^5 - 48439997760v^3 \\
& + 474137868960v) (\cos(v))^2 + ((1455008v^6 \\
& - 6907446960v^4 + 211658354880v^2 \\
& - 270935925120) \sin(v) + 1455008v^5 \\
& - 112613760v^3 - 10446186240v) \cos(v) \\
& + (-4365024v^6 - 337841280v^4 \\
& - 10446186240v^2) \sin(v) - 181876v^7 \\
& + 1141692670v^5 - 22742250720v^3 \\
& - 203201943840v, \\
T_{\text{denom2}} = & (45469v^7 + 1191127v^5 + 6478080v^3 \\
& - 4570206480v) (\cos(v))^2 + ((727504v^6 \\
& + 50850600v^4 + 1487650080v^2 - 2611546560) \\
& \cdot \sin(v) + 363752v^5 + 1724133600v^3 \\
& - 135467962560v) \cos(v) + (363752v^6 \\
& - 1718677320v^4 + 29638785120v^2 \\
& + 135467962560) \sin(v) + 90938v^7 + 12521841v^5 \\
& + 674562000v^3 + 7181753040v.
\end{aligned}$$

(B.1)

C. Formulae of the Asymptotic Form of the Local Truncation Errors

$$\text{LTE}_{\text{CL}} = \text{LTE}_{\text{NM2S5S3DV}} = a_0$$

Formulae of the asymptotic form of the local truncation errors are as follows:

LTE_{CL}

$$= \text{LTE}_{\text{NM2SS3DV}} = a_0$$

$$\begin{aligned}
&= \frac{134317 (g(x))^2 ((d/dx) y(x)) ((d^4/dx^4) g(x)) (d^3/dx^3) g(x)}{3390294398400} + \frac{14371919 g(x) ((d/dx) y(x)) ((d^3/dx^3) g(x))^2 (d/dx) g(x)}{153834608327400} \\
&+ \frac{222563269 (g(x))^2 y(x) ((d^7/dx^7) g(x)) (d/dx) g(x)}{22972634843558400} + \frac{3238785821 (g(x))^2 y(x) ((d^6/dx^6) g(x)) (d^2/dx^2) g(x)}{137835809061350400} \\
&+ \frac{42041221 (g(x))^4 y(x) ((d^2/dx^2) g(x))^2}{13127219910604800} + \frac{134317 ((d^3/dx^3) g(x)) ((d/dx) y(x)) (d^8/dx^8) g(x)}{36063790963200} \\
&+ \frac{166687397 g(x) y(x) ((d^5/dx^5) g(x)) ((d/dx) g(x)) (d^2/dx^2) g(x)}{1378358090613504} + \frac{757413563 (g(x))^2 y(x) ((d^3/dx^3) g(x)) ((d/dx) g(x)) (d^2/dx^2) g(x)}{5301377271590400} \\
&+ \frac{5917066801 g(x) y(x) ((d^4/dx^4) g(x)) ((d^3/dx^3) g(x)) (d/dx) g(x)}{34458952265337600} + \frac{5506997 (g(x))^3 ((d/dx) y(x)) ((d^4/dx^4) g(x)) (d/dx) g(x)}{61533843309600} \\
&+ \frac{447409927 (g(x))^2 y(x) ((d^5/dx^5) g(x)) (d^3/dx^3) g(x)}{11486317421779200} + \frac{11954213 (g(x))^2 y(x) (d^{10}/dx^{10}) g(x)}{45945269687116800} \\
&+ \frac{6312899 g(x) ((d/dx) y(x)) (d^{11}/dx^{11}) g(x)}{68917904530675200} + \frac{134317 (g(x))^6 y(x) (d^2/dx^2) g(x)}{2187869985100800} \\
&+ \frac{7118801 (g(x))^3 ((d/dx) y(x)) ((d^3/dx^3) g(x)) (d^2/dx^2) g(x)}{492270746647680} + \frac{189252653 ((d/dx) g(x))^2 y(x) ((d^3/dx^3) g(x))^2}{2812975695129600} \\
&+ \frac{2552023 (g(x))^5 y(x) ((d/dx) g(x))^2}{9845414932953600} + \frac{5506997 (g(x))^2 y(x) ((d/dx) g(x))^4}{984541493295360} \\
&+ \frac{68367353 ((d/dx) g(x))^2 ((d/dx) y(x)) (d^7/dx^7) g(x)}{6265264048243200} + \frac{6312899 ((d/dx) g(x))^2 y(x) (d^8/dx^8) g(x)}{1790075442355200} \\
&+ \frac{134317 (g(x))^3 ((d/dx) y(x)) ((d/dx) g(x))^3}{70324392378240} + \frac{99260263 ((d/dx) g(x))^4 y(x) (d^2/dx^2) g(x)}{4922707466476800} \\
&+ \frac{4969729 (g(x))^4 ((d/dx) y(x)) (d^5/dx^5) g(x)}{6563609955302400} + \frac{134317 (g(x))^5 y(x) (d^4/dx^4) g(x)}{307669216654800} \\
&+ \frac{3089291 ((d^2/dx^2) g(x)) y(x) ((d^4/dx^4) g(x))^2}{108191372889600} + \frac{2011665709 g(x) y(x) ((d^3/dx^3) g(x)) ((d/dx) g(x))^3}{34458952265337600} \\
&+ \frac{2283389 g(x) y(x) ((d^2/dx^2) g(x)) ((d^3/dx^3) g(x))^2}{18031895481600} + \frac{686494187 g(x) y(x) ((d^2/dx^2) g(x))^2 ((d/dx) g(x))^2}{6265264048243200} \\
&+ \frac{8999239 ((d^2/dx^2) g(x))^2 ((d/dx) y(x)) (d^5/dx^5) g(x)}{168297691161600} + \frac{134317 (g(x))^4 ((d/dx) y(x)) ((d/dx) g(x)) (d^2/dx^2) g(x)}{70324392378240} \\
&+ \frac{13834651 (g(x))^4 y(x) ((d/dx) g(x)) (d^3/dx^3) g(x)}{2812975695129600} + \frac{75620471 ((d^2/dx^2) g(x)) y(x) ((d^3/dx^3) g(x)) (d^5/dx^5) g(x)}{1514679220454400} \\
&+ \frac{59502431 ((d/dx) g(x)) ((d/dx) y(x)) ((d^5/dx^5) g(x)) (d^3/dx^3) g(x)}{703243923782400} + \frac{6312899 ((d/dx) g(x)) y(x) ((d^5/dx^5) g(x)) (d^4/dx^4) g(x)}{162734131123200} \\
&+ \frac{429411449 ((d/dx) g(x))^2 ((d/dx) y(x)) ((d^3/dx^3) g(x)) (d^2/dx^2) g(x)}{246135733238400} + \frac{1112010443 ((d/dx) g(x))^2 y(x) ((d^4/dx^4) g(x)) (d^2/dx^2) g(x)}{9845414932953600} \\
&+ \frac{134317 (g(x))^6 ((d/dx) y(x)) (d/dx) g(x)}{9845414932953600} + \frac{29952691 g(x) y(x) ((d^6/dx^6) g(x)) (d^4/dx^4) g(x)}{1566316012060800}
\end{aligned}$$

$$\begin{aligned}
& + \frac{134317 ((d/dx) g(x)) ((d/dx) y(x)) (d^{10}/dx^{10}) g(x)}{255725063193600} + \frac{134317 ((d^3/dx^3) g(x)) y(x) (d^9/dx^9) g(x)}{233027572377600} + \frac{134317 (g(x))^8 y(x)}{551343236245401600} \\
& + \frac{134317 ((d/dx) g(x))^5 (d/dx) y(x)}{44751886058880} + \frac{134317 ((d^{14}/dx^{14}) g(x)) y(x)}{551343236245401600} + \frac{134317 ((d^{13}/dx^{13}) g(x)) (d/dx) y(x)}{39381659731814400} \\
& + \frac{134317 ((d^3/dx^3) g(x))^3 (d/dx) y(x)}{4507973870400} + \frac{134317 ((d^2/dx^2) g(x))^4 y(x)}{8975876861952} + \frac{134317 ((d^6/dx^6) g(x))^2 y(x)}{183597481267200} \\
& + \frac{155673403 g(x) y(x) ((d^6/dx^6) g(x)) ((d/dx) g(x))^2}{5301377271590400} + \frac{671585 ((d^2/dx^2) g(x))^2 y(x) (d^6/dx^6) g(x)}{40391445878784} + \frac{134317 ((d/dx) g(x)) y(x) (d^{11}/dx^{11}) g(x)}{1458579990067200} \\
& + \frac{671585 ((d/dx) g(x))^3 ((d/dx) y(x)) (d^4/dx^4) g(x)}{17900754423552} + \frac{20013233 ((d/dx) g(x))^3 y(x) (d^5/dx^5) g(x)}{895037721177600} + \frac{3089291 g(x) y(x) (d^{12}/dx^{12}) g(x)}{137835809061350400} \\
& + \frac{123437323 (g(x))^3 y(x) ((d^3/dx^3) g(x))^2}{8614738066334400} + \frac{1581851309 (g(x))^2 y(x) ((d^4/dx^4) g(x))^2}{68917904530675200} + \frac{134317 (g(x))^5 ((d/dx) y(x)) (d^3/dx^3) g(x)}{703243923782400} \\
& + \frac{134317 ((d^2/dx^2) g(x)) y(x) (d^{10}/dx^{10}) g(x)}{504893073484800} + \frac{2552023 ((d^2/dx^2) g(x)) ((d/dx) y(x)) (d^3/dx^3) g(x)}{1514679220454400} \\
& + \frac{134317 ((d^5/dx^5) g(x)) ((d/dx) y(x)) (d^6/dx^6) g(x)}{17212263868800} + \frac{136869023 g(x) y(x) ((d^5/dx^5) g(x))^2}{12530528096486400} \\
& + \frac{134317 ((d/dx) g(x)) ((d/dx) y(x)) ((d^4/dx^4) g(x))^2}{2712235518720} + \frac{59502431 (g(x))^3 y(x) (d^8/dx^8) g(x)}{68917904530675200} + \frac{2283389 (g(x))^3 ((d/dx) y(x)) (d^7/dx^7) g(x)}{2153684516583600} \\
& + \frac{2552023 ((d^5/dx^5) g(x)) y(x) (d^7/dx^7) g(x)}{1927773553305600} + \frac{53861117 g(x) ((d/dx) y(x)) ((d^4/dx^4) g(x)) ((d/dx) g(x)) (d^2/dx^2) g(x)}{351621961891200} \\
& + \frac{279782311 (g(x))^4 y(x) (d^6/dx^6) g(x)}{275671618122700800} + \frac{134317 ((d^4/dx^4) g(x)) y(x) (d^8/dx^8) g(x)}{137698110950400} \\
& + \frac{4163827 (g(x))^2 ((d/dx) y(x)) (d^9/dx^9) g(x)}{7657544947852800} + \frac{165344227 g(x) y(x) ((d^2/dx^2) g(x))^2 (d^4/dx^4) g(x)}{1566316012060800} \\
& + \frac{426187841 (g(x))^3 y(x) ((d^5/dx^5) g(x)) (d/dx) g(x)}{34458952265337600} + \frac{134317 ((d/dx) g(x)) ((d/dx) y(x)) ((d^2/dx^2) g(x))^3}{1823224987584} \\
& + \frac{4160200441 (g(x))^2 y(x) ((d^2/dx^2) g(x))^3}{137835809061350400} + \frac{134317 ((d^3/dx^3) g(x))^2 y(x) (d^4/dx^4) g(x)}{4161206649600} \\
& + \frac{134317 ((d^4/dx^4) g(x)) ((d/dx) y(x)) (d^7/dx^7) g(x)}{21906517651200} + \frac{159702913 (g(x))^2 ((d/dx) y(x)) ((d^3/dx^3) g(x)) ((d/dx) g(x))^2}{4922707466476800} \\
& + \frac{1578090433 (g(x))^2 y(x) ((d^4/dx^4) g(x)) ((d/dx) g(x))^2}{34458952265337600} + \frac{13566017 (g(x))^2 ((d/dx) y(x)) ((d^6/dx^6) g(x)) (d/dx) g(x)}{1093934992550400} \\
& + \frac{89589439 (g(x))^2 ((d/dx) y(x)) ((d^5/dx^5) g(x)) (d^2/dx^2) g(x)}{3281804977651200} + \frac{432635057 g(x) y(x) ((d^8/dx^8) g(x)) (d^2/dx^2) g(x)}{68917904530675200} \\
& + \frac{876955693 g(x) y(x) ((d^7/dx^7) g(x)) (d^3/dx^3) g(x)}{68917904530675200} + \frac{84754027 (g(x))^3 y(x) ((d/dx) g(x))^2 (d^2/dx^2) g(x)}{4922707466476800} \\
& + \frac{6312899 g(x) y(x) ((d^9/dx^9) g(x)) (d/dx) g(x)}{2871579355444800} + \frac{589248679 g(x) ((d/dx) y(x)) ((d^2/dx^2) g(x))^2 (d^3/dx^3) g(x)}{4922707466476800} \\
& + \frac{60308333 g(x) ((d/dx) y(x)) ((d^8/dx^8) g(x)) (d/dx) g(x)}{11486317421779200} + \frac{248352133 g(x) ((d/dx) y(x)) ((d^7/dx^7) g(x)) (d^2/dx^2) g(x)}{17229476132668800} \\
& + \frac{66218281 g(x) ((d/dx) y(x)) ((d^6/dx^6) g(x)) (d^3/dx^3) g(x)}{2461353733238400} + \frac{50906143 g(x) ((d/dx) y(x)) ((d^2/dx^2) g(x)) ((d/dx) g(x))^3}{1230676866619200}
\end{aligned}$$

$$\begin{aligned}
& + \frac{37743077 (g(x))^2 ((d/dx) y(x)) ((d^2/dx^2) g(x))^2 (d/dx) g(x)}{895037721177600} + \frac{22430939 g(x) ((d/dx) y(x)) ((d^5/dx^5) g(x)) ((d/dx) g(x))^2}{546967496275200} \\
& + \frac{41235319 ((d/dx) g(x)) y(x) ((d^2/dx^2) g(x))^2 (d^3/dx^3) g(x)}{262544398212096} + \frac{170716907 ((d/dx) g(x)) ((d/dx) y(x)) ((d^6/dx^6) g(x)) (d^2/dx^2) g(x)}{3281804977651200} \\
& + \frac{30758593 ((d/dx) g(x)) y(x) ((d^7/dx^7) g(x)) (d^2/dx^2) g(x)}{1837810787484672} + \frac{64337843 ((d/dx) g(x)) y(x) ((d^6/dx^6) g(x)) (d^3/dx^3) g(x)}{2187869985100800} \\
& + \frac{28340887 ((d^2/dx^2) g(x)) ((d/dx) y(x)) ((d^3/dx^3) g(x)) (d^4/dx^4) g(x)}{189334902556800} \\
& + \frac{80455883 (g(x))^3 y(x) ((d^4/dx^4) g(x)) (d^2/dx^2) g(x)}{3445895226533760} + \frac{1477487 g(x) ((d/dx) y(x)) ((d^5/dx^5) g(x)) (d^4/dx^4) g(x)}{40683532780800}.
\end{aligned} \tag{C.1}$$

D. Formulae for the Stability Polynomials

T_k , $k = 8, 9$, and $T_{\text{denom}3}$

$$T_8 = 159532850484000v^2s^2$$

$$+ 26588808414000s^4v^2$$

$$+ 285508033854s^6v^2$$

$$- 30236885s^8v^2 + 1881961910s^6v^4$$

$$- 7406900100s^2v^8$$

$$- 766584691740s^2v^6$$

$$- 47158235397000s^2v^4$$

$$+ 17776560240 \sin(v) v^9$$

$$+ 17776560240 \cos(v) v^8$$

$$- 83991760628400 \sin(v) v^7$$

$$+ 84258409032000 \cos(v) v^6$$

$$+ 1448447428814400 \sin(v) v^5$$

$$- 6620319330307200 \cos(v) v^4$$

$$+ 6620319330307200 \sin(v) v^3$$

$$+ 33124136824800v^6$$

$$+ 239299275726000v^4$$

$$+ 641047557915v^8$$

$$- 17776560240 \sin(v) s^2v^7$$

$$- 124435921680 \cos(v) s^2v^6$$

$$+ 84382844953680 \sin(v) s^2v^5$$

$$+ 421292045160000 \cos(v) s^2v^4$$

$$- 2628065155262400 \sin(v) s^2v^3$$

$$- 6620319330307200 \cos(v) s^2v^2$$

$$+ 6620319330307200 \sin(v) s^2v$$

$$- 15953285048400s^4$$

$$- 171982326600s^6$$

$$+ 5555175075v^{10}$$

$$+ 18142131s^8$$

$$+ 1111035015v^{10} \cos(2v)$$

$$- 18142131s^8 \cos(2v)$$

$$+ 29105188245v^8 \cos(2v)$$

$$+ 171982326600s^6 \cos(2v)$$

$$+ 158291884800v^6 \cos(2v)$$

$$+ 15953285048400s^4 \cos(2v)$$

$$- 111672995338800v^4 \cos(2v)$$

$$+ 17776560240v^9 \sin(2v)$$

$$+ 1242534411000v^7 \sin(2v)$$

$$+ 36350729704800v^5 \sin(2v)$$

$$- 63813140193600v^3 \sin(2v)$$

$$- 17776560240s^2v^7 \sin(2v)$$

$$- 1438076573640s^2v^5 \sin(2v)$$

$$\begin{aligned}
& -45981739994400s^2v^3 \sin(2v) \\
& -63813140193600s^2v \sin(2v) \\
& -6047377s^8v^2 \cos(2v) \\
& +376392382s^6v^4 \cos(2v) \\
& -1481380020s^2v^8 \cos(2v) \\
& +58456619346s^6v^2 \cos(2v) \\
& -140873346180s^2v^6 \cos(2v) \\
& +5317761682800s^4v^2 \cos(2v) \\
& -9775611732600s^2v^4 \cos(2v) \\
& -31906570096800v^2s^2 \cos(2v), \\
T_9 = & 9930478995460800v^2s^2 \\
& -2779874954539200s^4v^2 \\
& -571016067708s^6v^2 \\
& +60473770s^8v^2 \\
& -3763923820s^6v^4 \\
& +14813800200s^2v^8 \\
& -105011921485800s^2v^6 \\
& +4569025673646000s^2v^4 \\
& -204430442760 \sin(v)v^9 \\
& +44441400600 \cos(v)v^8 \\
& -15689049845400 \sin(v)v^7 \\
& -3439646532000 \cos(v)v^6 \\
& -483042711060000 \sin(v)v^5 \\
& -319065700968000 \cos(v)v^4 \\
& +63813140193600 \sin(v)v^3 \\
& -2295045137952000v^6 \\
& +1655079832576800v^4 \\
& +70008688347210v^8 \\
& +204430442760 \sin(v)s^2v^7 \\
& -311089804200 \cos(v)s^2v^6 \\
& +15884592008040 \sin(v)s^2v^5 \\
& -17198232660000 \cos(v)s^2v^4 \\
& +492673721349600 \sin(v)s^2v^3 \\
& -319065700968000 \cos(v)s^2v^2 \\
& +63813140193600 \sin(v)s^2v \\
& +1655079832576800s^4 \\
& +343964653200s^6 \\
& -11110350150v^{10} \\
& -36284262s^8 \\
& -2222070030v^{10} \cos(2v) \\
& +36284262s^8 \cos(2v) \\
& +14214167564310v^8 \cos(2v) \\
& -343964653200s^6 \cos(2v) \\
& -1183631345265600v^6 \cos(2v) \\
& -1655079832576800s^4 \cos(2v) \\
& +11585558828037600v^4 \cos(2v) \\
& +35553120480v^9 \sin(2v) \\
& -168783466467600v^7 \sin(2v) \\
& +5171871901492800v^5 \sin(2v) \\
& -6620319330307200v^3 \sin(2v) \\
& -35553120480s^2v^7 \sin(2v) \\
& +168392382142320s^2v^5 \sin(2v) \\
& -3992254175044800s^2v^3 \sin(2v) \\
& -6620319330307200s^2v \sin(2v) \\
& +12094754s^8v^2 \cos(2v) \\
& -752784764s^6v^4 \cos(2v) \\
& +2962760040s^2v^8 \cos(2v) \\
& -116913238692s^6v^2 \cos(2v) \\
& -21126820218840s^2v^6 \cos(2v) \\
& -530284710614400s^4v^2 \cos(2v) \\
& +1208709566341200s^2v^4 \cos(2v) \\
& +3310159665153600v^2s^2 \cos(2v)
\end{aligned}$$

$$\begin{aligned}
& + 35680944852000s^4v^4 & - 6620319330307200 \cos(v)v^4 \\
& + 3439646532000s^2v^4 \cos(3v) & - 111672995338800v^4 \cos(2v) \\
& + 63813140193600v^2s^2 \cos(3v) & + 6620319330307200 \sin(v)v^3 \\
& + 63813140193600v^3 \sin(3v) & - 63813140193600v^3 \sin(2v) \\
& + 821253508200v^7 \sin(3v) & + 239299275726000v^4. \\
& + 27462410488800v^5 \sin(3v) & \\
& + 8888280120v^9 \sin(3v) & \\
& + 63813140193600v^4 \cos(3v) & \\
& - 8888280120v^8 \cos(3v) & \\
& + 687929306400v^6 \cos(3v) & \\
& - 8888280120s^2v^7 \sin(3v) & \\
& + 62217960840s^2v^6 \cos(3v) & \\
& + 7136188970400s^4v^4 \cos(2v) & \\
& - 625711345560s^2v^5 \sin(3v) & \\
& - 17831400199200s^2v^3 \sin(3v) & \\
& + 63813140193600s^2v \sin(3v), & \\
T_{\text{denom}3} & \\
& = 1111035015v^{10} \cos(2v) & \\
& + 17776560240 \sin(v)v^9 & \\
& + 17776560240v^9 \sin(2v) & \\
& + 5555175075v^{10} & \\
& + 17776560240 \cos(v)v^8 & \\
& + 29105188245v^8 \cos(2v) & \\
& - 83991760628400 \sin(v)v^7 & \\
& + 1242534411000v^7 \sin(2v) & \\
& + 641047557915v^8 & \\
& + 84258409032000 \cos(v)v^6 & \\
& + 158291884800v^6 \cos(2v) & \\
& + 1448447428814400 \sin(v)v^5 & \\
& + 36350729704800v^5 \sin(2v) & \\
& + 33124136824800v^6 &
\end{aligned}
\tag{D.1}$$

Additional Points

Theodore E. Simos is highly cited researcher, 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.

Competing Interests

The authors declare that they have no competing interests.

References

- [1] A. C. Allison, "The numerical solution of coupled differential equations arising from the Schrödinger equation," *Journal of Computational Physics*, vol. 6, no. 3, pp. 378–391, 1970.
- [2] J. D. Lambert and I. A. Watson, "Symmetric multistep methods for periodic initial values problems," *Journal of the Institute of Mathematics and Its Applications*, vol. 18, no. 2, pp. 189–202, 1976.
- [3] T. E. Simos and P. S. Williams, "A finite-difference method for the numerical solution of the Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 79, no. 2, pp. 189–205, 1997.
- [4] R. M. Thomas, "Phase properties of high order, almost P -stable formulae," *BIT Numerical Mathematics*, vol. 24, no. 2, pp. 225–238, 1984.
- [5] A. D. Raptis and T. E. Simos, "A four-step phase-fitted method for the numerical integration of second order initial value problems," *BIT Numerical Mathematics*, vol. 31, no. 1, pp. 160–168, 1991.
- [6] Z. A. Anastassi and T. E. Simos, "A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems," *Journal of Computational and Applied Mathematics*, vol. 236, no. 16, pp. 3880–3889, 2012.
- [7] Z. A. Anastassi and T. E. Simos, "An optimized Runge-Kutta method for the solution of orbital problems," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 1–9, 2005.
- [8] P. Atkins and R. Friedman, *Molecular Quantum Mechanics*, Oxford University Press, Oxford, UK, 2011.
- [9] M. M. Chawla and P. S. Rao, "A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems. II: explicit method," *Journal of Computational and Applied Mathematics*, vol. 15, no. 3, pp. 329–337, 1986.
- [10] M. M. Chawla and P. S. Rao, "An explicit sixth-order method with phase-lag of order eight for $y'' = f(t, y)$," *Journal of*

- Computational and Applied Mathematics*, vol. 17, no. 3, pp. 363–368, 1987.
- [11] C. J. Cramer, *Essentials of Computational Chemistry*, John Wiley & Sons, Chichester, UK, 2004.
 - [12] J. M. Franco and M. Palacios, “High-order P -stable multistep methods,” *Journal of Computational and Applied Mathematics*, vol. 30, no. 1, pp. 1–10, 1990.
 - [13] L. G. Ixaru and M. Rizea, “Comparison of some four-step methods for the numerical solution of the Schrödinger equation,” *Computer Physics Communications*, vol. 38, no. 3, pp. 329–337, 1985.
 - [14] L. G. Ixaru and M. Micu, *Topics in Theoretical Physics*, Central Institute of Physics, Bucharest, Romania, 1978.
 - [15] L. G. Ixaru and M. Rizea, “A Runge-Kutta-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies,” *Computer Physics Communications*, vol. 19, no. 1, pp. 23–27, 1980.
 - [16] F. Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons, Chichester, UK, 2007.
 - [17] Z. Kalogiratou, T. Monovasilis, and T. E. Simos, “New modified Runge-Kutta-Nyström methods for the numerical integration of the Schrödinger equation,” *Computers & Mathematics with Applications*, vol. 60, no. 6, pp. 1639–1647, 2010.
 - [18] A. A. Kosti, Z. A. Anastassi, and T. E. Simos, “Construction of an optimized explicit Runge-Kutta-Nyström method for the numerical solution of oscillatory initial value problems,” *Computers & Mathematics with Applications*, vol. 61, no. 11, pp. 3381–3390, 2011.
 - [19] J. D. Lambert, *Numerical Methods for Ordinary Differential Systems. The Initial Value Problem*, John Wiley & Sons, New York, NY, USA, 1991.
 - [20] A. R. Leach, *Molecular Modelling—Principles and Applications*, Pearson, Essex, UK, 2001.
 - [21] T. Lyche, “Chebyshevian multistep methods for ordinary differential equations,” *Numerische Mathematik*, vol. 19, no. 1, pp. 65–75, 1972.
 - [22] T. Monovasilis, Z. Kalogiratou, and T. E. Simos, “A family of trigonometrically fitted partitioned Runge-Kutta symplectic methods,” *Applied Mathematics and Computation*, vol. 209, no. 1, pp. 91–96, 2009.
 - [23] T. Monovasilis, Z. Kalogiratou, and T. E. Simos, “Exponentially fitted symplectic Runge-Kutta-Nyström methods,” *Applied Mathematics & Information Sciences*, vol. 7, no. 1, pp. 81–85, 2013.
 - [24] G. A. Panopoulos and T. E. Simos, “An eight-step semi-embedded predictor-corrector method for orbital problems and related IVPs with oscillatory solutions for which the frequency is unknown,” *Journal of Computational and Applied Mathematics*, vol. 290, pp. 1–15, 2015.
 - [25] G. A. Panopoulos and T. E. Simos, “An optimized symmetric 8-step semi-embedded predictor-corrector method for IVPs with oscillating solutions,” *Applied Mathematics & Information Sciences*, vol. 7, no. 1, pp. 73–80, 2013.
 - [26] G. A. Panopoulos and T. E. Simos, “A new optimized symmetric Embedded Predictor-Corrector Method (EPCM) for initial-value problems with oscillatory solutions,” *Applied Mathematics and Information Sciences*, vol. 8, no. 2, pp. 703–713, 2014.
 - [27] D. F. Papadopoulos and T. E. Simos, “A modified Runge-Kutta-Nyström method by using phase lag properties for the numerical solution of orbital problems,” *Applied Mathematics & Information Sciences*, vol. 7, no. 2, pp. 433–437, 2013.
 - [28] D. F. Papadopoulos and T. E. Simos, “The use of phase lag and amplification error derivatives for the construction of a modified Runge-Kutta-Nyström method,” *Abstract and Applied Analysis*, vol. 2013, Article ID 910624, 11 pages, 2013.
 - [29] G. D. Quinlan and S. Tremaine, “Symmetric multistep methods for the numerical integration of planetary orbits,” *Astronomical Journal*, vol. 100, no. 5, pp. 1694–1700, 1990.
 - [30] A. D. Raptis and A. C. Allison, “Exponential-fitting methods for the numerical solution of the Schrödinger equation,” *Physics Communications*, vol. 14, no. 1-2, pp. 1–5, 1978.
 - [31] D. P. Sakas and T. E. Simos, “Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation,” *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 161–172, 2005.
 - [32] T. E. Simos, “Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution,” *Applied Mathematics Letters*, vol. 17, no. 5, pp. 601–607, 2004.
 - [33] T. E. Simos, “Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems,” *Applied Mathematics Letters*, vol. 22, no. 10, pp. 1616–1621, 2009.
 - [34] T. E. Simos, “Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation,” *Acta Applicandae Mathematicae*, vol. 110, no. 3, pp. 1331–1352, 2010.
 - [35] T. E. Simos, “New stable closed Newton-Cotes trigonometrically fitted formulae for long-time integration,” *Abstract and Applied Analysis*, vol. 2012, Article ID 182536, 15 pages, 2012.
 - [36] 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,” *Journal of Applied Mathematics*, vol. 2012, Article ID 420387, 17 pages, 2012.
 - [37] T. E. Simos, “High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation,” *Applied Mathematics and Computation*, vol. 209, no. 1, pp. 137–151, 2009.
 - [38] H. Ramos, Z. Kalogiratou, Th. Monovasilis, and T. E. Simos, “An optimized two-step hybrid block method for solving general second order initial-value problems,” *Numerical Algorithms*, vol. 72, no. 4, pp. 1089–1102, 2016.
 - [39] T. Monovasilis, Z. Kalogiratou, and T. E. Simos, “Construction of exponentially fitted symplectic Runge-Kutta-Nyström methods from partitioned Runge-Kutta methods,” *Mediterranean Journal of Mathematics*, vol. 13, no. 4, pp. 2271–2285, 2016.
 - [40] T. E. Simos, “On the explicit four-step methods with vanished phase-lag and its first derivative,” *Applied Mathematics & Information Sciences*, vol. 8, no. 2, pp. 447–458, 2014.
 - [41] T. E. Simos, “Exponentially fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation and related problems,” *Computational Materials Science*, vol. 18, no. 3-4, pp. 315–332, 2000.
 - [42] S. Stavroyiannis and T. E. Simos, “Optimization as a function of the phase-lag order of nonlinear explicit two-step P -stable method for linear periodic IVPs,” *Applied Numerical Mathematics*, vol. 59, no. 10, pp. 2467–2474, 2009.
 - [43] E. Stiefel and D. G. Bettis, “Stabilization of Cowell’s method,” *Numerische Mathematik*, vol. 13, pp. 154–175, 1969.
 - [44] K. Tselios and T. E. Simos, “Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics,” *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 173–181, 2005.

- [45] C. Tsitouras, I. T. Famelis, and T. E. Simos, "On modified Runge-Kutta trees and methods," *Computers & Mathematics with Applications*, vol. 62, no. 4, pp. 2101–2111, 2011.
- [46] R. Vujasin, M. Senčanski, J. Radić-Perić, and M. Perić, "A comparison of various variational approaches for solving the one-dimensional vibrational Schrödinger equation," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 63, no. 2, pp. 363–378, 2010.
- [47] A. D. Raptis and J. R. Cash, "A variable step method for the numerical integration of the one-dimensional Schrödinger equation," *Computer Physics Communications*, vol. 36, no. 2, pp. 113–119, 1985.
- [48] J. R. Dormand, M. E. A. El-Mikkawy, and P. J. Prince, "Families of Runge-Kutta-Nyström formulae," *IMA Journal of Numerical Analysis*, vol. 7, no. 2, pp. 235–250, 1987.
- [49] J. R. Dormand and P. J. Prince, "A family of embedded Runge-Kutta formulae," *Journal of Computational and Applied Mathematics*, vol. 6, no. 1, pp. 19–26, 1980.
- [50] K. Mu and T. E. Simos, "A Runge-Kutta type implicit high algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of coupled differential equations arising from the Schrödinger equation," *Journal of Mathematical Chemistry*, vol. 53, no. 5, pp. 1239–1256, 2015.
- [51] H. Ning and T. E. Simos, "A low computational cost eight algebraic order hybrid method with vanished phase-lag and its first, second, third and fourth derivatives for the approximate solution of the Schrödinger equation," *Journal of Mathematical Chemistry*, vol. 53, no. 6, pp. 1295–1312, 2015.
- [52] M. Liang and T. E. Simos, "A new four stages symmetric two-step method with vanished phase-lag and its first derivative for the numerical integration of the Schrödinger equation," *Journal of Mathematical Chemistry*, vol. 54, no. 5, pp. 1187–1211, 2016.
- [53] X. Xi and T. E. Simos, "A new high algebraic order four stages symmetric two-step method with vanished phase-lag and its first and second derivatives for the numerical solution of the Schrödinger equation and related problems," *Journal of Mathematical Chemistry*, vol. 54, no. 7, pp. 1417–1439, 2016.
- [54] Z. Zhou and T. E. Simos, "A new two stage symmetric two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of the radial Schrödinger equation," *Journal of Mathematical Chemistry*, vol. 54, no. 2, pp. 442–465, 2016.
- [55] T. E. Simos, "Multistage symmetric two-step P -stable method with vanished phase-lag and its first, second and third derivatives," *Applied and Computational Mathematics*, vol. 14, no. 3, pp. 296–315, 2015.
- [56] R. B. Bernstein, A. Dalgarno, H. Massey, and I. C. Percival, "Thermal scattering of atoms by homonuclear diatomic molecules," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 274, no. 1359, pp. 427–442, 1963.
- [57] R. B. Bernstein, "Quantum mechanical (phase shift) analysis of differential elastic scattering of molecular beams," *The Journal of Chemical Physics*, vol. 33, no. 3, pp. 795–804, 1960.

Hindawi

Submit your manuscripts at
<http://www.hindawi.com>