Research Article

An Efficient Numerical Method for the Solution of the Schrödinger Equation

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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:

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

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

\[
y_{ij} = 0 \quad \text{at} \quad x = 0
\]

\[
y_{ij} \sim k_i x j_i (k_i x) \delta_{ij} + \left( \frac{k_i}{k_j} \right)^{1/2} K_{ij} k_j x n_{ij} (k_j x),
\]

where \(j_i(x)\) and \(n_i(x)\) 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])

\[
K'_{ij} = \left( \frac{k_i}{k_j} \right)^{1/2} K_{ij},
\]

\[
M_{ij} = k_i x j_i (k_i x) \delta_{ij},
\]

\[
N_{ij} = k_i x n_{ij} (k_i x) \delta_{ij}
\]

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

\[
y \sim M + N K'.
\]

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

\[
\left[ \frac{d^2}{dx^2} + k^2_{j'j} - \frac{l'(l' + 1)}{x^2} \right] y_{j'j}^{ij}(x) = \frac{2\mu}{\hbar^2} \sum_{j'} \langle j' l'; | V | j'' l''; j \rangle y_{j'j}^{ij}(x),
\]

(6)

where

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

(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 \(\mu\) 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

\[
\sum_{i=1}^{m} c_i y_{n+i} = \hbar^2 \sum_{i=1}^{m} b_i f(x_{n+i}, y_{n+i}),
\]

(8)

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

**Remark 1.** A method (8) is called symmetric multistep method or symmetric 2m-step method if \(c_i = c_j\) and \(b_j = b_i, i = 0(1)m\).

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

\[
y'' = -\phi^2 y,
\]

(9)

we obtain the difference equation

\[
A_m (v) y_{n+m} + \cdots + A_1 (v) y_{n+1} + A_0 (v) y_n + A_1 (v) y_{n-1} + \cdots + A_m (v) y_{n-m} = 0
\]

(10)

and the associated characteristic equation

\[
A_m (v) \lambda^m + \cdots + A_1 (v) \lambda + A_0 (v) + A_1 (v) \lambda^{-1} + \cdots + A_m (v) \lambda^{-m} = 0,
\]

(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 \((0, \nu_0^2)\) if, for all \(v \in (0, \nu_0^2)\), the roots \(\lambda_i, i = 1(1)2m,\) of (11) satisfy

\[
\lambda_1 = e^{i\theta(v)}, \quad \lambda_2 = e^{-i\theta(v)},
\]

(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

\[
t = v - \theta (v).
\]

(13)

Then, if the quantity \(t = O(v^{q+1})\) as \(v \to \infty\), 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

\[
C = 2A_m (v) \cos (mv) + \cdots + 2A_1 (v) \cos (jv) + \cdots + 2A_0 (v),
\]

(14)

and

\[
C = 2m^2 A_m (v) + \cdots + 2j^2 A_1 (v) + \cdots + 2A_1 (v).
\]

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:

\[
\tilde{y}_n = y_n - a_0 h^2 \left( f_{n+1} - 2f_n + f_{n-1} \right),
\]

\[
\tilde{y}_n = y_n - a_1 h^2 \left( f_{n+1} - 2\tilde{f}_n + f_{n-1} \right) - 2a_2 h^2 \tilde{f}_n,
\]

(11)

\[
\tilde{y}_{n+1/2} = \frac{1}{2} (y_n + y_{n+1}) - h^2 \left[ a_3 \tilde{f}_n + \left( \frac{1}{8} - a_5 \right) f_{n+1} \right],
\]

(15)

\[
\tilde{y}_{n-1/2} = \frac{1}{2} (y_n + y_{n-1}) - h^2 \left[ a_3 \tilde{f}_n + \left( \frac{1}{8} - a_5 \right) f_{n-1} \right],
\]

\[
y_{n+1} + a_4 y_n + y_{n-1} = h^2 \left[ b_1 (f_{n+1} + f_{n-1}) + b_0 f_n + b_2 (\tilde{f}_{n+1/2} + \tilde{f}_{n-1/2}) \right],
\]
where \( a_0 = \frac{45469}{862066800}, a_1 = -\frac{2793}{26878564}, a_2 = -\frac{86919}{13439282}, a_3 = \frac{6719641}{52720800}, \) 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

\[
A_1(v) = 1 + v^2 \left( b_1 + \frac{1}{2} b_2 \right) - v^4 b_2 \left( a_3 - \frac{1}{8} \right) + 2v^6 b_2 a_1 a_3 + 4v^8 b_2 a_3 (a_2 - a_1),
\]

\[
A_0(v) = a_4 + v^2 (b_0 + b_2) + 2v^4 b_3 a_3 (a_2 - a_1) - 8v^6 b_2 a_5 (a_2 - a_1).
\]

(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:

Phase-Lag (PL) = \( \frac{T_0}{T_{\text{denom}}} \),

First Derivative of the Phase-Lag = \( \frac{T_1}{T_{\text{denom}}} \),

Second Derivative of the Phase-Lag = \( \frac{T_2}{T_{\text{denom}}} \),

Third Derivative of the Phase-Lag = \( \frac{T_3}{T_{\text{denom}}} \)

(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:

\[
b_0 = \frac{1}{136407} \frac{T_4}{T_{\text{denom}_1}},
\]

\[
b_1 = \frac{1}{136407} \frac{T_5}{T_{\text{denom}_1}},
\]

\[
b_2 = \frac{1}{45469} \frac{T_6}{T_{\text{denom}_1}},
\]

\[
a_4 = \frac{T_2}{T_{\text{denom}_2}},
\]

(18)

where the formulae \( T_j, j = 4(1)7, T_{\text{denom}_1}, \) and \( T_{\text{denom}_2} \) 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):

\[
b_0 = \frac{73205}{63882} + \frac{268231049\nu^{10}}{6206331977892448} + \frac{47394640283\nu^{12}}{7245329438658249446400}
\]

\[
- \frac{841146961608850447\nu^{14}}{268766351049739245873408000}
\]

\[
- \frac{3471125215555020493\nu^{16}}{23840650403457053406595478323200}
\]

\[
- \frac{450175574700292070703419\nu^{18}}{7016973932030008047188109768345600000}
\]

\[
+ \cdots,
\]

\[
b_1 = \frac{51911}{383292} + \frac{268231049\nu^{10}}{1572361991867354688}
\]

\[
+ \frac{61738277963993\nu^{12}}{134719975463194946678400}
\]

\[
- \frac{559868876269811659\nu^{14}}{16125981062944345752404480000}
\]

\[
- \frac{60276057897670659833\nu^{16}}{3576097560518558010989321748480000}
\]

\[
+ \frac{526348577422138492034251\nu^{18}}{84203687184360096566257317220147200000}
\]

\[
+ \cdots,
\]

\[
b_2 = -\frac{19970}{95823} - \frac{268231049\nu^{10}}{393090497966838672}
\]

\[
+ \frac{1579002931233\nu^{12}}{336799383657987374169600}
\]

\[
+ \frac{1815411510701831\nu^{14}}{40314952657361088688101120}
\]

\[
+ \frac{21664254981643052111\nu^{16}}{89402439012963950274733043712000}
\]

\[
+ \frac{83649553946931897393718}{84203687184360096566257317220147200000}
\]

\[
+ \cdots,
\]

\[
a_4 = -2 + \frac{134317\nu^{16}}{15752663892725760}
\]

\[
+ \frac{117002347\nu^{18}}{42177757572773222400000}
\]

(19)

The behavior of the coefficients is given in Figure 1.
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 NM2SS53DV, is given by

$$\text{LTE}_{NM2SS53DV} = \frac{134317}{55134323645401600} h^{16} \left( y_n^{(16)} \right) + 56 \phi^{10} y_n^{(6)} + 140 \phi^{12} y_n^{(4)} + 120 \phi^{14} y_n^{(2)} + 35 \phi^{16} y_n^{(0)} + O \left( h^{18} \right).$$

3. Analysis of the Method

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

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

(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)

$$\text{LTE}_{\text{cls}} = \frac{134317}{55134323645401600} h^{16} y_n^{(16)} + O \left( h^{18} \right).$$

(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

\[ \text{LTE}_{\text{NM2SSSSDV}} = \frac{134317}{551343236245401600} h^{16} \left( y^{(16)} + 56 \phi y^{(6)} + 140 \phi y^{(4)} + 120 \phi y^{(2)} + 35 \phi y^{(1)} \right) + O \left( h^{18} \right). \]

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

\[ \text{LTE} = h^p \sum_{i=0}^{m} a_i G^i, \]

where \( a_i \) are constant numbers (classical methods) or formulae of \( \phi \) (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, \( G = V_c - E = 0 \Rightarrow G^2 = 0 \), \( i = 1, 2, \ldots \).

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., 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

\[ \text{LTE}_{\text{CL}} = \frac{134317}{551343236245401600} h^{16} \left( y(x) G^8 + \cdots \right) + O \left( h^{18} \right). \]

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

\[ \text{LTE}_{\text{NM2SSSSDV}} = \frac{134317}{9845414932953600} h^{16} \left( \left( 20g(x) y(x) \frac{d^2}{dx^2} g(x) + 15 \left( \frac{d}{dx} g(x) \right)^2 y(x) + 10 \left( \frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) + 31 \left( \frac{d^5}{dx^5} g(x) \right) y(x) \right) G^5 + \cdots \right) + O \left( h^{18} \right). \]

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:

\[ y'' = -\omega^2 y. \]

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

\[ A_1 (s, v) (y_{n+1} + y_{n-1}) + A_0 (s, v) y_n = 0, \]

where

\[ A_1 (s, v) = 1 + \frac{1}{8} (8b_1 + 4b_2) s^2 + \frac{1}{8} b_2 (-8a_3 + 1) s^4 + 4a_3 b_2 \left( v^2 a_0 a_2 + \frac{1}{2} a_1 \right) s^6 - 4a_0 a_1 a_2 b_2 s^8, \]

\[ A_0 (s, v) = a_6 + (b_0 + b_2) s^2 + 4a_0 b_2 \left( v^2 a_2 + \frac{1}{2} \right) s^4 \]
We will present the numerical solution of the coupled Schrödinger equations from the Schrödinger equation and related problems (in newstabilitypolynomialsareproduced: itsfirst, second, and third derivatives.

\[-8a_3b_2\left(v^2a_0a_2 + \frac{1}{2}a_1\right)s^6 + 8a_3a_1b_3s^8, \]

where the formulae

\[s = \omega h, \text{and } v = \phi h.\]

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

\[A_1 (s, v) = \frac{T_8}{\text{denom3}}, \tag{30}\]

\[A_0 (s, v) = \frac{T_9}{\text{denom3}}, \tag{31}\]

where the formulæ \(T_k, k = 8,9,\) and \(\text{denom3}\) 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

\[\text{LTE} = \left|y_{n+1}^L - y_{n+1}^H\right|, \tag{31}\]

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 LTE \(\leq\) acc then the step size is halved; that is, \(h_{n+1} = \frac{1}{2}h_n.\)

(ii) If acc \(\leq\) LTE \(\leq\) 100 acc then the step size remains stable; that is, \(h_{n+1} = h_n.\)

(iii) If 100 acc \(\leq\) LTE then the step size is halved and the step is repeated; that is, \(h_{n+1} = \frac{1}{2}h_n.\)

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
(i) 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])

\[
V(x, \hat{\mathbf{k}}_{ij}, \hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{ij}, \hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{ij}, \hat{\mathbf{k}}_{jj}),
\]

(32)

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

\[
\langle f'f''|V|f''f'''f''|f' \rangle = \delta_{f'f''} \delta_{f''f'''}V_0(x) + f_2(\langle f'f', f''f''', f'' \rangle) V_2(x),
\]

(33)

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

\[
y_{jij}^{ij}(x) = 0 \quad \text{at} \quad x = 0
\]

(34)

\[
y_{jij}^{ij}(x) \approx \delta_{jij} \delta_{y''} \exp \left[ -i \left( k_{ij}x - \frac{1}{2} j \pi \right) \right],
\]

\[
-\left( \frac{k_i}{k_j} \right)^{1/2} S'(j\ell) \exp \left[ i \left( k_{ij}x - \frac{1}{2} j \pi \right) \right],
\]

(35)

where

\[
S = (I + iK)(I - iK)^{−1}.
\]

(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:

\[
\frac{2\mu}{\hbar^2} = 1000.0,
\]

\[
\frac{\mu}{I} = 2.351,
\]

\[
E = 1.1,
\]

\[
V_0(x) = \frac{1}{x^{12}} - 2 \frac{1}{x^5},
\]

\[
V_2(x) = 0.2283V_0(x).
\]

(37)

For our test we take \( J = 6 \) and we will consider excitation of the rotator from \( j = 0 \) state to levels up to \( f = 2, 4, \) 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>
<thead>
<tr>
<th>Method</th>
<th>( N )</th>
<th>( h_{\text{max}} )</th>
<th>RTC</th>
<th>MErr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method I</td>
<td>4</td>
<td>0.014</td>
<td>3.25</td>
<td>( 1.2 \times 10^{-3} )</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.014</td>
<td>23.51</td>
<td>( 5.7 \times 10^{-3} )</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>0.014</td>
<td>99.15</td>
<td>( 6.8 \times 10^{-3} )</td>
</tr>
<tr>
<td>Method II</td>
<td>4</td>
<td>0.056</td>
<td>1.55</td>
<td>( 8.9 \times 10^{-4} )</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.056</td>
<td>8.43</td>
<td>( 7.4 \times 10^{-3} )</td>
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<tr>
<td></td>
<td>16</td>
<td>0.056</td>
<td>43.32</td>
<td>( 8.6 \times 10^{-2} )</td>
</tr>
<tr>
<td>Method III</td>
<td>4</td>
<td>0.007</td>
<td>45.15</td>
<td>( 9.0 \times 10^{-3} )</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Method IV</td>
<td>4</td>
<td>0.112</td>
<td>0.39</td>
<td>( 1.1 \times 10^{-5} )</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.112</td>
<td>3.48</td>
<td>( 2.8 \times 10^{-4} )</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>0.112</td>
<td>19.31</td>
<td>( 1.3 \times 10^{-3} )</td>
</tr>
<tr>
<td>Method V</td>
<td>4</td>
<td>0.448</td>
<td>0.14</td>
<td>( 3.4 \times 10^{-7} )</td>
</tr>
<tr>
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<td>9</td>
<td>0.448</td>
<td>1.37</td>
<td>( 5.8 \times 10^{-7} )</td>
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<tr>
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<td>16</td>
<td>0.448</td>
<td>9.58</td>
<td>( 8.2 \times 10^{-7} )</td>
</tr>
<tr>
<td>Method VI</td>
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<td>0.448</td>
<td>0.06</td>
<td>( 2.9 \times 10^{-7} )</td>
</tr>
<tr>
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<td>9</td>
<td>0.448</td>
<td>1.10</td>
<td>( 4.5 \times 10^{-7} )</td>
</tr>
<tr>
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<td>16</td>
<td>0.448</td>
<td>8.57</td>
<td>( 7.4 \times 10^{-7} )</td>
</tr>
<tr>
<td>Method VII</td>
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<td>0.448</td>
<td>0.04</td>
<td>( 8.8 \times 10^{-8} )</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.448</td>
<td>1.02</td>
<td>( 9.2 \times 10^{-8} )</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>0.448</td>
<td>7.48</td>
<td>( 8.9 \times 10^{-8} )</td>
</tr>
<tr>
<td>Method VIII</td>
<td>4</td>
<td>0.448</td>
<td>0.04</td>
<td>( 9.7 \times 10^{-8} )</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>0.448</td>
<td>1.01</td>
<td>( 1.2 \times 10^{-7} )</td>
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<tr>
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<td>16</td>
<td>0.448</td>
<td>7.15</td>
<td>( 2.3 \times 10^{-7} )</td>
</tr>
<tr>
<td>Method IX</td>
<td>4</td>
<td>0.896</td>
<td>0.02</td>
<td>( 7.0 \times 10^{-8} )</td>
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<tr>
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<td>9</td>
<td>0.896</td>
<td>0.45</td>
<td>( 5.7 \times 10^{-8} )</td>
</tr>
<tr>
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<td>16</td>
<td>0.896</td>
<td>6.11</td>
<td>( 6.5 \times 10^{-8} )</td>
</tr>
</tbody>
</table>

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

\[
y_{jij}^{ij}(x_0) = 0.
\]

(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 $\text{S}$ 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 $\text{S}$ 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 $T_{\text{denom}}$

$$T_0 = \left(45469v^8b_2 + 7038360b_2v^6 + 652886640b_2v^4 - 265712832000ight) + \left(-265712832000b_1 - 132856416000b_2\right)v^2 \cos(v) - 45469v^8b_2$$

$$+ 431033400b_2v^6 - 33866990640b_2v^4 + \left(-132856416000b_0 - 132856416000b_2\right)v^2$$

$$- 132856416000a_i,$$

$$T_1 = -2067429961\left(-\frac{265712832000}{45469} + \frac{v^8b_2}{45469} + \frac{7038360b_2v^6}{45469} + \frac{652886640b_2v^4}{45469}\right)\sin(v) - 39837369710880$$

$$+ \left(-\frac{265712832000b_1}{45469} - \frac{132856416000b_0}{45469}\right)v^2 + \left(-\frac{4393400v^{10}b^2}{28973} - \frac{26360400v^8b_2}{28973}ight)\left(b_0 + 2b_1 + \frac{153226717033b_2}{4994087615}\right)$$

$$- \frac{17669903328000b_2v^6}{188196191}\left(b_0 + \frac{45469a_i}{3519180} - \frac{16290b_1}{133} - \frac{8012b_2}{133} + \frac{45469}{1759590}\right)$$

$$- \frac{819540618336000b_2v^4}{188196191}\left(b_0 + \frac{8379a_i}{259082} + \frac{13439282b_1}{129541} + \frac{6849182b_2}{129541} - \frac{513135}{129541}\right).$$
\[
\begin{align*}
&\left(- \frac{1639081236672000}{188196191} v^2 b_2^2 \left(a_4 + \frac{13439282}{129541}\right) \\
&+ \left(\frac{166768965158400000 a_4}{188196191} - \frac{333537930316800000}{188196191}\right) b_2 \\
&+ \frac{333537930316800000 a_4 b_1}{188196191} - \frac{333537930316800000 b_0}{188196191}\right) v^6,
\end{align*}
\]

\[
T_2 = -94003972896709 \left(\frac{265712832000}{45469} + v^6 b_2 + \frac{7038360 b_6 v^6}{45469} + \frac{652886640 b_7 v^6}{45469}\right) \cos (v) + 5434096090152008160 v^{20} b_2^3
\]

\[\cdot \left( b_0 + 2 b_1 + \frac{227930737228 b_1}{4994087615}\right) v^{16} - 2295953942267723189760000 b_2^2
\]

\[\cdot \left( b_0 + \frac{45469 a_4}{5278770} - \frac{16290 b_0}{133} - \frac{7009130426558198 b_5}{125536380378255} + \frac{45469}{2639385}\right) v^{14}
\]

\[-194734009025380053800960000 b_2^2 \left( b_0 + \frac{6730730601 a_4}{290822990464} + \frac{379717697333 b_1}{18176436904}\right)
\]

\[\cdot \left( b_0 + 127130652893979671 b_1 \frac{536864310411}{145411495232} - \frac{356864310411}{15971271578806720}\right) v^{12}
\]

\[-48153927914830003875840000000 b_2 \left( 541122054664 b_2^2 \frac{24970438075}{24970438075}\right)
\]

\[+ \left( \frac{72734780969 b_0}{99881752300} + \frac{12770448547 a_4}{119881027600} + \frac{2191635189987 b_1}{49940876150} + \frac{63965810599}{599290513800}\right)
\]

\[\cdot \left( b_0 + b_1 + \frac{2 b_1}{129541}\right) v^{10} - 2981589039377359573155584000000000 b_2
\]

\[-\left(\frac{1773970067669 b_2}{73624597200} - \frac{90405467881 b_0}{147249194400} + \frac{58393539227 a_4}{1684466164800}\right)
\]

\[\cdot \left( b_0 + \frac{141363876421 b_0}{114527151200} - \frac{8073535624019 b_0}{73624597200} + \frac{114527151200}{147249194400} \right) b_2 - \frac{16290 b_0^2}{133} + \left( b_0 - \frac{45469 a_4}{14076720} + \frac{591097}{7038360}\right) b_1
\]

\[+ \frac{45469 b_2}{1005480} v^8 - 46095957244299145061007360000000000 b_2 \left( 3424591 b_2^2 \frac{129541}{129541}\right)
\]

\[+ \left( \frac{1}{2} b_0 - \frac{126696861899 a_4}{682950515280} + \frac{13568823 b_0}{129541} - \frac{2869992664019}{341475257640}\right) b_2 + \frac{13439282 b_2^2}{129541}
\]

\[+ \left( b_0 - \frac{11172 a_4}{129541} - \frac{2907765}{129541}\right) b_1 + \frac{69825 b_0}{259082} + \frac{45469 a_4}{23317380} + \frac{45469}{11658690} v^6
\]
\begin{align*}
-5531514869315897407320883200000000b_2^2 & \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} \right) v^4 
+ \left( -1407015390504886310279577600000000a_4 \right) b_1 + 2814030781009772620559155200000000b_0 \\
- 27657543465794870366044160000000a_4 & = -28693459297029315946323643023200000000b_2 \\
+ 5628061562019545241118310400000000b_1 \left( -a_4 b_1 + b_0 \right) v^2 \\
+ (93801026336590873519718400000000a_4 - 1876020520673181747039436800000000b_2 \\
+ 1876020520673181747039436800000000a_4 b_1 - 1876020520673181747039436800000000b_0, \\
T_3 = 4274266643640461521 & \left( -\frac{265712832000}{45469} + \frac{7038360b_2 v^6}{45469} + \frac{652886640b_2 v^4}{45469} \\
+ \left( -\frac{265712832000b_1}{45469} - \frac{1328564160000b_2}{45469} \right) v^2 \right)^4 
\cdot \sin(v) \quad - 988331660492486636108160 \\
\cdot \left( v^2 b_2^4 - \frac{703331165780v^2 b_2^4}{1317373337} - \frac{17573600b_1^2 v^2}{4139} \left( b_0 + 2b_1 + \frac{52341891953b_2}{998817523} \right) \\
- \frac{229708743264000v^2 b_2}{188196191} b_0 \left( b_0 + \frac{45469a_4}{6099912} - \frac{16290b_1}{133} \cdot \frac{36266054426070}{3049956} + \frac{45469}{36266054426070} \right) \\
- \frac{1218751529857909344000v^2 b_2}{8557092608579} b_0 \left( b_0 + \frac{8254669605a_4}{385284849578} - \frac{66316829662b_1}{192642424789} \\
\frac{2052773129961092548765b_2}{192414629552462777647} - \frac{394861571517}{192642424789} + \frac{52341891953b_2}{998817523} \right) \\
- \frac{11673827561088000000b_2^2 v^{16}}{188196191} \left( \frac{25981841558644066102303b_2}{997636442512855529000} \\
+ \frac{14436736503248b_0}{20643288160585} + \frac{67209544881a_4}{8390671932000} + \frac{61372103581289784b_1}{1135380848832175} \right. \\
\left. + \frac{6194383101859}{41950335966000} b_2 \right) b_2 \\
+ b_1 \left( b_0 + 2b_1 \right) \right) \right) = \frac{84512160980083888128000000b_2^2 v^{14}}{8557092608579} \right) - \frac{200253323882994581b_2^2}{1506436564539060000} 
\end{align*}
\[
\begin{align*}
&+ \left( \frac{17737276391689996}{301873290781200} + \frac{4562576732722819a_4}{63230335706405200} - \frac{5606745847270819b_1}{792861349757400} + \frac{170062020887713063}{316351678553202600} \right) b_2 \\
&- \frac{105220a^2}{1197} + \left( b_0 + \frac{45649a_4}{12669048} + \frac{591097}{15836310} \right) b_1 + \frac{45649b_0}{3016440} \\
&- \frac{24441425578632065770546790400000b^2_vb_1^2}{38082443819478551} - \frac{187867872296658547b_1^2}{7985635789403360} \\
&+ \left( \frac{8969884197456053b_3}{15971271578806720} + \frac{3422548322166571a_4}{38330157891361280} + \frac{136160476468092927b_1}{7985635789403360} + \frac{280627620486327149}{19165525894680640} \right) b_2 \\
&- \frac{222153379571b_2^2}{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} - \frac{651265402149779258800000000b_1v^0}{8557092608579} \\
&- \frac{15313712383120673847b_0}{43882049054820000} + \frac{144221396158735377}{87764098110964000} - \frac{339180954813}{499408761500} \\
&+ \frac{72734780969b_0}{499408761500} + \frac{7528738019a_4}{1997635046000} - \frac{100387}{2196700} \\
&+ \frac{9856938253b_0}{1997635046000} + \frac{49343a_4}{8786800} - \frac{100387}{2196700} \\
&- \frac{62377682312383293089061273600000000000b_1v^0}{389082443819478551} - \frac{665172562469b_3^3}{73624597200} \\
&+ \left( \frac{53593169281b_0}{147249194400} + \frac{255436772783415a_4}{1811388909895488000} + \frac{547869492173b_1}{8180510800} + \frac{267706836641709133}{143004387623328000} \right) b_2^2 \\
&+ \left( \frac{5855940613619b_0}{36812298600} + \frac{90405467881b_0}{73624597200} + \frac{23902606957a_4}{309922308240} + \frac{1205462023201}{386529153500} \right) b_1 \\
&+ \left( \frac{284403838933b_0}{202873791600} + \frac{12770484547a_4}{7421359397760} + \frac{109882438403}{3710679698800} \right) b_2^2 + \left( \frac{16290h_2^2}{133} + \left( b_0 + \frac{45469a_4}{1407672} + \frac{45469}{185220} \right) b_1 + \frac{45469b_0}{502740} \right) b_1 \\
&+ \frac{1421741999377084654844751052800000000000b_1v^0}{389082443819478551} - \frac{26839722353533}{839043353405} \\
&+ \left( \frac{96906582357a_4}{83904353405} - \frac{14553382412876}{83904353405} \right) b_1 + \frac{5839339227a_4}{1761991421505} + \frac{439542930952}{251713060215} b_2 \\
&+ \left( \frac{29449838880a_4}{16780870681} - \frac{3607051694400}{16780870681} \right) b_1^2 + \left( \frac{399527092a_4}{352398284301} + \frac{51938511196}{352398284301} \right) b_1 \left( \frac{9988175230b_2}{117466094767} \right) \\
&+ \frac{231449118350975844469748269056000000000b_1v^0}{389082443819478551} - \frac{1}{4} a_4 + \frac{1}{2} b_0^2 \\
&+ \left( b_0 - \frac{1}{2} b_0 + \frac{16678686199a_4}{2731802061120} + \frac{430638152579}{13659010350560} \right) b_2 \\
&- a_4 b_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} \\
\end{align*}
\]
\[
\begin{align*}
T_\text{denom} &= 45469\nu^2b_2 + 703860b_2\nu^4 - 65288640b_2\nu^4 - 265712832000 + (-265712832000b_1 + 132856416000b_2)\nu^2.
\end{align*}
\]

(A.1)

**B. Formulae for the Coefficients of the Produced Method**

\[ T_j, j = 4(1)7, T_\text{denom1}, \text{ and } T_\text{denom2} \]

\[
T_4 = (15277584\nu^6 + 844603200\nu^4)
+ 1566927936\nu^2 (\cos (\nu)) + \left((-2182512\nu^2\right)
- 153643056\nu^5 - 4378489920\nu^3
\]

\[
+ \left(\frac{294361019840198453122964870400000000000a_4}{389082443819478551} - \frac{5887220396803969062459329740800000000000b_1}{389082443819478551}\right)b_1^2
\]

\[
+ \left(\frac{176616611904119071873779822240000000000a_4}{389082443819478551} - \frac{23548881587215876249837318963200000000000b_1}{389082443819478551}\right)b_1
\]

\[
+ \frac{661502702451465533560772198400000000000}{948915702914111} - \frac{5887220396803969062459329740800000000000b_1}{389082443819478551}
\]

\[
+ \frac{1735868387632318835231120179200000000000}{389082443819478551} b_2^2
\]

\[
+ \left(\frac{3532322380823814374755978444800000000000a_4}{389082443819478551} - \frac{23548881587215876249837318963200000000000b_1}{389082443819478551}\right)b_1^2
\]

\[
+ \left(\frac{6002944955979456946942038753280000000000}{389082443819478551} - \frac{23548881587215876249837318963200000000000b_1}{389082443819478551}\right)b_1^2
\]

\[
+ \frac{3471736775264637670465243058400000000000}{389082443819478551}_1 + \frac{38200467852207663240905318400000000000b_0}{389082443819478551}_2
\]

\[
- \frac{3118841561916465445306368000000000000}{389082443819478551} b_2^2
\]

\[
+ \frac{23548881587215876249837318963200000000000b_0}{389082443819478551} b_2^2
\]

\[
+ \frac{2893113979381980587153636320000000000b_0}{389082443819478551} b_2^2
\]

\[
+ \frac{11774440793607938124918659481600000000000}{389082443819478551} b_2^2
\]

\[
+ \frac{6029449559794569469420387532800000000000}{389082443819478551} b_2^2
\]

\[
+ \frac{11774440793607938124918659481600000000000}{389082443819478551} b_2^2
\]

\[
- \frac{578622795877439611743706726400000000000}{389082443819478551} b_2^2
\]

\[
+ \frac{2354888158721587624983731896320000000000b_0}{389082443819478551} b_2^2
\]

\[
+ \frac{15669279360\nu\sin(\nu) + 363752\nu^8}{15669279360\nu^8 - 2593839192\nu^6 + 148398964560\nu^4 + 672116719680\nu^2 + 797138496000(\cos(\nu))^2}
+ \frac{64390147842240\nu^3 - 81280777360\nu}{490147842240\nu^3 - 30555168\nu - 1689206400\nu^4}
\]
\[
T_5 = \left( -181876 \nu^8 - 1729568 \nu^6 - 1200197880 \nu^4 + 128939096160 \nu^2 + 39856924800 \right) (\cos (\nu))^2 \\
+ \left( -2182512 \nu^7 - 176559432 \nu^5 - 56455184 \nu^3 - 7834639680 \nu \right) (\sin (\nu)) - 7638792 \nu^6 \\
+ 2568204000 \nu^4 - 40643887680 \nu^2 \cos (\nu) \\
+ \left( -1091256 \nu^7 + 518003952 \nu^5 \right) \\
- 161329966560 \nu^6 + 40643887680 \nu \sin (\nu) \\
- 363752 \nu^8 - 38410764 \nu^6 - 229488420 \nu^4 + 27746791520 \nu^2 - 398569248000, \\
T_6 = \left( -88570944000 \nu^2 - 265712832000 \right) (\cos (\nu))^2 \\
- 177141888000 \nu^2 + 265712832000, \\
T_{\text{denom}1} = \nu^3 (\nu^6 + \frac{1191127 \nu^4}{45469} + \frac{6478080 \nu^2}{45469} \\
- \frac{4570206480}{45469}) (\cos (\nu))^2 + \left( \frac{16 \nu^6}{45469} \right) \\
+ \frac{508506000 \nu^4}{45469} + \frac{1487650080 \nu^2}{45469} - \frac{2611546560}{45469} \right) \sin (\nu) + 8 \nu^5 + \frac{1724133600 \nu^3}{45469} \\
- \frac{135467962560 \nu}{45469} \cos (\nu) + \left( \frac{8 \nu^6}{45469} \right) \\
- \frac{1718677320 \nu^4}{45469} + \frac{29638785120 \nu^2}{45469} \right) \sin (\nu) + 2 \nu^7 + \frac{12521841 \nu^5}{45469} + 674562000 \nu^3 + 7181753040 \nu^5, \\
T_{\text{denom}2} = \left( 45469 \nu^7 + 1191127 \nu^5 + 6478080 \nu^3 \\
- 4570206480 \nu \right) (\cos (\nu))^2 + \left( \frac{727504 \nu^6}{45469} + \frac{508506000 \nu^4 + 1487650080 \nu^2 - 2611546560}{45469} \right) \sin (\nu) + 363752 \nu^5 + 1724133600 \nu^3 \cos (\nu) + \left( \frac{363752 \nu^6}{45469} \right) \\
- \frac{135467962560 \nu}{45469} \sin (\nu) + 90938 \nu^7 + 12521841 \nu^5 + 674562000 \nu^3 + 7181753040 \nu^5, \\
\end{equation}

\textbf{C. Formulae of the Asymptotic Form of the Local Truncation Errors}

\[ \text{LTE}_{\text{CL}} = \text{LTE}_{\text{NM2SSS3DV}} = a_0 \]

Formulae of the asymptotic form of the local truncation errors are as follows:
$$\begin{align*}
&\frac{134317}{255725663193600} (d^2/dx^2) g(x) y(x) (d^{10}/dx^{10}) g(x) + \frac{233027572357600}{5534326245401600} (d^3/dx^3) g(x) y(x) + \frac{134317}{5534326245401600} (d^4/dx^4) g(x) y(x) + \frac{134317}{5534326245401600} (g(x))^3 y(x) \\
&\frac{134317}{4475188058880} (d^5/dx^5) g(x) y(x) + \frac{233027572357600}{5758197981318400} (d^6/dx^6) g(x) y(x) + \frac{134317}{5534326245401600} (d^7/dx^7) g(x) y(x) + \frac{134317}{5534326245401600} (d^8/dx^8) g(x) y(x) + \frac{134317}{5534326245401600} (g(x))^3 y(x) \\
&\frac{134317}{4507973870400} (d^9/dx^9) g(x) y(x) + \frac{233027572357600}{5758197981318400} (d^{10}/dx^{10}) g(x) y(x) + \frac{134317}{5534326245401600} (d^11/dx^{11}) g(x) y(x) + \frac{134317}{5534326245401600} (g(x))^3 y(x) \\
&\frac{134317}{530137727590400} (d^{12}/dx^{12}) g(x) y(x) + \frac{233027572357600}{5758197981318400} (d^{13}/dx^{13}) g(x) y(x) + \frac{134317}{5534326245401600} (d^{14}/dx^{14}) g(x) y(x) + \frac{134317}{5534326245401600} (g(x))^3 y(x)
\end{align*}$$
D. Formulae for the Stability Polynomials

\( T_k, k = 8, 9, \) and \( T_{\text{denom3}} \)

\[
T_8 = 159532850484000v^2s^2 + 26588808414000s^4v^2 + 285508323854v^2s^2 - 302368858s^2 + 1881961910s^4v^4 - 7406900100v^2s^4 - 766584691740v^2s^2 - 4715823539700v^2s^2 + 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 - 662031933037200\cos(v)v^4 + 662031933037200\sin(v)v^3 + 33124136824800v^6 + 23929927572600v^4 + 641047557915v^8 - 17776560240\sin(v)s^2v^7 - 124435921680\cos(v)s^2v^5 + 37743077456037721177600 \quad + \frac{22430939456037721177600}{1895037721177600} \quad + \frac{170716907456037721177600}{262544398212096} \quad + \frac{64373843456037721177600}{1837810787484672} \quad + \frac{1477487456037721177600}{189334902556800} \quad + \frac{84382844953680\sin(v)s^2v^9}{895037721177600} + 421292045160000\cos(v)s^2v^4 - 2628065155262400\sin(v)s^2v^3 - 662031933037200\cos(v)s^2v^2 + 662031933037200\sin(v)s^2v + 15953285048400s^2 - 171982326600s^6 + 5555175075\sin(v)\cos^2(v) - 181421318s^8 - 1111035015\sin^2(v)\cos^2(v) + 29105188245\cos(v)s^2v^6 + 171982326600\cos^2(v)s^2v^2 + 15953285048400s^2\cos^2(v) + 181421318s^8\cos^2(v) - 111672995338800\sin^2(v)s^2v^4 + 17776560240\sin(v)s^2v^7 + 1242534411000v^7 \sin(v) + 36350729704800v^5 \sin(v) - 63813140193600v^3 \sin(v) - 17776560240s^2v^7 \sin(v) - 1438076573640s^2v^5 \sin(v) - 5469746275200 \quad + \frac{30758593456037721177600}{1837810787484672} \quad + \frac{64373843456037721177600}{1837810787484672} \quad + 3895037721177600 \quad + 5469746275200}
\begin{equation}
+ \frac{35680944852000\nu^4}{3!} + \frac{3439645320000\nu^4 \cos (3\nu)}{3!} + \frac{6381314019360\nu^3 \nu^4}{3!} \\
+ \frac{6381314019360\nu^3 \sin (3\nu)}{3!} + \frac{821255508200\nu^7 \sin (3\nu)}{3!} \\
+ \frac{2746241048800\nu^5 \sin (3\nu)}{3!} + \frac{8888280120\nu^9 \sin (3\nu)}{3!} \\
+ \frac{6381314019360\nu^4 \cos (3\nu)}{3!} - \frac{8888280120\nu^8 \cos (3\nu)}{3!} \\
+ \frac{687929306400\nu^6 \cos (3\nu)}{3!} - \frac{8888280120\nu^2 \nu^7 \sin (3\nu)}{3!} \\
+ \frac{62217960840\nu^6 \cos (3\nu)}{3!} + \frac{7136188970400\nu^4 \cos (2\nu)}{3!} \\
- \frac{625711345600\nu^5 \nu^5 \sin (3\nu)}{3!} - \frac{1783140019200\nu^2 \nu^3 \sin (3\nu)}{3!} \\
+ \frac{6381314019360\nu^3 \nu \sin (3\nu)}{3!} \\
T_{\text{denom}}^3 \\
= \frac{1111035015\nu^4 \cos (2\nu)}{3!} + \frac{17776560240 \sin (\nu) \nu^9}{3!} + \frac{17776560240\nu^9 \sin (2\nu)}{3!} \\
+ \frac{5555175075\nu^{10}}{3!} + \frac{17776560240 \cos (\nu) \nu^8}{3!} + \frac{2910518245\nu^8 \cos (2\nu)}{3!} \\
- \frac{83991760628400 \sin (\nu) \nu^7}{3!} + \frac{1242534411000 \nu^7 \sin (2\nu)}{3!} \\
+ \frac{641047557915\nu^8}{3!} + \frac{84258409032000 \cos (\nu) \nu^6}{3!} \\
+ \frac{158291884800 \nu^6 \cos (2\nu)}{3!} + \frac{1448447428814400 \sin (\nu) \nu^5}{3!} \\
+ \frac{36350729704800 \nu^5 \sin (2\nu)}{3!} + \frac{33124136824800 \nu^6}{3!} \\
- \frac{6620319330307200 \cos (\nu) \nu^4}{3!} - \frac{11167299533880 \nu^4 \cos (2\nu)}{3!} + \frac{6620319330307200 \sin (\nu) \nu^3}{3!} \\
- \frac{6381314019360 \nu^3 \sin (2\nu)}{3!} + \frac{239299275726000 \nu^4}{3!}.
\end{equation}

### 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


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