A New Methodology for the Development of Numerical Methods for the Numerical Solution of the Schrödinger Equation

Z.A. Anastassi*, D.S. Vlachos† and T.E. Simos‡

Laboratory of Computational Sciences, Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece

Abstract. In the present paper we introduce a new methodology for the construction of numerical methods for the approximate solution of the one-dimensional Schrödinger equation. The new methodology is based on the requirement of vanishing the phase-lag and its derivatives. The efficiency of the new methodology is proved via error analysis and numerical applications.

Keywords: Numerical solution, Schrödinger equation, multistep methods, hybrid methods, P-stability, phase-lag, phase-fitted

PACS: 02.60, 02.70.Bf, 95.10.Ce, 95.10.Eg, 95.75.Pq

1. Introduction

The radial Schrödinger equation can be written as:

\[ y''(x) = \frac{l(l + 1)}{x^2} + V(x) - k^2 y(x). \]  

(1)

Many problems in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. can be express via the above boundary value problem (see for example [1] - [4]).

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

- The function \( W(x) = \frac{l(l + 1)}{x^2} + V(x) \) is called the effective potential. This satisfies \( W(x) \to 0 \) as \( x \to \infty \)

- The quantity \( k^2 \) is a real number denoting the energy

* e-mail: zackanas@uop.gr
† e-mail: dvlachos@uop.gr
‡ Highly Cited Researcher, Active Member of the European Academy of Sciences and Arts. Corresponding Member of the European Academy of Sciences Corresponding Member of European Academy of Arts, Sciences and Humanities, Please use the following address for all correspondence: Dr. T.E. Simos, 10 Konitsis Street, Amfithea - Paleo Faliro, GR-175 64 Athens, Greece, Tel: 0030 210 94 20 091, e-mail: tsimos.conf@gmail.com, tsimos@mail.ariadne-t.gr

© 2008 Kluwer Academic Publishers. Printed in the Netherlands.
The quantity \( l \) is a given integer representing the angular momentum.

\( V \) is a given function which denotes the potential.

The boundary conditions are:

\[ y(0) = 0 \quad (2) \]

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

The last years an extended study on the development of numerical methods for the solution of the Schrödinger equation has been done. The aim of this research is the development of fast and reliable methods for the solution of the Schrödinger equation and related problems (see for example [5] - [18], [24] - [127]).

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

1. Methods with constant coefficients

2. Methods with coefficients depending on the frequency of the problem \(^1\).

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

More specifically, we will develop a family of hybrid Numerov-type methods of sixth algebraic order. The development of the new family is based on the requirement of vanishing the phase-lag and its derivatives. We will investigate the stability and the error of the methods of the new family. Finally, we will apply both categories of methods the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The paper is organized as follows. In Section 2 we present the theory of the new methodology. In section 3 we present the development of the new family of methods. The error analysis is presented in section 4. In section 5 we will investigate the stability properties of the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The paper is organized as follows. In Section 2 we present the theory of the new methodology. In section 3 we present the development of the new family of methods. The error analysis is presented in section 4. In section 5 we will investigate the stability properties of the new

\(^1\) When using a functional fitting algorithm for the solution of the radial Schrödinger equation, the fitted frequency is equal to: \( \sqrt{\frac{l(l + 1)}{x^2} + V(x) - k^2} \)
developed methods. In Section 6 the numerical results are presented. Finally, in Section 7 remarks and conclusions are discussed.

2. Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

\[ y'' = f(x, y) \]  \hfill (3)

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

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

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

\[ y'' = -\omega^2 y \]  \hfill (4)

a difference equation of the form

\[ A_k(H) y_{n+k} + \ldots + A_1(H) y_{n+1} + A_0(H) y_n + \]
\[ + A_1(H) y_{n-1} + \ldots + A_k(H) y_{n-k} = 0 \]  \hfill (5)

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

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

\[ A_k(H) \lambda^k + \ldots + A_1(H) \lambda + A_0(H) + A_1(H) \lambda^{-1} + \ldots \]
\[ + A_k(H) \lambda^{-k} = 0 \]  \hfill (6)

THEOREM 1. \[ 102 \] The symmetric \( 2k \)-step method with characteristic equation given by (6) has phase-lag order \( q \) and phase-lag constant \( c \) given by

\[ -c H^{q+2} + O(H^{q+4}) = \frac{2 A_k(H) \cos(kH) + \ldots + 2 A_1(H) \cos(jH) + \ldots + A_0(H)}{2k^2 A_k(H) + \ldots + 2j^2 A_j(H) + \ldots + 2 A_1(H)} \]  \hfill (8)

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric \( 2k \)-step method.
3. The New Family of Numerov-Type Hybrid Methods -
Construction of the New Methods

3.1. First Method of the Family

We introduce the following family of methods to integrate \( y'' = f(x, y) \):

\[
\bar{y}_n = y_n - a_0 h^2 \left( y''_{n+1} - 2y''_n + y''_{n-1} \right)
\]

\[
y_{n+1} + c_1 y_n + y_{n-1} = h^2 \left[ b_0 \left( y''_{n+1} + y''_{n-1} \right) + b_1 \bar{y}_n \right]
\]

The application of the above method to the scalar test equation (4) gives the following difference equation:

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

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

The characteristic equation associated with (10) is given by:

\[
A_1(H) \lambda + A_0(H) + A_1(H) \lambda^{-1} = 0
\] (10)

where

\[
A_1(H) = 1 + H^2 b_0 + H^4 b_1 a_0 \\
A_0(H) = c_1 + H^2 b_1 - 2 H^4 b_1 a_0
\]

By applying \( k = 1 \) in the formula (8), we have that the phase-lag is equal to:

\[
phl = \frac{2 A_1(H) \cos(H) + A_0(H)}{2 A_1(H)}
\]

\[
= \frac{1}{2} \frac{2 \left( 1 + H^2 b_0 + H^4 b_1 a_0 \right) \cos(H) + c_1 + H^2 b_1 - 2 H^4 b_1 a_0}{1 + H^2 b_0 + H^4 b_1 a_0}
\] (11)

We demand that the phase-lag is equal to zero and we consider that:

\[
b_0 = \frac{1}{12}, \ b_1 = \frac{5}{6}, \ c_1 = -2
\] (12)

Then we find out that:

\[
a_0 = \frac{-12 \cos(H) - \cos(H) H^2 + 12 - 5 H^2}{10 \cos(H) H^4 - 10 H^4}
\] (13)
For small values of $|H|$ the formulae given by (13) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

\[
a_0 = \frac{1}{200} + \frac{1}{5040} H^2 + \frac{1}{14400} H^4 + \frac{1}{4435200} H^6
\]
\[
+ \frac{3617}{592812380160000} H^{12} + \frac{43867}{250445794959360000} H^{14}
\]
\[
+ \frac{352130553815040000}{174611} H^{16} + \ldots
\]

(14)

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

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

\[
\text{LTE} = \frac{h^8}{6048} \left( y_n^{(8)} + \omega^2 y_n^{(6)} \right)
\]

(15)

REMARK 1. The method developed in this section is the same with the obtained by Simos in [116]

3.2. SECOND METHOD OF THE FAMILY

Consider the family of methods presented in (9).

The application of the above method to the scalar test equation (4) gives the difference equation (10) and the characteristic equation (10).

By applying $k = 1$ in the formula (8), we have that the phase-lag is given by (11). The first derivative of the phase-lag is given by:

\[
\dot{\phi}_l = \frac{1}{2} \left( \frac{T_4 - 2 T_0 \sin(H)}{T_0} \right) + \frac{1}{2} \left( \frac{2 T_0 \cos(H) + c_1 + H^2 b_1 - 2 H^4 b_1 a_0}{T_0^2} \right)
\]

\[
T_0 = 1 + H^2 b_0 + H^4 b_1 a_0
\]
\[
T_4 = 2 (2 H b_0 + 4 H^3 b_1 a_0) \cos(H)
\]

(16)

We demand that the phase-lag and its derivative are equal to zero and we consider that:

\[
b_0 = \frac{1}{12}, \quad b_1 = \frac{5}{6}
\]

(17)
Then we find out that:

\[ a_0 = \frac{-\sin(H) H^2 + 10 H + 2 \cos(H) H \cdot 12 \sin(H)}{10 \sin(H) H^4 - 40 \cos(H) H^3 + 40 H^4} \]

\[ c_1 = \frac{(24 \cos(2H) + 24 - 48 \cos(H) + H^2 \cos(2H) - 9 H^2 + 8 \cos(H) H^2 - 6 H^3 \sin(H)}{12 \sin(H) H \cdot (6 \sin(H) H - 24 \cos(H) + 24)} \quad (18) \]

Figure 1. Behavior of the coefficient \( a_0 \) of the new method given by (13) for several values of \( H \).
For small values of $|H|$ the formulae given by (18) are subject to heavy cancelations. In this case the following Taylor series expansions should be used:

$$a_0 = \frac{1}{200} + \frac{1}{3780} H^2 + \frac{73}{5443200} H^4 + \frac{509}{2833543} H^6$$

$$+ \frac{8826801984000}{4912333} H^8$$

$$+ \frac{31764871424000}{16509555251} H^{10}$$

$$+ \frac{2288303913}{3889422026229760000} H^{12} + \frac{15619496804053}{46556621053970227200000} H^{14}$$

$$+ \frac{921821096868610498560000000}{1059216238080000} H^{16} + \ldots$$

$$c_1 - 2 + \frac{1}{18144} H^8 + \frac{13}{16329600} H^{10} + \frac{31}{461894400} H^{12}$$

$$+ \frac{308851}{3813178457088000} H^{14} + \frac{537907}{3813178457088000} H^{16} + \ldots$$

The behavior of the coefficients is given in the following Figure 2.

**Figure 2.** Behavior of the coefficients of the new method given by (18) for several values of $H$.

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

$$LTE = \frac{h^8}{18144} \left( 3 y_n^{(8)} + 4 \omega^2 y_n^{(6)} + \omega^8 y_n \right)$$

(21)
3.3. **Third Method of the Family**

Consider the family of methods presented in (9).

The application of the above method to the scalar test equation (4) gives the difference equation (10) and the characteristic equation (10).

By applying $k = 1$ in the formula (8), we have that the phase-lag is given by (11). The first derivative of the phase-lag is given by (16). The second derivative of the phase-lag can be written as:

\[
\ddot{\phi}_l = \frac{1}{2} \frac{T_3 - 4T_2 \sin(H) - 2T_1 \cos(H) + 2b_1 - 24b_1a_0H^2}{T_1} \\
- \frac{(2T_2 \cos(H) - 2T_1 \sin(H) + 2Hb_1 - 8H^3b_1a_0)T_2}{T_1^2} \\
+ \frac{(2T_1 \cos(H) + c_1 + H^2b_1 - 2H^4b_1a_0)T_2^2}{T_1^3} \\
- \frac{1}{2} \frac{(2T_1 \cos(H) + c_1 + H^2b_1 - 2H^4b_1a_0)(2b_0 + 12b_1a_0H^2)}{T_1^2}
\]

We demand that the phase-lag and its first and second derivative are equal to zero and we consider that:

\[
b_0 = \frac{1}{12}
\]

Then we find out that:
A New Methodology for the Development of Numerical Methods

\[ a_0 = \frac{1}{2} \left( \cos(H)H^3 + 12\cos(H)H - 12\sin(H) + 3\sin(H)H^2 \right) / \left( (\cos(H))^2 H^3 + 16\cos(H)^2 H + 5\cos(H)H^2 \sin(H) + 72\cos(H)\sin(H) + 2\cos(H)H^3 + 32\cos(H)H + 2\sin(H)H^2 - 48H - 2H^3 - 72\sin(H)H^2 \right) \]

\[ c_1 = \frac{1}{6} \left( 24\cos(H)^2 H^2 + \cos(H)^2 H^4 + 96\cos(H)^2 + \cos(H)\sin(H)H^3 + 12\cos(H)H^2 - 24\cos(H)\sin(H)H - 96\cos(H) + \cos(H)H^4 - \sin(H)H^3 - 2H^4 - 60\sin(H)H - 48H^2 \right) / \left( \cos(H)H^2 + 7\sin(H)H + 8 - 8\cos(H) \right) \]

\[ b_1 = -\frac{1}{6} \left( \cos(H)^2 H^3 + 16\cos(H)^2 H + 5\cos(H)H^2 \sin(H) + 72\cos(H)\sin(H) + 2\cos(H)H^3 + 32\cos(H)H + 2\sin(H)H^2 - 48H - 2H^3 - 72\sin(H) \right) / \left( H (\cos(H)H^2 + 7\sin(H)H + 8 - 8\cos(H)) \right) \] (24)

For small values of \(|H|\) the formulae given by (24) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:
The behavior of the coefficients is given in the following Figure 3.

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

\[
LTE = \frac{h^8}{6048} \left( y^{(8)}_n + 2\omega^2 y^{(6)}_n - 2\omega^6 y^{(2)}_n - \omega^8 y_n \right)
\]  

(26)

3.4. Fourth Method of the Family

Consider the family of methods presented in (9).

The application of the above method to the scalar test equation (4) gives the difference equation (10) and the characteristic equation (10).

By applying \( k = 1 \) in the formula (8), we have that the phase-lag is given by (11). The first derivative of the phase-lag is given by (16). The second derivative of the phase-lag is given by (22). The third derivative of the phase-lag can be written as:
We demand that the phase-lag and its first, second and third derivative are equal to zero and we find out that:

\[ phl = \frac{1}{2} \frac{T_9 - 6 T_8 \cos(H) + 2 T_5 \sin(H) - 48 b_1 a_0 H}{T_5} \]
\[ + \frac{3 (2 T_7 \cos(H) - 4 T_8 \sin(H) - 2 T_5 \cos(H) + 2 b_1 - 24 b_1 a_0 H^2) T_8}{T_5^2} \]
\[ + \frac{3 (2 T_8 \cos(H) - 2 T_5 \sin(H) + 2 H b_1 - 8 H^3 b_1 a_0) T_8^2}{T_5^3} \]
\[ - \frac{3 (2 T_8 \cos(H) - 2 T_5 \sin(H) + 2 H b_1 - 8 H^3 b_1 a_0) T_7}{T_5^2} \]
\[ + \frac{3 T_6 T_8 T_7}{T_5^3} - \frac{12 T_6 b_1 a_0 H}{T_5^2} \]
\[ T_5 = 1 + H^2 b_0 + H^4 b_1 a_0 \]
\[ T_6 = 2 T_5 \cos(H) + c_1 + H^2 b_1 - 2 H^4 b_1 a_0 \]
\[ T_7 = 2 b_0 + 12 b_1 a_0 H^2 \]
\[ T_8 = 2 H b_0 + 4 H^3 b_1 a_0 \]
\[ T_9 = 48 b_1 a_0 H \cos(H) - 6 T_7 \sin(H)^2 \]
\[ a_0 = \frac{1}{4} \left( 3 \cos(H)^2 + \cos(H)^2 H^2 + 2 H^2 - 3 \right) \]
\[ / \left( (6 \cos(H)^3 H + 6 \sin(H) \cos(H)^2 - 2 \cos(H)^2 H^2 \sin(H) + \cos(H)^2 H^3 + 3 \cos(H)^2 H - 6 \cos(H) \sin(H) - 4 \cos(H) H^2 \sin(H) - 12 \cos(H) H + 2 H^3 + 3 H + 12 \sin(H) H^2 \right) \]
\[ c_1 = -2 \left( -12 \cos(H)^3 H + \cos(H)^2 H^3 - 21 \cos(H)^2 H - 12 \sin(H) \cos(H)^2 - 4 \cos(H)^2 H^2 \sin(H) + 12 \cos(H) \sin(H) - 8 \cos(H) H^2 \sin(H) + 24 \cos(H) H + 2 H^3 + 9 H + 24 \sin(H) H^2 \right) / \]
\[ (\cos(H)^2 H^3 - 21 \cos(H)^2 H + 8 \cos(H) H^2 \sin(H) - 12 \cos(H) H - 12 \cos(H) \sin(H) + 4 \sin(H) H^2 + 33 H + 12 \sin(H) + 2 H^3) \]
\[ b_0 = -2 \left( 3 \cos(H)^2 H + \cos(H)^2 H^3 + 6 \cos(H) \sin(H) + 4 \cos(H) H^2 \sin(H) + 6 \cos(H) H + 2 \sin(H) H^2 - 9 H - 6 \sin(H) + 2 H^3 \right) / \]
\[ (\cos(H)^2 H^3 - 21 \cos(H)^2 H + 8 \cos(H) H^2 \sin(H) - 12 \cos(H) H - 12 \cos(H) \sin(H) + 4 \sin(H) H^2 + 33 H + 12 \sin(H) + 2 H^3) H^2 \]
\[ b_1 = 4 \left( 6 \cos(H)^3 H + 6 \sin(H) \cos(H)^2 - 2 \cos(H)^2 H^2 \sin(H) + \cos(H)^2 H^3 + 3 \cos(H)^2 H - 6 \cos(H) \sin(H) - 4 \cos(H) H^2 \sin(H) - 12 \cos(H) H + 2 H^3 + 3 H + 12 \sin(H) H^2 \right) / \]
\[ (\cos(H)^2 H^3 - 21 \cos(H)^2 H + 8 \cos(H) H^2 \sin(H) - 12 \cos(H) H - 12 \cos(H) \sin(H) + 4 \sin(H) H^2 + 33 H + 12 \sin(H) + 2 H^3) H^2 \] (28)

For small values of \(|H|\) the formulae given by (28) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:
\[a_0 = \frac{1}{200} + \frac{1}{1260} H^2 + \frac{29}{504000} H^4 + \frac{1433}{1164240000} H^6 - \frac{36324288000000}{63101} H^8 - \frac{127135008000000}{222861} H^{10} - \frac{8804897780662489600000000}{360497} H^{12} + \frac{20489596601126400000000}{240953700049} H^{14} + \frac{8195838640045056000000000}{9699610781879} H^{16} + \ldots\]

\[c_1 = -2 + \frac{1}{6048} H^8 + \frac{1}{43200} H^{10} + \frac{1}{53224} H^{12} - \frac{41}{5943974400} H^{14} - \frac{601}{24141680640} H^{16} + \ldots\]

\[b_0 = \frac{1}{12} - \frac{1}{1008} H^4 - \frac{31}{181440} H^6 - \frac{221}{1368576} H^8 - \frac{1345344000}{84256583} H^{10} + \frac{25031}{174356582400} H^{12} + \frac{2667655710720000}{1030007057} H^{14} + \frac{290284441574400000}{290289444157440000} H^{16} + \ldots\]

\[b_1 = \frac{5}{6} + \frac{1}{504} H^4 - \frac{29}{90720} H^6 - \frac{3271}{47900160} H^8 - \frac{35293}{4540536000} H^{10} - \frac{36019}{87178291200} H^{12} + \frac{13382785360000}{294008389} H^{14} + \frac{24562952967168000}{24562952967168000} H^{16} + \ldots\] (29)

The behavior of the coefficients is given in the following Figure 4.

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

\[\text{LTE} = \frac{h^8}{6048} \left( y^{(8)} + 4 \omega^2 y^{(6)} + 6 \omega^4 y^{(4)} + 4 \omega^6 y^{(2)} + \omega^8 y_n \right) \] (30)

4. Error Analysis

We will study the following methods:
The error analysis is based on the following steps:

- The radial time independent Schrödinger equation is of the form

\[ y''(x) = f(x) y(x) \]  \hspace{1cm} (31)

- Based on the paper of Ixaru and Rizea [25], the function \( f(x) \) can be written in the form:

\[ f(x) = g(x) + G \]  \hspace{1cm} (32)
where \( g(x) = V(x) - V_c = g \), where \( V_c \) is the constant approximation of the potential and \( G = v^2 = V_c - E \).

- We express the derivatives \( y_n^{(i)} \), \( i = 2, 3, 4, \ldots \), which are terms of the local truncation error formulae, in terms of the equation (31). The expressions are presented as polynomials of \( G \).

- Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae.

Based on the procedure mentioned above and on the formulae:

\[
\begin{align*}
y_n^{(2)} &= (V(x) - V_c + G) y(x) \\
y_n^{(4)} &= (\frac{d^2}{dx^2} V(x)) y(x) + 2(\frac{d}{dx} V(x)) (\frac{d}{dx} y(x)) \\
&\quad + (V(x) - V_c + G) (\frac{d^2}{dx^2} y(x)) \\
y_n^{(6)} &= (\frac{d^4}{dx^4} V(x)) y(x) + 4(\frac{d^3}{dx^3} V(x)) (\frac{d}{dx} y(x)) \\
&\quad + 3(\frac{d^2}{dx^2} V(x)) (\frac{d^2}{dx^2} y(x)) \\
&\quad + 4(\frac{d}{dx} V(x))^2 y(x) \\
&\quad + 6 (V(x) - V_c + G) (\frac{d}{dx} y(x)) (\frac{d}{dx} V(x)) \\
&\quad + 4 (U(x) - V_c + G) y(x) (\frac{d^2}{dx^2} V(x)) \\
&\quad + (V(x) - V_c + G)^2 (\frac{d^2}{dx^2} y(x)) \ldots
\end{align*}
\]

we obtain the following expressions:
\[
\text{LTE}_{PL1} = h^8 \left[ -\frac{1}{6048} g(x) y(x) G^3 + \left( -\frac{5}{2016} \left( \frac{d^2}{dx^2} g(x) \right) y(x) \right. \right. \\
\left. \left. - \frac{1}{1008} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) - \frac{1}{2016} g(x)^2 y(x) \right) G^2 + \left( \right. \right. \\
\left. \left. - \frac{5}{2016} \left( \frac{d^4}{dx^4} g(x) \right) y(x) - \frac{5}{1512} \left( \frac{d^3}{dx^3} g(x) \right) \left( \frac{d}{dx} y(x) \right) \right. \right. \\
\left. \left. - \frac{1}{336} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) - \frac{37}{6048} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right) \right. \right. \\
\left. \left. - \frac{1}{252} \left( \frac{d}{dx} g(x) \right)^2 y(x) - \frac{1}{2016} g(x)^3 y(x) \right) \right. \right. \\
\left. \left. G \right. \right. \\
\left. \left. - \frac{1}{6048} \left( \frac{d^6}{dx^6} g(x) \right) y(x) - \frac{1}{1008} \left( \frac{d^5}{dx^5} g(x) \right) \left( \frac{d}{dx} g(x) \right) \right. \right. \\
\left. \left. - \frac{1}{378} g(x) y(x) \left( \frac{d^4}{dx^4} g(x) \right) - \frac{75}{2016} \left( \frac{d^2}{dx^2} g(x) \right)^2 y(x) \right. \right. \\
\left. \left. - \frac{13}{3024} \left( \frac{d}{dx} g(x) \right) y(x) \left( \frac{d^3}{dx^3} g(x) \right) - \frac{1}{252} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^3}{dx^3} g(x) \right) \right. \right. \\
\left. \left. - \frac{1}{504} g(x)^2 \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \right. \right. \\
\left. \left. - \frac{1}{126} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^2}{dx^2} g(x) \right) \right. \right. \\
\left. \left. - \frac{11}{3024} g(x)^2 y(x) \left( \frac{d^2}{dx^2} g(x) \right) - \frac{223}{126} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right)^2 \right. \right. \\
\left. \left. - \frac{1}{6048} g(x)^4 y(x) \right]\right. \right. (33)
\]
The Second Method of the Family

\[ \text{LTE}_{PL2} = \hbar^8 \left[ \frac{19}{9072} \left( \frac{d^2}{dx^2} g(x) \right) y(x) + \frac{1}{1512} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) \right. \\
+ \frac{1}{3024} g(x)^2 y(x) \right] \left( G^2 + \left( \frac{d^4}{dx^4} g(x) \right) y(x) \right) \\
+ \frac{1}{324} \left( \frac{d^3}{dx^3} g(x) \right) \left( \frac{d}{dx} y(x) \right) + \frac{1}{378} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \right. \\
+ \frac{13}{2268} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{17}{4536} \left( \frac{d}{dx} g(x) \right)^2 y(x) \right. \\
+ \frac{1}{2268} g(x)^3 y(x) G + \frac{1}{6048} \left( \frac{d^6}{dx^6} g(x) \right) y(x) \left. \right. \\
+ \frac{1}{1008} \left( \frac{d^5}{dx^5} g(x) \right) \left( \frac{d}{dx} y(x) \right) + \frac{1}{378} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^3}{dx^3} g(x) \right) \right. \\
+ \frac{5}{2016} \left( \frac{d^2}{dx^2} g(x) \right)^2 y(x) + \frac{13}{3024} \left( \frac{d}{dx} g(x) \right) \left( \frac{d^3}{dx^3} g(x) \right) \right. \\
+ \frac{1}{252} \left( \frac{d}{dx} y(x) \right) \left( \frac{d^3}{dx^3} g(x) \right) + \frac{1}{504} g(x)^2 \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \right. \\
+ \frac{1}{12} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{11}{3024} \left( \frac{d}{dx} g(x) \right)^2 \left( \frac{d^2}{dx^2} g(x) \right) \right. \\
+ \frac{1}{216} g(x) y(x) \left( \frac{d}{dx} g(x) \right)^2 + \frac{1}{6048} \left( \frac{d}{dx} g(x) \right)^4 y(x) \right] \] (34)
\[
\text{LTE}_{PL3} = h^8 \left[ \frac{1}{1756} \left( \frac{d^2}{dx^2} g(x) \right) y(x) G^2 + \left( \frac{1}{432} \left( \frac{d^4}{dx^4} g(x) \right) y(x) + \frac{1}{378} \left( \frac{d^3}{dx^3} g(x) \right) \left( \frac{d}{dx} y(x) \right) \right) + \frac{1}{504} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) + \frac{5}{1008} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{5}{1512} \left( \frac{d}{dx} g(x) \right)^2 y(x) + \frac{1}{3024} g(x)^3 y(x) \right] G + \frac{1}{6048} \left( \frac{d^6}{dx^6} g(x) \right) y(x) + \frac{1}{1008} \left( \frac{d^5}{dx^5} g(x) \right) \left( \frac{d}{dx} y(x) \right) + \frac{1}{378} g(x) y(x) \left( \frac{d^4}{dx^4} g(x) \right) + \frac{5}{2016} \left( \frac{d^2}{dx^2} g(x) \right)^2 y(x) + \frac{13}{3024} \left( \frac{d}{dx} g(x) \right) y(x) \left( \frac{d^3}{dx^3} g(x) \right) + \frac{1}{252} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^3}{dx^3} g(x) \right) + \frac{1}{504} g(x)^2 \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) + \frac{1}{126} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{11}{3024} g(x)^2 y(x) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{1}{216} g(x) y(x) \left( \frac{d}{dx} g(x) \right)^2 + \frac{1}{6048} g(x)^4 y(x) \right] (35)
\]
The Fourth Method of the Family

\[ \text{LTE}_{PL4} = h^8 \left[ \frac{1}{504} \left( \frac{d^4}{dx^4} g(x) \right) y(x) + \frac{1}{756} \left( \frac{d^3}{dx^3} g(x) \right) \left( \frac{d}{dx} y(x) \right) \right. \]
\[ \left. + \frac{1}{378} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{1}{504} \left( \frac{d}{dx} g(x) \right)^2 y(x) \right] G \]
\[ + \frac{1}{6048} \left( \frac{d^6}{dx^6} g(x) \right) y(x) + \frac{1}{1008} \left( \frac{d^5}{dx^5} g(x) \right) \left( \frac{d}{dx} y(x) \right) \]
\[ + \frac{1}{378} g(x) y(x) \left( \frac{d^4}{dx^4} g(x) \right) + \frac{5}{2016} \left( \frac{d^2}{dx^2} g(x) \right)^2 y(x) \]
\[ + \frac{13}{3024} \left( \frac{d}{dx} g(x) \right) y(x) \left( \frac{d^3}{dx^3} g(x) \right) \]
\[ + \frac{1}{252} g(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^3}{dx^3} g(x) \right) + \frac{1}{504} g(x)^2 \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \]
\[ + \frac{1}{126} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^2}{dx^2} g(x) \right) \]
\[ + \frac{11}{3024} g(x)^2 y(x) \left( \frac{d^2}{dx^2} g(x) \right) \]
\[ + \frac{1}{216} g(x) y(x) \left( \frac{d}{dx} g(x) \right)^2 + \frac{1}{6048} g(x)^4 y(x) \right] (36) \]

We consider two cases in terms of the value of \( E \):

- The Energy is close to the potential, i.e. \( G = V_c - E \approx 0 \). So only the free terms of the polynomials in \( G \) are considered. Thus for these values of \( G \), the methods are of comparable accuracy. This is because the free terms of the polynomials in \( G \), are the same for the cases of the classical method and of the new developed methods.

- \( G \gg 0 \) or \( G \ll 0 \). Then \( |G| \) is a large number. So, we have the following asymptotic expansions of the equations (33), (34), (35) and (36).

The First Method of the Family

\[ \text{LTE}_{PL1} = h^8 \left( -\frac{1}{6048} g(x) y(x) G^3 + \ldots \right) \] (37)
The Second Method of the Family

\[ \text{LTE}_{PL2} = h^8 \left( \frac{19}{9072} \left( \frac{d^2}{dx^2} g(x) \right) y(x) + \frac{1}{1512} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) + \frac{1}{3024} g(x)^2 y(x) \right) G^2 + \ldots \]  

The Third Method of the Family

\[ \text{LTE}_{PL3} = h^8 \left( \frac{1}{756} \left( \frac{d^2}{dx^2} g(x) \right) y(x) G^2 + \ldots \right) \] (38)

The Fourth Method of the Family

\[ \text{LTE}_{PL4} = h^8 \left( \left( \frac{1}{504} \left( \frac{d^4}{dx^4} g(x) \right) y(x) + \frac{1}{756} \left( \frac{d^3}{dx^3} g(x) \right) \left( \frac{d}{dx} y(x) \right) + \frac{1}{378} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right) + \frac{1}{504} \left( \frac{d}{dx} g(x) \right)^2 y(x) \right) G + \ldots \right) \] (39)

From the above equations we have the following theorem:

**THEOREM 2.** For the First Method of the New Family of Methods the error increases as the third power of \( G \). For the Second and Third Methods of the New Family of Methods the error increases as the second power of \( G \). For the Fourth Method of the New Family of Methods the error increases as the first power of \( G \). It is easy one to see that the coefficient of the second power of \( G \) in the case of the second method of the New Family of Methods is 1.583333333 times larger than the coefficient of the second power of \( G \) in the case of the third method of the New Family of Methods. So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Fourth Method of the New Family of Methods is the most accurate one, especially for large values of \( |G| = |V_c - E| \).

5. Stability Analysis

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

\[ y'' = -t^2 y, \] (40)
where $t \neq \omega$. We obtain the following difference equation:

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

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

The characteristic equation associated with (41) is given by:

$$A_1(H, s) s + A_0(H, s) + A_1(H, s) s^{-1} = 0 \quad (41)$$

where

$$A_1(H, s) = 1 + s^2 b_0 + s^4 b_1 a_0$$

$$A_0(H, s) = c_1 + s^2 b_1 - 2 s^4 b_1 a_0 \quad (42)$$

**DEFINITION 1.** (see [19]) A symmetric four-step method with the characteristic equation given by (41) is said to have an interval of periodicity $(0, w^2_0)$ if, for all $w \in (0, w^2_0)$, the roots $z_i, i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i \theta(t h)}, \quad |z_i| \leq 1, \quad i = 3, 4 \quad (43)$$

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

**DEFINITION 2.** (see [19]) A method is called $P$-stable if its interval of periodicity is equal to $(0, \infty)$.

**THEOREM 3.** (see [20]) A symmetric two-step method with the characteristic equation given by (41) is said to have a nonzero interval of periodicity $(0, s^2_0)$ if, for all $s \in (0, s^2_0)$ the following relations are hold

$$P_1(H, s) > 0, \quad P_2(H, s) > 0, \quad (44)$$

where $H = \omega h$, $s = t h$ and:

$$P_1(H, s) = A_0(H, s) + 2 A_1(H, s) > 0,$$

$$P_2(H, s) = A_0(H, s) - 2 A_1(H, s) > 0, \quad (45)$$

**DEFINITION 3.** A method is called singularly almost $P$-stable if its interval of periodicity is equal to $(0, \infty) - S^2$ only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $H = s$. 

---

2 where $S$ is a set of distinct points
Based on (42) the stability polynomials (45) for the new developed methods take the form:

\[
P_1(H, s) = c_1 + v^2 b_1 + 2 + 2 v^2 b_0, \\
P_2(H, s) = c_1 + v^2 b_1 - 4 v^4 b_1 a_0 - 2 - 2 v^2 b_0 \tag{46}
\]

In Figures 5, 6, 7 and 8 we present the \( s - H \) planes for the methods developed in this paper. A shadowed area denotes the \( s - H \) region where the method is unstable, while a white area denotes the region where the method is stable. In Figure 5 we present the \( s - H \) plane for the first method of the new family of method developed in this paper (paragraph 3.1). In Figure 6 we present the \( s - H \) plane for the second method of the new family of method developed in this paper (paragraph 3.2). In Figure 7 we present the \( s - H \) plane for the third method of the new family of method developed in this paper (paragraph 3.3). Finally, in Figure 8 we present the \( s - H \) plane for the fourth method of the new family of method developed in this paper (paragraph 3.4).

\textit{Figure 5.} \( s - H \) plane of the first method of the new family of method developed in this paper (paragraph 3.1)
Figure 6. $s - H$ plane of the second method of the new family of method developed in this paper (paragraph 3.2)

In the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $H = s$, we have the following figure for the stability polynomials of the new developed methods. A method is P-stable if the $s - H$ plane is not shadowed. From the above diagrams it is easy for one to see that the interval of periodicity of all the new methods is equal to: $\left(0, \pi^2\right)$.

REMARK 2. For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the $w - H$ plane.
6. Numerical results - Conclusion

In order to illustrate the efficiency of the new methods obtained in paragraphs 3.1 - 3.4, we apply them to the radial time independent Schrödinger equation.

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

\[
v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|}
\]

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

6.1. Woods-Saxon potential

We use the well known Woods-Saxon potential given by

\[
V(x) = \frac{u_0}{1 + z} - \frac{u_0 z}{a (1 + z)^2}
\]

with \( z = \exp \left( \frac{x - X_0}{a} \right) \), \( u_0 = -50 \), \( a = 0.6 \), and \( X_0 = 7.0 \).
A New Methodology for the Development of Numerical Methods

Figure 8. $s - H$ plane of the fourth method of the new family of method developed in this paper (paragraph 3.4)

Figure 9. Stability polynomials of the new developed methods in the case that $H = s$

The behavior of Woods-Saxon potential is shown in the Figure 10.
It is well known that for some potentials, such as the Woods-Saxon potential, the definition of parameter $v$ is not given as a function of $x$ but it is based on some critical points which have been defined from the investigation of the appropriate potential (see for details [13]).

For the purpose of obtaining our numerical results it is appropriate to choose $v$ as follows (see for details [13]):

$$
v = \begin{cases} 
\sqrt{-50 + E}, & \text{for } x \in [0, 6.5 - 2h], \\
\sqrt{-37.5 + E}, & \text{for } x = 6.5 - h \\
\sqrt{-25 + E}, & \text{for } x = 6.5 \\
\sqrt{-12.5 + E}, & \text{for } x = 6.5 + h \\
\sqrt{E}, & \text{for } x \in [6.5 + 2h, 15] 
\end{cases} 
$$ (49)
6.2. Radial Schrödinger Equation - The Resonance Problem

Consider the numerical solution of the radial time independent Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (48). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as \( x \in [0, 15] \). We consider equation (1) in a rather large domain of energies, i.e. \( E \in [1, 1000] \).

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

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

for \( x > X \).

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

\[
y(x) \simeq A k x j_l(kx) - B k x n_l(kx)
\]

\[
\simeq A C \left[ \sin \left( kx - \frac{l\pi}{2} \right) + \tan \delta_l \cos \left( kx - \frac{l\pi}{2} \right) \right]
\]

where \( \delta_l \) is the phase shift, that is calculated from the formula

\[
tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)}
\]

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

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift \( \delta_l \) or finding those \( E \), for \( E \in [1, 1000] \), at which \( \delta_l = \frac{\pi}{2} \). We actually solve the latter problem, known as the resonance problem when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

\[
y(0) = 0, \; y(x) = \cos \left( \sqrt{E}x \right) \text{ for large } x.
\]
We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using:

- The Numerov’s method which is indicated as Method I

- The Exponentially-fitted four-step method developed by Raptis [16] which is indicated as Method II
Figure 12. Error Errmax for several values of n for the eigenvalue $E = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive.

- The Two-Step Numerov-type Method with minimum phase-lag produced by Chawla and Rao [23] which is indicated as Method III.

- The new Two-Step Numerov-Type Method with phase-lag equal to zero obtained in paragraph 3.1 which is indicated as Method IV.
− The new Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero obtained in paragraph 3.2 which is indicated as Method V.

− The new Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 3.3 which is indicated as Method VI.

− The new Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero obtained in paragraph 3.4 which is indicated as Method VII.

The computed eigenenergies are compared with exact ones. In Figure 11 we present the maximum absolute error $\log_{10}(Err)$ where

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

(54)

of the eigenenergy $E_1$, for several values of NFE = Number of Function Evaluations. In Figure 12 we present the maximum absolute error $\log_{10}(Err)$ where

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

(55)

of the eigenenergy $E_3$, for several values of NFE = Number of Function Evaluations.

7. Conclusions

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

More specifically we have developed:

1. A Two-Step Numerov-Type Method with phase-lag equal to zero

2. A Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero

3. A Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero

4. A Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero
We have applied the new method to the resonance problem of the radial Schrödinger equation.

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

- The Exponentially-fitted four-step method developed by Raptis [16] (denoted as Method II) is more efficient than the Numerov’s Method (denoted Method I).

- The Two-Step Numerov-type Method with minimum phase-lag produced by Chawla and Rao [23] (Method III) is more efficient than the Exponentially-fitted four-step method developed by Raptis [16] (Method II) for the energy $163.215341$ and less efficient for the energy $989.701916$.

- The new developed methods are much more efficient than the older ones.

- The Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero (Method V) is more efficient than the New Two-Step Numerov-Type Method with phase-lag equal to zero (Method IV)

- The Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero (Method VI) is more efficient than the Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero (Method V)

- The Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero (Method VII) is more efficient than the Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero (Method VI)

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

References

1. L.Gr. Ixaru and M. Micu, *Topics in Theoretical Physics*. Central Institute of Physics, Bucharest, 1978.
2. L.D. Landau and F.M. Lifshitz: *Quantum Mechanics*. Pergamon, New York, 1965.
3. I. Prigogine, Stuart Rice (Eds): Advances in Chemical Physics Vol. 93: New Methods in Computational Quantum Mechanics, John Wiley & Sons, 1997.
4. G. Herzberg, *Spectra of Diatomic Molecules*, Van Nostrand, Toronto, 1950.
5. T.E. Simos, Atomic Structure Computations in Chemical Modelling: Applications and Theory (Editor: A. Hinchliffe, UMIST), *The Royal Society of Chemistry* 38-142(2000).
6. T.E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems, *Chemical Modelling: Application and Theory*, The Royal Society of Chemistry, 2(2002),170-270.
7. T.E. Simos and P.S. Williams, On finite difference methods for the solution of the Schrödinger equation, *Computers & Chemistry* 23 513-554(1999).
8. T.E. Simos: *Numerical Solution of Ordinary Differential Equations with Periodical Solution*, Doctoral Dissertation, National Technical University of Athens, Greece, 1990 (in Greek).
9. A. Konguetsof and T.E. Simos, On the Construction of exponentially-fitted methods for the numerical solution of the Schrödinger Equation, *Journal of Computational Methods in Sciences and Engineering* 1 143-165(2001).
10. A.D. Raptis and A.C. Allison: Exponential - fitting methods for the numerical solution of the Schrödinger equation, *Computer Physics Communications*, 14 1-5(1978).
11. A.D. Raptis, Exponential multistep methods for ordinary differential equations, *Bull. Greek Math. Soc.* 25 113-126(1984).
12. L.Gr. Ixaru, Numerical Methods for Differential Equations and Applications, Reidel, Dordrecht - Boston - Lancaster, 1984.
13. L.Gr. Ixaru and M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. *Comput. Phys. Commun.* 19 23-27(1980).
14. T. E. Simos, P. S. Williams: A New Runge-Kutta-Nystrom Method with Phase-Lag of Order Infinity for the Numerical Solution of the Schrödinger Equation, *MATCH Commun. Math. Comput. Chem.* 45 123-137(2002).
15. T. E. Simos, Multiderivative Methods for the Numerical Solution of the Schrödinger Equation, *MATCH Commun. Math. Comput. Chem.* 45 7-26(2004).
16. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Shrödinger equation with automatic error control, *Computer Physics Communications*, 28 427-431(1983)
17. A.D. Raptis, On the numerical solution of the Schrodinger equation, *Computer Physics Communications*, 24 1-4(1981)
18. Zacharoula Kalogiratou and T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation, *Applied Mathematics and Computation*, 112 99-112(2000).
19. J.D. Lambert and I.A. Watson, Symmetric multistep methods for periodic initial values problems, *J. Inst. Math. Appl.* 18 189-202(1976).
20. A.D. Raptis and T.E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problem, *BIT*, 31 160-168(1991).
21. Peter Henrici, *Discrete variable methods in ordinary differential equations*, John Wiley & Sons, 1962.
22. M.M. Chawla, Uncoditionally stable Numerov-type methods for second order differential equations, *BIT*, 23 541-542(1983).
23. M. M. Chawla and P. S. Rao, A Numerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems, *Journal of Computational and Applied Mathematics* 11(3) 277-281(1984)
24. Liviu Gr. Ixaru and Guido Vanden Berghe, Exponential Fitting, Series on Mathematics and its Applications, Vol. 568, Kluwer Academic Publisher, The Netherlands, 2004.
25. L. Gr. Ixaru and M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation, *Computer Physics Communications*, **38**(3) 329-337 (1985)
26. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation, *J. Math. Chem* **41**(1) 79-100 (2007)
27. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation, *J. Math. Chem* **40**(3) 257-267 (2006)
28. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor-Corrector methods, *J. Math. Chem* **40**(3) 269-293 (2006)
29. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation, *J. Math. Chem* **40**(3) 305-318 (2006)
30. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation *J. Math. Chem* **37**(3) 263-270 (2005)
31. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods *J. Math. Chem* **37**(3) 271-279 (2005)
32. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation *J. Math. Chem* **37**(3) 281-293 (2005)
33. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation, *J. Math. Chem* **37**(3) 295-316 (2005)
34. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem* **37**(3) 317-331 (2005)
35. T.E. Simos, Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem* **36**(1) 13-27 (2004)
36. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation, *J. Math. Chem* **35**(1) 55-63 (2004)
37. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems *J. Math. Chem* **34**(1-2) 39-58 JUL 2003
38. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation, *J. Math. Chem* **34**(1-2) 83-94 (2003)
39. J. Vigo-Aguiar J, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation, *J. Math. Chem* **32**(3) 257-270 (2002)
40. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation, *J. Math. Chem* **31**(4) 371-404 (2002)
41. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. *J. Math. Chem* 31 (2) 135-144 (2002)

42. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nystrom methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. *J. Math. Chem* 31 (2) 211-232

43. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. *J. Math. Chem* 30 (1) 121-131 (2001)

44. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. *J. Math. Chem* 29 (4) 281-291 (2001)

45. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. *J. Math. Chem* 29 (4) 293-305 (2001)

46. J. Vigo-Aguiar, T.E. Simos, A family of P-stable eighth algebraic order methods with exponential fitting facilities. *J. Math. Chem* 29 (3) 177-189 (2001)

47. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. *J. Math. Chem* 27 (4) 343-356 (2000)

48. G. Avdelas, T.E. Simos, Embedded eighth order methods for the numerical solution of the Schrödinger equation. *J. Math. Chem* 26 (4) 327-341 (1999)

49. T.E. Simos, A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. *J. Math. Chem* 25 (1) 65-84 (1999)

50. T.E. Simos, Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. *J. Math. Chem* 24 (1-3) 23-37 (1998)

51. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. *J. Math. Chem* 21 (4) 359-372 (1997)

52. P. Amodio, I. Gladwell and G. Romanazzi, Numerical Solution of General Bordered ABD Linear Systems by Cyclic Reduction, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 5-12 (2006)

53. S. D. Capper, J. R. Cash and D. R. Moore, Lobatto-Obrechkoff Formulae for 2nd Order Two-Point Boundary Value Problems, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 13-25 (2006)

54. S. D. Capper and D. R. Moore, On High Order MIRK Schemes and Hermite-Birkhoff Interpolants, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 27-47 (2006)

55. J. R. Cash, N. Sumarti, T. J. Abdulla and I. Vieira, The Derivation of Interpolants for Nonlinear Two-Point Boundary Value Problems, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 49-58 (2006)

56. J. R. Cash and S. Girdlestone, Variable Step Runge-Kutta-Nystrom Methods for the Numerical Solution of Reversible Systems, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 59-80 (2006)
57. Jeff R. Cash and Francesca Mazzia, Hybrid Mesh Selection Algorithms Based on Conditioning for Two-Point Boundary Value Problems, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 81-90 (2006)

58. Felice Iavernaro, Francesca Mazzia and Donato Trigiante, Stability and Conditioning in Numerical Analysis, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 91-112 (2006)

59. Felice Iavernaro and Donato Trigiante, Discrete Conservative Vector Fields Induced by the Trapezoidal Method, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 113-130 (2006)

60. Francesca Mazzia, Alessandra Sestini and Donato Trigiante, BS Linear Multistep Methods on Non-uniform Meshes, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(1) 131-144 (2006)

61. L.F. Shampine, P.H. Muir, H. Xu, A User-Friendly Fortran BVP Solver, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(2) 201-217 (2006)

62. G. Vanden Berghe and M. Van Daele, Exponentially-fitted Störmer/Verlet methods, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 1(3) 241-255 (2006)

63. L. Aceto, R. Pandolfi, D. Trigiante, Stability Analysis of Linear Multistep Methods via Polynomial Type Variation, *JNAIAM J. Numer. Anal. Indust. Appl. Math* 2(1-2) 1-9 (2007)

64. G. Psihoyios, A Block Implicit Advanced Step-point (BIAS) Algorithm for Stiff Differential Systems, *Computing Letters* 2(1-2) 51-58(2006)

65. W.H. Enright, On the use of ‘arc length’ and ‘defect’ for mesh selection for differential equations, *Computing Letters* 1(2) 47-52(2005)

66. T.E. Simos, P-stable Four-Step Exponentially-Fitted Method for the Numerical Integration of the Schrödinger Equation, *Computing Letter* 1(1) 37-45(2005).

67. T.E. Simos, Stabilization of a Four-Step Exponentially-Fitted Method and its Application to the Schrödinger Equation, *International Journal of Modern Physics C* 18(3) 315-328(2007).

68. Zhongcheng Wang, P-stable linear symmetric multistep methods for periodic initial-value problems, *Computer Physics Communications* 171 162174(2005)

69. T.E. Simos, A Runge-Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution, *Computers and Mathematics with Applications* 25 95-101(1993).

70. T.E. Simos, Runge-Kutta interpolants with minimal phase-lag, *Computers and Mathematics with Applications* 26 43-49(1993).

71. T.E. Simos, Runge-Kutta-Nyström interpolants for the numerical integration of special second-order periodic initial-value problems, *Computers and Mathematics with Applications* 26 7-15(1993).

72. T.E. Simos and G.V. Mitsou, A family of four-step exponential fitted methods for the numerical integration of the radial Schrödinger equation, *Computers and Mathematics with Applications* 28 41-50(1994).

73. T.E. Simos and G. Mousadis, A two-step method for the numerical solution of the radial Schrdinger equation, *Computers and Mathematics with Applications* 29 31-37(1995).

74. G. Avdelas and T.E. Simos, Block Runge-Kutta methods for periodic initial-value problems, *Computers and Mathematics with Applications* 31 69-83(1996).

75. G. Avdelas and T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation, *Computers and Mathematics with Applications* 31 85-102(1996).
76. G. Papakaliatakis and T.E. Simos, A new method for the numerical solution of fourth order BVPs with oscillating solutions, *Computers and Mathematics with Applications* **32** 1-6 (1996).

77. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation, *Computers and Mathematics with Applications* **33** 67-78 (1997).

78. T.E. Simos, A new hybrid imbedded variable-step procedure for the numerical integration of the Schrödinger equation, *Computers and Mathematics with Applications* **36** 51-63 (1998).

79. T.E. Simos, Bessel and Neumann Fitted Methods for the Numerical Solution of the Schrödinger equation, *Computers & Mathematics with Applications* **42** 833-847 (2001).

80. A. Konguetsof and T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems, *Computers and Mathematics with Applications* **45** 547-554 (2003).

81. Z.A. Anastassi and T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *Journal of Computational and Applied Mathematics* **175**(1) 1-9 (2005).

82. G. Psihoyios and T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions, *Journal of Computational and Applied Mathematics* **175**(1) 137-147 (2005).

83. 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* **175**(1) 161-172 (2005).

84. 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* **175**(1) 173-181 (2005).

85. Z. Kalogiratou and T.E. Simos, Newton-Cotes formulae for long-time integration, *Journal of Computational and Applied Mathematics* **158**(1) 75-82 (2003).

86. Z. Kalogiratou, T. Monovasilis and T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* **158**(1) 83-92 (2003).

87. A. Konguetsof and T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* **158**(1) 93-106 (2003).

88. G. Psihoyios and T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions, *Journal of Computational and Applied Mathematics* **158**(1) 135-144 (2003).

89. Ch. Tsitouras and T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions, *Journal of Computational and Applied Mathematics* **147**(2) 397-409 (2002).

90. T.E. Simos, An exponentially fitted eighth-order method for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* **108**(1-2) 177-194 (1999).

91. T.E. Simos, An accurate finite difference method for the numerical solution of the Schrödinger equation, *Journal of Computational and Applied Mathematics* **91**(1) 47-61 (1998).

92. R.M. Thomas and T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial solution.
Schrödinger equation, *Journal of Computational and Applied Mathematics* 87(2) 215-226(1997)

93. Z.A. Anastassi and T.E. Simos: Special Optimized Runge-Kutta methods for IVPs with Oscillating Solutions, International Journal of Modern Physics C, 15, 1-15 (2004)

94. Z.A. Anastassi and T.E. Simos: A Dispersive-Fitted and Dissipative-Fitted Explicit Runge-Kutta method for the Numerical Solution of Orbital Problems, New Astronomy, 10, 31-37 (2004)

95. Z.A. Anastassi and T.E. Simos: A Trigonometrically-Fitted Runge-Kutta Method for the Numerical Solution of Orbital Problems, New Astronomy, 10, 301-309 (2005)

96. T.V. Triantafyllidis, Z.A. Anastassi and T.E. Simos: Two Optimized Runge-Kutta Methods for the Solution of the Schrödinger Equation, MATCH Commun. Math. Comput. Chem., 60, 3 (2008)

97. Z.A. Anastassi and T.E. Simos, A Family of Two-Stage Two-Step Methods for the Numerical Integration of The Schrödinger Equation, MATCH Commun. Math. Comput. Chem., 58(3) 337-344(1995)

98. Z.A. Anastassi and T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution, Journal of Mathematical Chemistry, Article in Press, Corrected Proof

99. 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* 58(3) 337-344(1995)
108. A.B. Sideridis and T.E. Simos, A Low-Order Embedded Runge-Kutta Method for Periodic Initial-Value Problems, *Journal of Computational and Applied Mathematics* **44**(2) 235-244(1992)

109. T.E. Simos and A.D. Raptis, A 4th-order Bessel Fitting Method for the Numerical-Solution of the Schrödinger-Equation, *Journal of Computational and Applied Mathematics* **43**(3) 313-322(1992)

110. T.E. Simos, Explicit 2-Step Methods with Minimal Phase-Lag for the Numerical-Integration of Special 2nd-order Initial-Value Problems and their Application to the One-Dimensional Schrödinger-Equation, *Journal of Computational and Applied Mathematics* **39**(1) 89-94(1992)

111. T.E. Simos, A 4-Step Method for the Numerical-Solution of the Schrödinger-Equation, *Journal of Computational and Applied Mathematics* **30**(3) 251-255(1990)

112. C.D. Papageorgiou, A.D. Raptis and T.E. Simos, A Method for Computing Phase-Shifts for Scattering, *Journal of Computational and Applied Mathematics* **29**(1) 61-67(1990)

113. A.D. Raptis, Two-Step Methods for the Numerical Solution of the Schrödinger Equation, *Computing* **28** 373-378(1982).

114. T.E. Simos, A new Numerov-type method for computing eigenvalues and resonances of the radial Schrödinger equation, International Journal of Modern Physics C-Physics and Computers, **7**(1) 33-41(1996)

115. T.E. Simos, Predictor Corrector Phase-Fitted Methods for $Y''=F(X,Y)$ and an Application to the Schrödinger-Equation, International Journal of Quantum Chemistry, **53**(5) 473-483(1995)

116. T.E. Simos, Two-step almost $P$-stable complete in phase methods for the numerical integration of second order periodic initial-value problems, *Inter. J. Comput. Math.* **46** 77-85(1992).

117. R. M. Corless, A. Shakoori, D.A. Aruliah, L. Gonzalez-Vega, Barycentric Hermite Interpolants for Event Location in Initial-Value Problems, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 1-16 (2008)

118. M. Dewar, Embedding a General-Purpose Numerical Library in an Interactive Environment, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 17-26 (2008)

119. J. Kierzenka and L.F. Shampine, A BVP Solver that Controls Residual and Error, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 27-41 (2008)

120. R. Knapp, A Method of Lines Framework in Mathematica, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 43-59 (2008)

121. N. S. Nedialkov and J. D. Pryce, Solving Differential Algebraic Equations by Taylor Series (III): the DAETS Code, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 61-80 (2008)

122. R. L. Lipsman, J. E. Osborn, and J. M. Rosenberg, The SCHOL Project at the University of Maryland: Using Mathematical Software in the Teaching of Sophomore Differential Equations, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 81-103 (2008)

123. M. Sofroniou and G. Spaletta, Extrapolation Methods in Mathematica, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 105-121 (2008)

124. R. J. Spiteri and Thian-Peng Ter, pythNon: A PSE for the Numerical Solution of Nonlinear Algebraic Equations, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 123-137 (2008)

125. S.P. Corwin, S. Thompson and S.M. White, Solving ODEs and DDEs with Impulses, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 139-149 (2008)
126. W. Weckesser, VGEN: A Code Generation Tool, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 151-165 (2008)

127. A. Wittkopf, Automatic Code Generation and Optimization in Maple, *JNAIAM J. Numer. Anal. Indust. Appl. Math*, 3, 167-180 (2008)
Behavior of the coefficient $a_0$
Behavior of the coefficient $a_0$
Behavior of the coefficient $c_1$
Behavior of the coefficient $b_1$
Behavior of the coefficient $a_0$
Behavior of the coefficient $c_1$
Behavior of the coefficient $b_0$
Behavior of the coefficient $b_1$
The Woods-Saxon Potential

![Graph of the Woods-Saxon Potential](image-url)