J Math Chem (2010) 48:224–252
DOI 10.1007/s10910-010-9664-8

ORIGINAL PAPER

Two-step high order hybrid explicit method for the numerical solution of the Schrödinger equation

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Received: 18 January 2010 / Accepted: 8 February 2010 / Published online: 4 March 2010

Abstract In this paper we present a new method for the numerical solution of the time-independent Schrödinger equation for one spatial dimension and related problems. A technique, based on the phase-lag and its derivatives, is used, in order to calculate the parameters of the new Numerov-type algorithm. We study the relation of the local truncation error with the energy of the model of the radial Schrödinger equation and via this investigation we examine how accurate is the new method compared with other well known numerical methods in the literature. We present also the stability analysis of the new method and the relation of the interval of periodicity with the frequency of the test problem and the frequency of the new developed method. We illustrate the accuracy and computational efficiency of the new developed method via numerical examples.

Keywords Multistep methods · Explicit methods · Hybrid methods · Phase-lag · Phase-fitted · Schrödinger equation

Abbreviations

LTE Local Truncation Error

1 Introduction

We will study the one-dimensional Schrödinger equation, which is a second order differential equation that describes the wave nature of matter (see [1–8]).

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It is the basic equation of quantum mechanics and we find it very frequently in physics and chemistry problems.

In particular, the subject of this paper is the numerical solution of the time-independent Schrödinger equation, which has the form

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

with one boundary condition

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

and another one taken from physical considerations.

There are numerical methods, developed for such problems, that need the frequency of the problem and others, where the knowledge of the frequency is not necessary for their application (see for details in the next paragraph in which we present the literature for these methods).

In this work an explicit Numerov-type sixth algebraic order family of methods with coefficients dependent on the frequency of the problem is presented. More analytically the paper has the following structure. The phase-lag analysis is given in paragraph 2. The construction of the new method is described in the 3rd paragraph. In paragraphs 4 and 5 we have the error and stability analysis respectively. In order to test the algorithm, it is applied to the resonance problem, as shown in the 6th paragraph. Finally, based on the numerical results given in paragraph 7, the 8th paragraph contains the conclusions extracted.

2 Description of the existed literature

There is an extended literature on the numerical methods for the radial time-independent Schrödinger equation and related problems.

More specifically, in [9] a description of finite difference methods for the solution of the Schrödinger equation was presented. In [10], symmetric multistep methods for periodic initial value problems are obtained. In [11], a modification of Numerov's method which produces a family of unconditionally stable fourth order methods for $y'' = f(t, y)$ was given.

In [12] Numerov-type methods which were made explicit with the help of the classical second order method. In [13–16] and [17] exponential-fitting methods for the numerical solution of the Schrödinger equation are developed. In [18] three four-step methods for the numerical solution of the radial Schrödinger equation.

In [19] a Runge-Kutta-Nyström fourth algebraic order method for the numerical solution of the Schrödinger equation was developed. The new method has phase-lag of order infinity and extended interval of periodicity. In [20] some multiderivative methods are developed. The methods are called multiderivative since derivatives of order two and four are used.

In [21] a P-stable exponentially fitted method was developed. In [22] a four-step method with phase-lag of infinite order for the numerical integration of second order

initial-value problems was introduced. This method was called "phase-fitted". This terminology was introduced in this paper.

In [23], three Runge-Kutta methods based on a classical method of Fehlberg with eight stages and sixth algebraic order are constructed. These methods are exponentially-fitted. In [24] exponentially fitted symplectic integrators are developed.

In [25] some seventh order trigonometrically fitted Adams-Bashforth-Moulton predictor–corrector algorithms are obtained. The predictor was based on the sixth algebraic order Adams-Bashforth scheme and the corrector on the seventh algebraic order Adams-Moulton scheme. In [26] an exponentially fitted four-step method for the numerical solution of the radial Schrödinger equation was introduced.

In [27] exponentially fitted and trigonometrically fitted symplectic integrators are obtained, by modification of the first and second order Yoshida symplectic methods for the computation of the energy eigenvalues of the one-dimensional time-independent Schrödinger equation. In [28] Numerov-type methods for the numerical solution of the two-dimensional time independent Schrödinger equation are presented.

In [29] two trigonometrically fitted methods based on a classical Runge-Kutta method of England with fifth algebraic order were obtained. In [30] trigonometrically fitted predictor–corrector schemes based on the well known Adams-Bashforth-Moulton methods were produced. The predictor was based on the fifth order Adams-Bashforth scheme and the corrector on the sixth order Adams-Moulton scheme.

In [31] a family of multiderivative methods with minimal phase-lag for the numerical solution of the Schrödinger equation is presented. In [32] exponentially fitted multiderivative methods are developed for the numerical solution of the one-dimensional Schrödinger equation. In [33] symplectic methods of fifth order for the numerical solution of the radial Shrödinger equation are obtained.

In [34] a family of trigonometrically-fitted symmetric ten-step methods for the efficient solution of the Schrödinger equation is produced. In [35] symplectic-schemes of second and third order for the numerical solution of the radial Shrödinger equation are presented. In [36] a family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation is constructed. In [37] exponentially-fitted multistep methods are developed. In [38] the general theory for the exponential fitting is presented.

In [39] a family of P-stable high algebraic order exponentially-fitted methods for the numerical solution of the Schrödinger equation is presented. In [40] an eighth algebraic order symmetric eight step methods for the numerical solution of the Schrödinger equation is obtained. In [41] trigonometrically and exponentially fitted Runge-Kutta-Nyström methods for the numerical solution of the Schrödinger equation and related problems are presented and a method of eighth algebraic order is obtained.

In [42] a modified phase-fitted Runge-Kutta method based on the Runge-Kutta fifth algebraic order method of Dormand and Prince for the numerical solution of the Schrödinger equation is developed. In [43] a generator of hybrid explicit methods of algebraic order ten for the numerical solution of the Schrödinger equation are produced. In [44] a generator of tenth-order hybrid explicit methods, the basic method of which has been developed in part 1, was constructed and also optimized, by maximization of the intervals of periodicity. In [45] a P-stable exponentially-fitted method

of algebraic order eight for the approximate numerical integration of the Schrödinger equation is presented.

In [46] an explicit eighth algebraic order Bessel and Neumann fitted method for the numerical solution of the Schrödinger equation is constructed. In [47] embedded eighth order methods for the numerical solution of the Schrödinger equation are developed. In [48] a family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation is produced. In [49] a new embedded modified Runge-Kutta 4(6) Fehlberg method with minimal phase-lag and a block embedded Runge-Kutta-Fenlberg method is obtained.

In [50] two new hybrid eighth algebraic order two-step methods with phase-lag of order twelve and fourteen for computing elastic scattering phase shifts of the radial Schrödinger equation is produced. In [51] two optimized eight-step symmetric implicit methods with phase-lag order ten and infinite (phase-fitted) for the numerical solution of the radial time-independent Schrödinger equation with the use of the Woods-Saxon potential and related IVPs with oscillating solutions is developed.

In [52] a family of six methods for the numerical integration of the Schrödinger equation and related initial value problems with oscillating solution is constructed. Three of the methods are P-stable, also two of these three methods are trigonometrically fitted with trigonometric orders one and two. The other three methods are constructed so that they are trigonometrically fitted with orders one, two and three.

In [53] a singularly almost P-stable exponentially-fitted four-step method for the approximate solution of the one-dimensional Schrödinger equation is obtained.

In [54] the closed Newton-Cotes formulae are written as symplectic multilayer structures. Some Trigonometrically-fitted symplectic methods which are based on the closed Newton-Cotes formulae are developed.

In [55] trigonometrically and exponentially fitted symplectic integrators for the solution of the one-dimensional time-independent Schrödinger equation are obtained.

In [56]–[60] trigonometrically and exponentially fitted and optimized multistep and Runge-Kutta methods are developed.

In [61] trigonometrically-fitted multiderivative methods are developed for the numerical solution of the radial Schrödinger equation. The methods are called multiderivative since they use derivatives of order two and four.

In [62] trigonometrically fitted Adams-Bashforth-Moulton predictor–corrector (P–C) methods are used to efficiently solve the resonance problem of the Schrödinger equation. The new trigonometrically fitted P–C schemes are based on the well known Adams-Bashforth-Moulton methods.

In [63] cyclic reduction algorithm to the solution of bordered ABD linear systems with blocks of different sizes and with different overlaps is presented. This kind of system often arises from the numerical approximation of BVPs with non separated boundary conditions.

In [64] methods based on a Lobatto-MIRK formula for finding $y'n$ and an Obrechkoff type formula for finding yn using the same values of y'' are derived and these methods are of sixth and of eighth order accuracy.

In [65] Mono-Implicit Runge-Kutta (MIRK) formulae of orders ten and twelve for solving general non-linear two-point boundary value problems are developed.

In [66] a survey of some of the approaches that are at present being used to derive interpolants and a new interpolant for use with TWPBVPL.f which was a highly stable deferred correction code based on Lobatto formulae is presented.

In [67] fixed step, symmetric Runge-Kutta-Nyström formulae very efficient for the numerical integration of a large class of reversible second order systems of ordinary differential equations of the special form $d^2y/dt^2 = f(t, y)$ is presented.

In [68] hybrid mesh selection strategies based on conditioning which are used in codes designed for the numerical solution of singularly perturbed boundary value problems are presented.

In [69] a review of the terms stability and conditioning by using simple examples taken from both linear algebra and numerical methods for ODEs is presented.

In [70] a symmetric formula, namely the trapezoidal method, which under certain circumstances, can attach to the discrete system a discrete energy function and therefore obtain a discrete conservative dynamical system is developed.

In [71] a study on BS methods in the general case of a non-uniform mesh is presented. BS methods are a special class of linear multistep methods defined using B-spline functions.

In [72] a BVP-SOLVER, which extends the class of BVPs solved by MIRKDC to problems with unknown parameters and problems with ODEs having a singular coefficient are presented.

In [73] exponentially-fitted Störmer/Verlet methods of order four taking into account a six-step flow chart are developed.

In [74] a rigorous analysis of the linear stability for some classes of BVMs is presented.

In [75] barycentric Hermite interpolants for event location in initial-value problems are developed.

In [76] software engineering and documentation issues which arise when trying to integrate a large general-purpose C or Fortran Library such as NAG into an interactive environment are presented.

In [77] a BVP Solver that controls residual and error is described.

In [78] a method of lines framework in Mathematica is developed.

In [79] a differential algebraic equations Taylor series code for solving DAE initial value problems by Taylor series expansion is presented.

In [80] the use of mathematical software in the teaching of Sophomore differential equations is presented.

In [81] extrapolation one step methods for solving ordinary differential equations in Mathematica are described.

In [82] a problem-solving environment (PSE) called pythNon for solving systems of NAEs is presented.

In [83] the solution of systems of ordinary differential equations (ODEs) and systems of delay differential equations (DDEs) in which solution impulses are applied at specific times is studied.

In [84] a code generation tool is presented.

In [85] an automatic code generation and optimization in Maple is studied.

In [86] an identification of stiffness is studied and the definition of A-stability is presented.

In [87] a technique for seismic waveform tomography on continental scales is studied. The present study is based on a fully numerical simulation of wave propagation in complex Earth models, the inversion of complete waveforms and the quantification of the waveform discrepancies through a specially designed phase misfit. The numerical approximation of the equations of motion allows to overcome the limitations of ray theory and of finite normal mode summations.

In [88] a family of L-stable general linear methods of arbitrarily high order is obtained. Moreover it is possible to define a corresponding Blended GLM for each one of such methods.

In [89] a study on the relation between the length T of the integration window of a linear differential equation $x' + A\,x = b$ and a spectral parameter s^* is described. The determination of the parameter is based on the comparison of the exact solution $x(T)$ at the end of the integration window and the solution of a linear system obtained from the Laplace transform of the differential equation by freezing the system matrix. In the paper a method to integrate the relation $s* = s*(T)$ into the determination of the interval of rapid convergence of waveform relaxation iterations is proposed.

In [90] variable step/order generalized upwind methods for the numerical solution of second order singular perturbation problems are obtained.

In [91] the behaviour of (R-K) geometric numerical integrators, symplectic and pseudo-symplectic, is studied. Numerical applications are presented.

In [92] a class of arbitrary high order symmetric one-step methods for the numerical approximation of Hamiltonian systems are obtained.

In [93] the stability of one-leg linear multistep methods applied to linear nonautonomous systems of equations is studied.

In [94] boundary value methods for Sturm-Liouville eigenvalue estimates with general boundary conditions are presented.

In [95] an algorithm for the efficient numerical solution of singular two-point boundary value problems is obtained. This algorithm is based on collocation at Gauss points.

In [96] a block implicit multistep algorithm is presented. This algorithm has been developed with the aim to successfully tackle the numerical solution of stiff ordinary differential equations.

In [97] mesh selection techniques for ordinary differential equations (ODEs) and for partial differential equations (PDEs) are presented. These techniques are based on arc length and defect.

In [98] a P-stable exponentially-fitted four-step method for the numerical solution of the radial Schrödinger equation is developed.

In [99] the definition of the singularly P-stable exponentially-fitted methods is given and a singularly P-stable exponentially-fitted four-step method for the numerical solution of the radial Schrödinger equation is produced.

In [100] some P-stable multistep methods for periodic initial-value problems are obtained.

In [101] an embedded Runge-Kutta method with phase-lag of order infinity is constructed. This methods is based on the Runge-Kutta Fehlberg 2(3) method.

In [102] an embedded Runge-Kutta 10(12) method is obtained and an explicit scaled Runge-Kutta method is produced.

In [103] the theory of the phase-lag analysis for Runge-Kutta-Nyström methods and Runge-Kutta-Nyström interpolants is obtained. A new Runge-Kutta-Nyström method with interpolation properties is constructed. This method is used for the integration of second-order differential equations of the form $u''(t) = f(t, u)$ with oscillating solutions.

In [104] a family of exponential four-step methods is constructed for the numerical integration of the one-dimensional Schrödinger equation. The characteristic of the new methods is that are very simple compared with the sixth algebraic order Runge-Kutta type methods.

In [105] a two-step method for the numerical solution of the radial Schrödinger equation is developed.

In [106] block Runge-Kutta methods with minimal phase-lag for first order periodic initial value problems are obtained. The new methods are based on the Runge-Kutta methods of algebraic order three, and on a new error estimate introduced in this paper.

In [107] some new embedded methods for the one-dimensional Schrödinger equation are constructed.

In [108] a finite difference scheme with minimal phase-lag, for the numerical solution of fourth-order differential equations is developed.

In [109] a method for computing eigenvalues of Schrödinger type equations is obtained. This methods is based on the new property of phase-lag.

In [110] a hybrid imbedded variable-step procedure for the numerical integration of the radial Schrödinger equation is obtained. The new imbedded method is based on P-stable methods of exponential order eight, ten, twelve, and fourteen.

In [111] Bessel and Neumann fitted methods of eighth algebraic order for the numerical solution of the Schrödinger equation are developed.

In [112] an explicit symmetric multistep exponentially fitted and trigonometrically-fitted and of algebraic order eight method for the numerical solution of periodic problems is produced.

In [113] an explicit Runge-Kutta method with algebraic order four, minimum error of the fifth algebraic order (the limit of the error is zero, when the step-size tends to zero), infinite order of dispersion and eighth order of dissipation for the solution of well-known periodic orbital problems is constructed.

In [114] trigonometrically fitted predictor–corrector (P–C) Adams-Bashforth-Moulton methods for the numerical solution of initial value problems with oscillating solutions are obtained.

In [115] multiderivative methods with minimal phase-lag for the numerical solution of the one-dimensional Schrödinger equation are presented.

In [116] Runge-Kutta method with minimal dispersion and dissipation error is developed. The Chebyshev pseudospectral method is utilized using spatial discretization and a new fourth-order six-stage Runge-Kutta scheme is used for time advancing. The proposed scheme is more efficient than the existing ones for acoustic computations.

In [117] Newton-Cotes formulae for long-time integration are produced.

In [118] asymptotic symplecticness is introduced and asymptotically symplectic methods of order up to 3 are developed.

In [119] a generator of hybrid explicit four-step methods of sixth algebraic order with minimal phase-lag for the numerical solution of the Schrödinger equation is obtained.

In [120] a trigonometrically fitted predictor–corrector (P–C) scheme, which is based on the well-known two-step second-order Adams-Bashforth method (as predictor) and on the third-order Adams-Moulton method (as corrector) is introduced.

In [121] three types of methods for integrating periodic initial value problems(oscillatory problems) are introduced. These methods are (i) phase-fitted, (ii) zero dissipation (iii) both zero dissipative and phase fitted. Some particular modifications of well known explicit Runge-Kutta pairs of orders five and four are constructed.

In [122] an eighth algebraic order exponentially fitted method for the numerical integration of the Schrödinger equation is developed.

In [123] an accurate finite difference approach for computing eigenvalues of Schrödinger equations is presented.

In [124] a family of hybrid, exponentially fitted, predictor–corrector methods is developed for the numerical integration of the one-dimensional Schrödinger equation. The new methods are of algebraic order six.

In [125] a finite-difference method for the numerical solution of the Schrödinger equation is obtained.

In [126] a generator of new embedded P-stable methods of order $2n+2$, where n is the number of layers used by the embedded methods, for the approximate numerical integration of the one-dimensional Schrödinger equation is presented.

In [127] a family of predictor–corrector exponential Numerov-type methods for the numerical integration of the one-dimensional Schrödinger equation is produced.

In [128] a family of predictor–corrector exponential four step methods is developed for the numerical integration of the one-dimensional Schrödinger equation is introduced.

In [129] an explicit four-step method with phase-lag of infinite order is developed for the numerical integration of second order initial value problems.

In [130] a new Runge-Kutta-Nyström fourth algebraic order method is developed to integrate second order differential equations of the form $u''(t) = f(t, u)$ when they posses an oscillatory solution.

In [131] an embedded Runge-Kutta-Fehlberg method is developed. It should be noted that this embedded method is produced using the Runge-Kutta-Fehlberg method with algebraic order four to estimate a truncation phase-lag error of algebraic order three.

In [132] a new fourth order method is developed for the numerical integration of the one-dimensional radial Schrödinger equation. This method integrates Bessel and Neumann functions exactly.

In [133] two step sixth order methods with phase-lag of order eight, ten and twelve are constructed for the numerical integration of the special second order initial-value sproblem.

In [134] a new four step exponentially-fitted method is obtained in this paper. The expressions for the coefficients of the method are found such as to ensure the optimal approximation to the eigenvalue Schrödinger equation.

In [135] a new approach is developed for the computation of the phase shifts of the one-dimensional Schrödinger equation. The method is applied to scattering problems. The algorithm is very simple to code and very efficient for computational purposes. The method is also general and can be applied to any kind of potential functions (Coulomb-type etc).

In [136] a two step exponentially-fitted formula is derived and applied to the Schrödinger equation.

In [137] some two step almost P-stable methods with phase-lag of order infinite are developed for the numerical integration of second order periodic initial-value problem. One of them has algebraic order four and the other has algebraic order six.

In [138] a dissipative trigonometrically-fitted two-step explicit hybrid method is constructed in this paper.

In [139] an exponentially-fitted Runge-Kutta-Nyström fourth algebraic order method is obtained for the numerical solution of initial-value problems with oscillating solutions.

In [140] a modified Runge-Kutta method with minimal phase-lag is developed for the numerical solution of ordinary differential equations with oscillating solutions. The method is based on the accurate Runge-Kutta method of Sharp and Smart RK4SS(5) of order five.

In [141] a Runge-Kutta type method is developed here. This method has an algebraic order eight, a large interval of periodicity and a phase-lag of order twelve.

In [142] a new variable-step method is developed for the numerical integration of special second-order initial value problems.

In [143–145] and [146] new insights in the subject of the numerical approximation of the 2nd order periodic initial value problems are expressed.

In [147] an extensive review for the multistelp methods for the numerical solution of the quantum mechanical problems and related applications is described. New results are also obtained.

In [148] a comparison of the two methodologies for the development of exponentially and trigonometrically fitted methods is presented.

In [149] a nonlinear explicit two-step P-stable method of fourth algebraic order and varying phase-lag order for solving one-dimensional second order linear periodic initial value problems (IVPs) of ordinary differential equations is obtained.

In [150] a Numerov-type method for the numerical solution of the radial Schrödinger equation is constructed.

In [151] the terminology of the phase-fitted methods is introduced. The definition of phase-fitted methods is also introduced. Finally, a four-step method with phase-lag of infinite order (phase-fitted) for the numerical integration of second order initial-value problems is produced.

In [152] an exponentially-fitted Runge-Kutta method for the numerical integration of the radial Schrödinger equation is developed.

In [153] a family of exponential fitting methods is produced.

In [154] an explicit Runge-Kutta type method which has an algebraic order six, a large interval of periodicity and a phase-lag of order eight is obtained.

In [155] a new explicit, zero dissipative, hybrid Numerov type method is produced. The method is of sixth algebraic order at a cost of seven stages per step while their phase-lag order is fourteen.

In [156] an algorithm for the numerical solution of the one-dimensional Schrödinger equation is obtained.

In [157] a two-step exponentially-fitted formula is derived and applied to the Schrödinger equation.

In [158–160] new contributions in the subject of the numerical solution of the initial and boundary value problems are presented.

3 Theory of the phase-lag analysis for symmetric multistep methods

For the numerical solution of the initial value problem

$$q''(r) = f(r, q(r)) \tag{3}$$

consider a multistep method (see [161]) with m steps which can be used over the equally spaced intervals $\{r_i\}_{i=0}^{m} \in [a, b]$ and $h = |r_{i+1} - r_i|, \ \ i = 0(1)m - 1$.

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

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

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

a difference equation of the form

$$\begin{aligned} C_k(H)\, q_{n+k} \ &+ \cdots + C_1(H)\, q_{n+1} + C_0(H)\, q_n \\ &+ C_1(H)\, q_{n-1} + \cdots + C_k(H)\, q_{n-k} = 0 \end{aligned} \tag{5}$$

is obtained, where $H = \omega h$, h is the step length and $C_0(H), C_1(H), \ldots, C_k(H)$ are polynomials of H.

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

$$C_k(H)\, \lambda^k + \cdots + C_1(H)\, \lambda + C_0(H) + C_1(H)\, \lambda^{-1} + \cdots + C_k(H)\, \lambda^{-k} = 0 \tag{6}$$

Theorem 1 [125] *The symmetric $2k$-step method with characteristic equation given by (6) has phase-lag order t and phase-lag constant c given by*

$$-c\, H^{t+2} + O\left(H^{t+4}\right) = \frac{D_1}{D_2}, \tag{7}$$

where

$$D_1 = 2\, C_k(H) \cos(kH) + \cdots + 2\, C_j(H) \cos(jH) + \cdots + C_0(H) \tag{8}$$

$$D_2 = 2\, k^2\, C_k(H) + \cdots + 2\, j^2\, C_j(H) + \cdots + 2C_1(H) \tag{9}$$

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

4 The high order new Numerov-type hybrid method—development of the new method

Consider the following family of three-stage Numerov-Type Hybrid Methods:

$$\begin{aligned} \overline{q}_{n+1} &= 2\,q_n - q_{n-1} + h^2\,q_n'' \\ \overline{q}_n &= q_n - a_0\,h^2\,\left(\overline{q}_{n+1}'' - 2\,q_n'' + q_{n-1}''\right) \\ q_{n+1} + c_1\,q_n + q_{n-1} &= h^2\,\left[b_0\,\left(\overline{q}_{n+1}'' + q_{n-1}''\right) + b_1\,\overline{q}_n''\right] \end{aligned} \tag{10}$$

Using the scalar test equation (4) to apply the above hybrid method, we obtain the difference equation of the form:

$$C_1(H)\,q_{n+1} + C_0(H)\,q_n + C_1(H)\,q_{n-1} = 0 \tag{11}$$

where $H = \omega h$, h is the step length and $C_0(H)$ and $C_1(H)$ are polynomials of H.

The difference equation (11) is related with the characteristic equation of the form:

$$C_1(H)\,\lambda + C_0(H) + C_1(H)\,\lambda^{-1} = 0 \tag{12}$$

where,

$$\begin{aligned} C_1(H) &= 1 \\ C_0(H) &= c_1 + (2\,b_0 + b_1)\;H^2 - b_0\,H^4 - b_1\,a_0\,H^6 \end{aligned}$$

In order to find the phase-lag and its derivatives we use the formula (7) with $k = 1$. So, we have:

$$PL = \cos(H) + \frac{1}{2}\,c_1 + \left(b_0 + \frac{1}{2}\,b_1\right)\,H^2 - \frac{1}{2}\,b_0\,H^4 - \frac{1}{2}\,b_1\,a_0\,H^6 \tag{13}$$

We differentiate formula (13) in order to acquire first, second and third derivatives of the phase-lag:

$$PL' = -\sin(H) + (2\,b_0 + b_1)\;H - 2\,b_0\,H^3 - 3\,b_1\,a_0\,H^5 \tag{14}$$

$$PL'' = -\cos(H) + b_1 + 2\,b_0 - 6\,b_0\,H^2 - 15\,b_1\,a_0\,H^4 \tag{15}$$

$$PL''' = \sin(H) - 12\,b_0\,H - 60\,b_1\,a_0\,H^3 \tag{16}$$

The coefficients a_0, b_0, b_1, c_1 are the solution of the system of equations, which arises when we set PL, PL', PL'', PL''' equal to zero. The above mentioned coefficients and their Taylor series expansions are presented in Appendices A and B. In the graphs in Fig. 1 we can observe the behavior of each coefficient of the method.

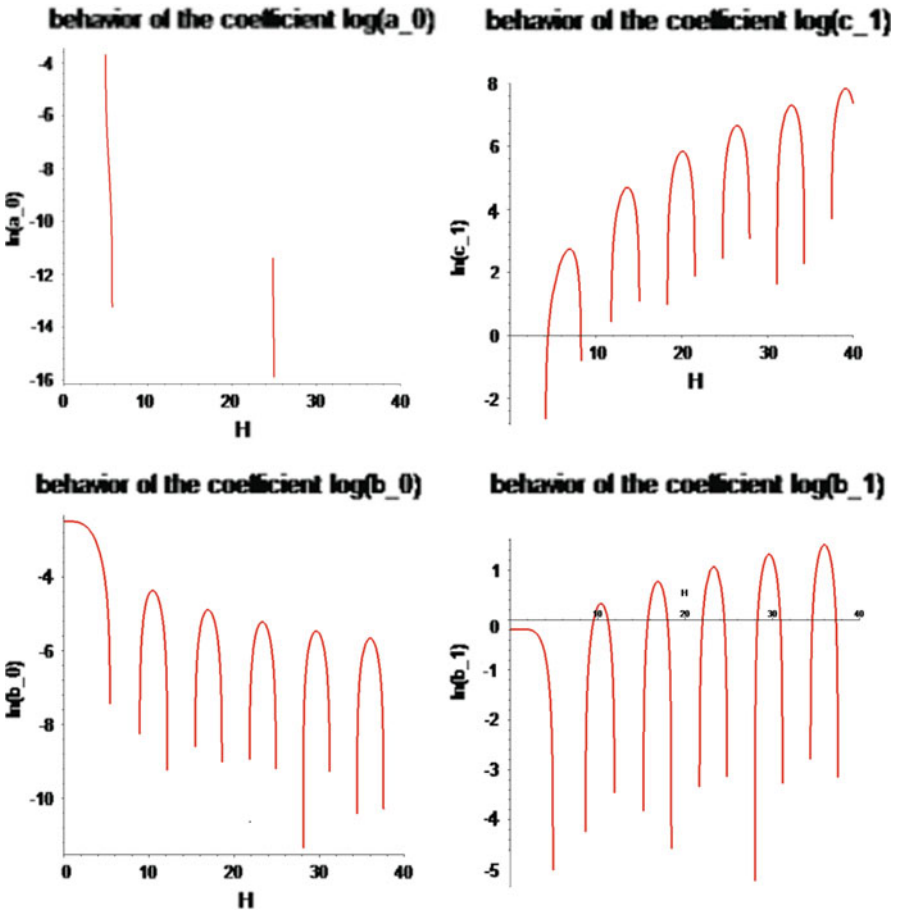

Fig. 1 Behavior of the coefficients of the new method given by (40)–(43) for several values of H

The local truncation error of the new method id given by:

$$\text{LTE} = \frac{h^8}{20160}\left(q_n^{(8)} + 4\omega^2\, q_n^{(6)} + 6\omega^4\, q_n^{(4)} + 4\omega^6\, q_n^{(2)} + \omega^8\, q_n\right) \tag{17}$$

Theorem 2 *The hybrid method given by* (10) *with coefficients determined in* (40), (41), (42) *and* (43) *is a sixth algebraic order method with phase-lag and its first three derivatives equal to zero.*

5 Comparative error analysis

We will study the following methods:

– The Numerov's Method (mentioned as $PL0$)

– The Method developed by Konguetsof in [156] (mentioned as $PL1$)
– The New Developed Method (mentioned as $PL2$)

The error analysis is based on the following steps:

– The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)\, y(x) \tag{18}$$

– Based on the paper of Ixaru and Rizea [18], the function f(x) can be written in the form:

$$f(x) = g(x) + G \tag{19}$$

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 $y_n^{(i)}$, $i = 2, 4, 6, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. (18). The expressions are presented as polynomials of G
– Finally, we substitute the derivatives, which are produced, into the local truncation error formulae

Based on the procedure mentioned above and on the formulae:

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

we obtain the expressions of the local truncation error mentioned in "Appendix C".

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

– The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. Thus for these values of G, the methods

are of comparable accuracy. This is because the free terms of the polynomials in G, are the same for the cases of the classical method and of the new developed methods.

– $G \gg 0$ or $G \ll 0$. Then $\mid G \mid$ is a large number. So, we have the following asymptotic expansions of the Eqs. (48) and (49).

The Numerov's method

$$\mathrm{LTE_{PL0}} = h^6 \left(\frac{1}{240}\, y(x)\, G^3 + \cdots \right) \tag{20}$$

The method developed by Konguetsof in [156]

$$\mathrm{LTE_{PL1}} = h^6 \left(\frac{1}{90} \left(\frac{d^2}{dx^2}\, g(x) \right) y(x)\, G + \cdots \right) \tag{21}$$

The new obtained method

$$\begin{aligned} \mathrm{LTE_{PL2}} = h^8 \Bigg[& \left(\frac{1}{1680} \left(\frac{d^4}{dx^4}\, \mathrm{g}(x) \right) \mathrm{y}(x) \right. \\ & + \frac{1}{2520} \left(\frac{d^3}{dx^3}\, \mathrm{g}(x) \right) \left(\frac{d}{dx}\, \mathrm{y}(x) \right) \\ & + \frac{1}{1260}\, \mathrm{g}(x)\, \mathrm{y}(x) \left(\frac{d^2}{dx^2}\, \mathrm{g}(x) \right) \\ & \left. + \frac{1}{1680} \left(\frac{d}{dx}\, \mathrm{g}(x) \right)^2 \mathrm{y}(x) \right) G + \cdots \Bigg] \end{aligned} \tag{22}$$

From the above equations we have the following theorem:

Theorem 3 *For the fourth order Numerov's Method the error increases as the third power of G. For the fourth algebraic order method developed by Konguetsof in* [156] *the error increases as the first power of G. For the new sixth algebraic order methods developed in this paper the error increases also as the first power of G. So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Method is the most accurate one, especially for large values of* $\mid G \mid = \mid V_c - E \mid$.

6 Stability analysis

The scalar test equation is given below

$$q''(x) = -v^2\, q(x), \quad v \neq \omega \tag{23}$$

where the new presented method is applied. The obtained difference equation is:

$$C_1(H, s)\, q_{n+1} + C_0(H, s)\, q_n + C_1(H, s)\, q_{n-1} = 0 \tag{24}$$

where $s = vh$, h is the step length and $C_0(H, s)$ and $C_1(H, s)$ are polynomials of s.

The characteristic equation associated with (24) is given by:

$$C_1(H, s)\, s + C_0(H, s) + C_1(H, s)\, s^{-1} = 0 \tag{25}$$

where

$$\begin{aligned} C_1(H, s) &= 1 \\ C_0(H, s) &= c_1 + s^2\ (2b_0 + b_1) - s^4\, b_0 - s^6\, b_1\, a_0 \end{aligned} \tag{26}$$

Definition 1 (*see* [10]) A symmetric four-step method with the characteristic equation given by (25) is said to have an *interval of periodicity* $\left(0, \omega_0^2\right)$ if, for all $\omega \in \left(0, \omega_0^2\right)$, the roots $z_i,\ i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i\, \phi(vh)},\ |z_i| \leq 1,\ i = 3, 4 \tag{27}$$

where $\phi(vh)$ is a real function of vh and $s = vh$.

Definition 2 (*see* [10]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Theorem 4 *(*see [22]*) A symmetric two-step method with the characteristic equation given by* (25) *is said to have a nonzero interval of periodicity* $\left(0, s_0^2\right)$ *if, for all* $s \in \left(0, s_0^2\right)$ *the following relations are hold*

$$P_1(H, s)\, P_2(H, s) < 0, \tag{28}$$

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

$$\begin{aligned} P_1(H, s) &= C_0(H, s) + 2\, C_1(H, s), \\ P_2(H, s) &= C_0(H, s) - 2\, C_1(H, s) \end{aligned} \tag{29}$$

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $H = s$.

Based on (26) the stability polynomials (29) for the new developed methods take the form:

$$\begin{aligned} P_1(H, s) &= 2 + c_1 + (2\, b_0 + b_1)\ s^2 - b_0\, s^4 - b_1\, a_0\, s^6, \\ P_2(H, s) &= -2 + c_1 + (2\, b_0 + b_1)\ s^2 - b_0\, s^4 - b_1\, a_0\, s^6 \end{aligned} \tag{30}$$

In the Fig. 2 we present the $s - H$ plane for the new method of the new family of methods developed in this paper (Sect. 4).

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

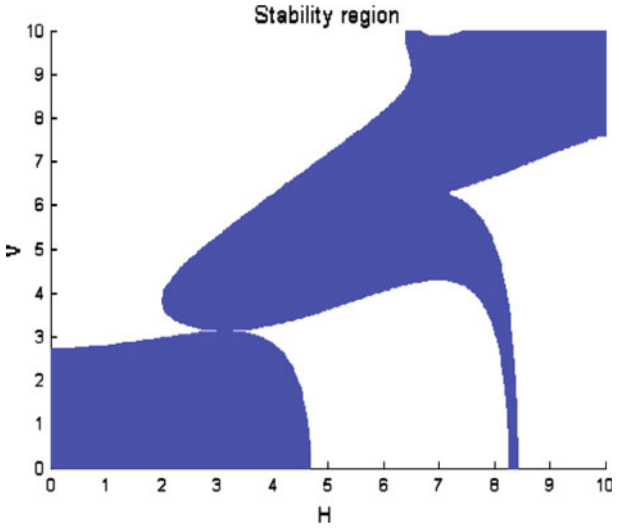

Fig. 2 $s - H$ plane of the new method of the family of methods developed in this paper

A method is P-stable if the $s - H$ plane is completely shadowed. From the above diagram it is easy for one to see that the present method is singularly almost P-stable. The method cannot be P-stable since it is explicit.

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

7 Numerical illustrations

The radial time independent Schrödinger equation is used to check the efficiency of the new method obtained in Sect. 4.

We base our tests on the radial time-independent Schrödinger equation presented in (1). For this equation we give some definitions: The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(r) \to 0$ as $r \to \infty$. The quantity k^2 is a real number denoting *the energy*. The quantity l is a given integer representing the *angular momentum* and finally the quantity V is a given function which denotes the potential.

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

$$v = \sqrt{|q(r)|} = \sqrt{|V(r) - E|} \tag{31}$$

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

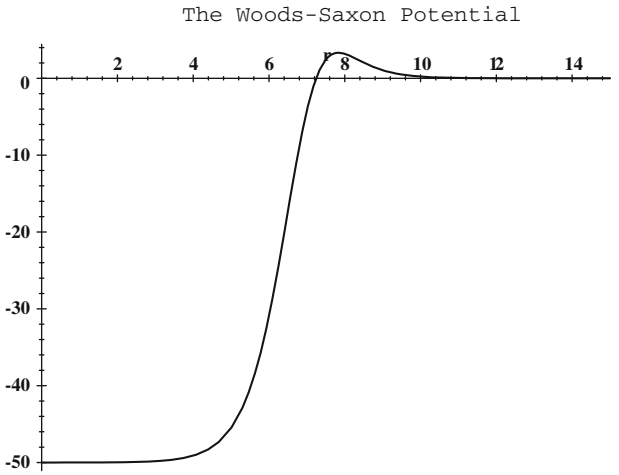

Fig. 3 The Woods-Saxon potential

7.1 Woods-Saxon potential

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

$$V(r) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{32}$$

with $z = exp\left[(r - R_0)/a\right]$, $u_0 = -50$, $a = 0.6$, and $R_0 = 7.0$.

The behavior of Woods-Saxon potential is shown in the Fig. 3.

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 r but based on some critical points which have been defined from the investigation of the appropriate potential (see for details [17]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [17]):

$$v = \begin{cases} \sqrt{-50+E}, & \text{for r} \in [0, 6.5-2\text{h}], \\ \sqrt{-37.5+E}, & \text{for r} = 6.5-h \\ \sqrt{-25+E}, & \text{for r} = 6.5 \\ \sqrt{-12.5+E}, & \text{for r} = 6.5+h \\ \sqrt{E}, & \text{for r} \in [6.5+2\text{h}, 15] \end{cases} \tag{33}$$

7.2 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 (32). 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 $r \in [0, 15]$. We consider Eq. 1 in a rather large domain of energies, i.e. $E \in [1, 1000]$.

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

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{34}$$

for r greater than some value R.

The above equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$ where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. 1 has (when $r \to \infty$) the asymptotic form

$$\begin{aligned} q(r) &\simeq Akrj_l(kr) - Bkrn_l(kr) \\ &\simeq AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{35}$$

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

$$\tan\delta_l = \frac{q(r_2)S(r_1) - q(r_1)S(r_2)}{q(r_1)C(r_1) - q(r_2)C(r_2)} \tag{36}$$

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need q_0 before starting a one-step method. From the initial condition we obtain q_0. With these starting values we evaluate at r_1 of the asymptotic region the phase shift δ_l.

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

The boundary conditions for this problem are:

$$q(0) = 0,\ q(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{37}$$

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

- the Numerov's method which is indicated as **Method I**
- The two-step method developed by Raptis and Allison (which is indicated as **Method II**) [14]
- The two-step method developed by Ixaru and Rizea (which is indicated as **Method III**) [17]
- The Method developed by Konguetsof in [156] (which is indicated as **Method IV**)
- The two-step method developed by Raptis (which is indicated as **Method V**) [157]

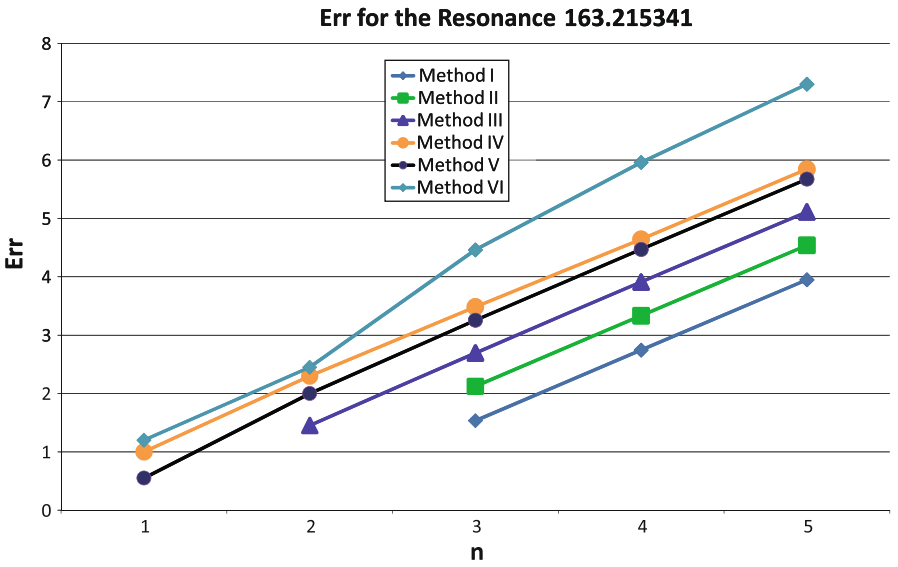

Fig. 4 Error Errmax for several values of n for the eigenvalue $E_1 = 163.215341$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

– the new Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero obtained in Sect. 4 which is indicated as **Method VI**.

for several step sizes $h = \frac{3}{10}\frac{1}{2^n}$.

The computed eigenenergies are compared with exact ones. In Fig. 4 we present the maximum absolute error $log_{10}(Err)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{38}$$

of the eigenenergy E_2, for several values of NFE = Number of Function Evaluations. In Figs. 5 and 6 we present the maximum absolute error $log_{10}(Err)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{39}$$

of the eigenenergies E_3 and E_4, for several values of n.

8 Conclusions

In the present paper we have developed a hybrid two-step method of sixth algebraic order for the numerical solution of the radial Schrödinger equation.

More specifically we have developed a hybrid 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.

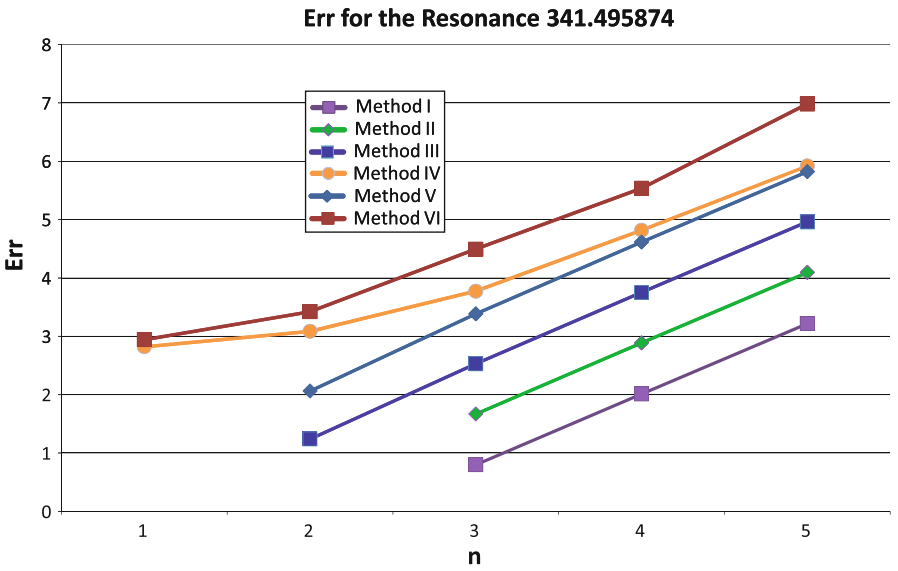

Fig. 5 Error Errmax for several values of n for the eigenvalue $E_3 = 341.495874$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

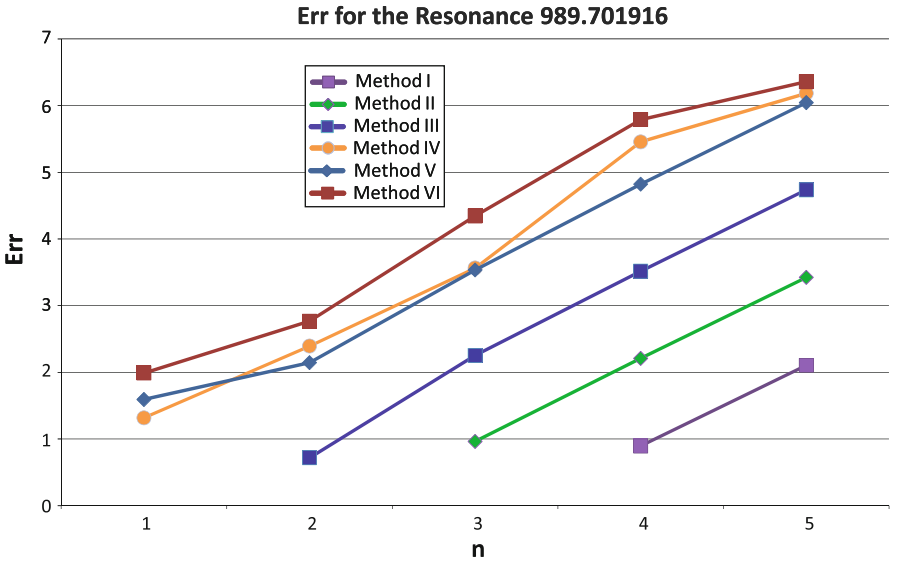

Fig. 6 Error Errmax for several values of n for the eigenvalue $E_4 = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

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

– The two-step method developed by Raptis and Allison [14] (Method II) is more efficient than Numerov's Method (Method I) but less efficient than the other two methods.

– The two-step method developed by Ixaru and Rizea [17] (Method III) is more efficient than Numerov's Method (Method I) and method developed by Raptis and Allison (Method II) but less efficient than the new obtained method.
– The Method developed by Konguetsof in [156] (Method IV) is more efficient than is more efficient than Numerov's Method (Method I), method developed by Raptis and Allison (Method II) but less efficient than the new obtained method and generally the two-step method developed by Raptis [157] (Method V)
– Finally the new developed two-step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero (Method VI) is the most efficient than all the other methods.

Acknowledgments The author wishes to thank the anonymous referee and the Editor-in-Chief of the Journal for their careful reading of the manuscript and their fruitful comments and suggestions. All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

Appendix A

$$a_0 = -\frac{1}{3}\,\frac{H^2\sin(H) + 3H\cos(H) - 3\sin(H)}{10\,H^2\sin(H) - 10\,H^3\cos(H) - 17H^4\sin(H) + 7\,H^5\cos(H) + H^6\sin(H)} \tag{40}$$

$$c_1 = -2\cos(H) - \frac{11}{8}\,H\sin(H) + \frac{3}{8}\,H^2\cos(H) + \frac{1}{24}\,H^3\sin(H) \tag{41}$$

$$b_0 = -\frac{1}{8}\,\frac{H^2\sin(H) + 5H\cos(H) - 5\sin(H)}{H^3} \tag{42}$$

$$b_1 = -\frac{1}{8}\,\frac{10\sin(H) - 10H\cos(H) - 17H^2\sin(H) + 7H^3\cos(H) + H^4\sin(H)}{H^3} \tag{43}$$

Appendix B

$$\begin{aligned} a_0 = {} & \frac{-1}{300} + \frac{1}{4200}\,H^2 - \frac{1}{236250}\,H^4 - \frac{277}{291060000}\,H^6 \\ & + \frac{18847}{189189000000}\,H^8 - \frac{31463}{8939180250000}\,H^{10} \\ & - \frac{13888499}{60786425700000000}\,H^{12} + \frac{6659696851}{1778610815982000000000}\,H^{14} \\ & - \frac{58988516273}{30014057519696250000000}\,H^{16} + \cdots \\ c_1 = {} & -2 + \frac{1}{20160}\,H^8 - \frac{1}{453600}\,H^{10} + \frac{1}{23950080}\,H^{12} \\ & - \frac{1}{2179457280}\,H^{14} + \frac{1}{298896998400}\,H^{16} \end{aligned} \tag{44}$$

$$- \frac{1}{57164050944000} H^{18} + \cdots \tag{45}$$

$$b_0 = \frac{1}{12} - \frac{1}{3360} H^4 + \frac{1}{90720} H^6 - \frac{1}{5322240} H^8 + \frac{1}{518918400} H^{10} - \frac{1}{74724249600} H^{12} + \frac{1}{14820309504000} H^{14} - \frac{1}{3861749219328000} H^{16} + \frac{1}{1277273554292736000} H^{18} + \cdots \tag{46}$$

$$b_1 = \frac{5}{6} + \frac{1}{1680} H^4 - \frac{1}{4536} H^6 + \frac{23}{2661120} H^8 - \frac{1}{6486480} H^{10} + \frac{61}{37362124800} H^{12} - \frac{43}{3705077376000} H^{14} + \frac{23}{386174921932800} H^{16} - \frac{37}{159659194286592000} H^{18} + \cdots \tag{47}$$

Appendix C

The Numerov's Method

$$\begin{aligned} LTE_{PL0} = h^6 \Bigg[& \frac{1}{240} \mathrm{y}(x) G^3 + \frac{1}{80} \mathrm{g}(x) \mathrm{y}(x) G^2 \\ & + \left(\frac{1}{40} \left(\frac{d}{dx} \mathrm{g}(x) \right) \left(\frac{d}{dx} \mathrm{y}(x) \right) + \frac{7}{240} \left(\frac{d^2}{dx^2} \mathrm{g}(x) \right) \mathrm{y}(x) \right. \\ & \left. + \frac{1}{80} \mathrm{g}(x)^2 \mathrm{y}(x) \right) G + \frac{1}{240} \left(\frac{d^4}{dx^4} \mathrm{g}(x) \right) \mathrm{y}(x) \\ & + \frac{1}{60} \left(\frac{d^3}{dx^3} \mathrm{g}(x) \right) \left(\frac{d}{dx} \mathrm{y}(x) \right) + \frac{7}{240} \mathrm{g}(x) \mathrm{y}(x) \left(\frac{d^2}{dx^2} \mathrm{g}(x) \right) \\ & + \frac{1}{240} \mathrm{g}(x)^3 \mathrm{y}(x) + \frac{1}{60} \left(\frac{d}{dx} \mathrm{g}(x) \right)^2 \mathrm{y}(x) \\ & + \frac{1}{40} \mathrm{g}(x) \left(\frac{d}{dx} \mathrm{y}(x) \right) \left(\frac{d}{dx} \mathrm{g}(x) \right) \Bigg] \end{aligned} \tag{48}$$

The method developed by Konguetsof in [156]

$$\begin{aligned} LTE_{PL1} = h^6 \Bigg[& \frac{1}{90} \left(\frac{d^2}{dx^2} \mathrm{g}(x) \right) \mathrm{y}(x) G + \frac{7}{360} \mathrm{g}(x) \mathrm{y}(x) \left(\frac{d^2}{dx^2} \mathrm{g}(x) \right) \\ & + \frac{1}{360} \mathrm{g}(x)^3 \mathrm{y}(x) + \frac{1}{360} \left(\frac{d^4}{dx^4} \mathrm{g}(x) \right) \mathrm{y}(x) \\ & + \frac{1}{90} \left(\frac{d^3}{dx^3} \mathrm{g}(x) \right) \left(\frac{d}{dx} \mathrm{y}(x) \right) + \frac{1}{90} \left(\frac{d}{dx} \mathrm{g}(x) \right)^2 \mathrm{y}(x) \end{aligned}$$

$$+\frac{1}{60}\,\mathrm{g}(x)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\Bigg] \tag{49}$$

The new developed method

$$\begin{aligned}
LTE_{PL2} = h^8 \Bigg[& \left(\frac{1}{1680}\left(\frac{d^4}{dx^4}\,\mathrm{g}(x)\right)\mathrm{y}(x) + \frac{1}{2520}\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\right. \\
& \left. + \frac{1}{1260}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right) + \frac{1}{1680}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)^2\mathrm{y}(x)\right) G \\
& + \frac{1}{20160}\left(\frac{d^6}{dx^6}\,\mathrm{g}(x)\right)\mathrm{y}(x) + \frac{1}{3360}\left(\frac{d^5}{dx^5}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right) \\
& + \frac{1}{1260}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d^4}{dx^4}\,\mathrm{g}(x)\right) + \frac{1}{1344}\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)^2\mathrm{y}(x) \\
& + \frac{13}{10080}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\mathrm{y}(x)\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right) \\
& + \frac{1}{840}\,\mathrm{g}(x)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right) \\
& + \frac{1}{1680}\,\mathrm{g}(x)^2\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d}{dx}\,\mathrm{g}(x)\right) \\
& + \frac{1}{420}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\mathrm{y}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right) \\
& + \frac{11}{10080}\,\mathrm{g}(x)^2\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right) \\
& + \frac{1}{720}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d}{dx}\,\mathrm{g}(x)\right)^2 + \frac{1}{20160}\,\mathrm{g}(x)^4\,\mathrm{y}(x)\Bigg]
\end{aligned} \tag{50}$$

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