Hybrid Multistep Multiderivative Methods for the Schrödinger Equation and Related Problems

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***Abstract*—In this paper we will present a new methodology for the development of efficient hybrid multiderivative multistep methods for the approximate solution of the Schrödinger equation and related initial-value or boundary-value problems with solutions, which their behavior is periodical or oscillating. The main characteristics of this new methodology are (1) the vanishing of the phase-lag on its level of the hybrid multiderivative method and (2) the vanishing of the its derivatives on its level of the hybrid multiderivative method. We apply the new methodology on a four-step hybrid type multiderivative method. A comparative error and stability analysis will be presented for the new produced method. The new constructed method will finally be applied to the resonance problem of the Schrödinger equation in order to show its efficiency.**

Keywords*—Numerical solution, Schrödinger equation, multistep methods, hybrid methods, multiderivative methods, interval of periodicity, P-stability, phase-lag, phase-fitted, derivatives of the phase-lag

I. INTRODUCTION

The Schrödinger equation is a very important mathematical model in quantum mechanics, which describes how the quantum state of some physical system changes with time. This mathematical model was first formulated in late 1925, and published in 1926, by the Austrian physicist Erwin Schrödinger (see for details [1])

The numerical solution of the the radial time-independent Schrödinger equation and of the related initial-value or boundary-value problems with periodical and/or oscillating solutions is investigated in this paper.

The radial time independent Schrödinger equation :

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

is a boundary value problem. The one boundary condition is the following:

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

and the other boundary condition, for large values of r, determined by the physical conditions and parameters of the specific problem.

In order to have the completion of the above mentioned mathematical model, we have give the following definitions of the functions, quantities and parameters presented in Equation 1 :

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

The main purposes of this paper are (1) to introduce a new procedure in order to obtain efficient methods for the numerical solution of second order initial or boundary value problems of the form $q''(x) = f(x, q(x))$ with periodical and/or oscillating solutions and (2) to develop (based on the previous mentioned procedure) an efficient hybrid four-step multiderivative method.

II. DESCRIPTION OF THE METHODOLOGY

In Sciences and Engineering there are a significant number of real problems, which have models, which can be expressed as initial or boundary value problems of the above mentioned category (for example, the Schrödingers equation, Duffings equation, etc).

The new procedure for the development of efficient multiderivative multistep methods consists the following stages:

- The determination of the form of the hybrid multiderivative multistep method (i.e., method with more that one stage, higher order derivatives and more than one step)
- On each level of the hybrid multiderivative multistep method the vanishing of the phase-lag

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- On each level of the hybrid multiderivative multistep method the vanishing of the derivatives of the derivatives (the order of the derivatives depends from the free parameters that the hybrid multiderivative multistep method has)
- The determination of how much more efficient are the new developed methods i.e., the investigation on how the vanishing of the phase-lag and its derivative affects the efficiency of the produced numerical methods
- The determination of how much more efficient are the new developed methods compared with those developed via the vanishing of the phase-lag and its derivatives in the whole of the method (and not on each stage).

Problems for which the algorithms presented in this paper are efficient for this approximate solution are:

1) problems with oscillating and / or periodical solutions,
2) problems in which the functions $\cos$ and $\sin$ are presented in their analytical solution,
3) problems in which combination of the functions $\cos$ and $\sin$ are presented in their analytical solution.

The aim and scope of the present research is the construction of a two-stage, four-step hybrid multiderivative method with the following properties:

1) the maximum possible algebraic order
2) the vanishing of the phase-lag on each stage of the method
3) the vanishing of the derivatives of the phase-lag on each stage of the method. The maximum order of the derivatives to be vanished is dependent on the free parameters which we have. The number of free parameters is dependent by the form of the hybrid two-stage, four-step multiderivative method

The satisfaction of the above purposes requires the computation of the phase-lag and its derivatives for the specific method. In [2] and [3], Simos and co-authors has proved a direct formula for the computation of the phase-lag for a $2\,n$-step method. We mention here that the computation of the derivatives of the phase-lag is based on the previously mentioned formula.

In order to investigate the efficiency of the new produced method, we will apply the following studies:

1) The local truncation of the new developed method will be compared with those of other methods of the same form (comparative error analysis),
2) The Stability (interval of periodicity) of the new obtained method will be determined and
3) Finally, the new produced method will be applied to the resonance problem of the radial time independent Schrödinger equation (see for more details [4]) and the results will be compared with those of other well known methods in the literature.

III. Study of the Phase-lag of Symmetric $2\,n$-step Methods

The general problem we face in the paper is the numerical solution of the the initial or boundary value problem of the form $q''(x) = f(x, q(x))$ via multistep multiderivative finite difference methods.

In order to investigate the above mentioned problem we apply the follow procedure

- We divide the interval of integration $[a,b]$ into $n+1$ intervals $\{x_i\}_{i=0}^{n}$ of equal length. The length $h = |x_{i+1} - x_i|$ is called step-size of the integration.
- For the approximate solution of the above described problem we consider the general $2\,n$-step finite difference multistep multiderivative method of the form:

$$\sum_{i=-n}^{n} a_i\, q_{k+i} = h^2 \sum_{i=-n}^{n} b_i^j\, f^{(j)}\Big(x_{k+i}, q(x_{k+i})\Big), \quad j = 0, 1, \dots \qquad (3)$$

where $f^{(j)}\Big(x_{k+i}, q(x_{k+i})\Big)$ is the derivative of j order of: $f\Big(x_{k+i}, q(x_{k+i})\Big)$ and $f^{(0)}\Big(x_{k+i}, q(x_{k+i})\Big) = f\Big(x_{k+i}, q(x_{k+i})\Big)$.
Using the integration step-size defined above, the method (Equation 3) is applied over the above mentioned integration area. In this paper we will study the specific category of methods (Equation 3), which are symmetric i.e., the category of methods for which: $a_i = a_{-i}$, $b_i = b_{-i}$, $i = -n(1)n$.
- We investigate now the phase-lag of the above mentioned method. The study demands the following procedure:
- In order to define the phase-lag for the above category of methods, we use the scalar test equation:

$$q'' = -\phi^2\, q \qquad (4)$$

- If we apply a symmetric $2\,n$-step multiderivative method to the above test equation (Equation 4), the following difference equation is produced:

$$A_n(w)\, q_{k+n} + \ldots + A_1(w)\, q_{k+1} + A_0(w)\, q_k + +A_1(w)\, q_{k-1} + \ldots + A_n(w)\, q_{k-n} = 0 \qquad (5)$$

where $w = \phi\, h$, h is the step length and $A_0(w)$, $A_1(w), \ldots, A_n(w)$ are polynomials of $w = \phi\, h$.
- We note here that in our analysis the corresponding characteristic equation is also required. The characteristic equation of the difference equation (5) is given by:

$$A_n(w)\,\lambda^n + \ldots + A_1(w)\,\lambda + A_0(w) + +A_1(w)\,\lambda^{-1} + \ldots + A_n(w)\,\lambda^{-n} = 0 \qquad (6)$$

- The calculation of the phase-lag can be done via the following theorem which is proved by Simos and coworkers (see [2] and [3]):

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Theorem 1: [2] and [3] The symmetric $2\,n$-step method with characteristic equation given by Equation 6 has phase-lag order q and phase-lag constant c given by:

$$-c\,w^{q+2} + O\left(w^{q+4}\right) = \frac{T_0}{T_1} \quad (7)$$

where

$$T_0 = 2\,A_n\,(w)\,\cos\,(n\,w) + \ldots + \\ +2\,A_j\,(w)\,\cos\,(j\,w) + \ldots + A_0\,(w) \quad (8)$$
$$T_1 = 2\,n^2\,A_n\,(w) + \ldots + \\ +2\,j^2\,A_j\,(w) + \ldots + 2\,A_1\,(w) \quad (9)$$

where the polynomials $A_0(w)$, $A_1(w), \ldots, A_n(w)$ are given above (see Equation 5 and Equation 6).
Remark 1: It is easy to see that from the above formulae Equations 7, 8 and 9 we can compute the phase-lag of any symmetric $2\,n$-step multiderivative method.

IV. THE NEW ALGORITHM

The construction of a hybrid type symmetric four-step multiderivative method for the numerical solution of problems of the form $p'' = f\,(x,p)$ is presented in this section.

Consider the method:

$$\begin{aligned}\hat{p}_{n+2} &= c_0\,p_{n+1} + c_0\,p_{n-1} - p_{n-2} + \\ &+h^2\Big(a_0\,p''_{n+1} + a_1\,p''_n + a_0\,p''_{n-1}\Big) + \\ &+h^4\Big(b_0\,p^{(4)}_{n+1} + b_1\,p^{(4)}_n + b_0\,p^{(4)}_{n-1}\Big)\\ p_{n+2} - c_1\,p_{n+1} - c_1\,p_{n-1} + p_{n-2} &= \\ = h^2\Bigg[a_4\,\left(\hat{p}''_{n+2} + p''_{n-2}\right) &+ \\ +a_3\,\left(p''_{n+1} + p''_{n-1}\right) + a_2\,p''_n\Bigg] &+ \\ +h^4\Bigg[b_4\,\left(\hat{p}^{(4)}_{n+2} + p^{(4)}_{n-2}\right) &+ \\ +b_3\,\left(p^{(4)}_{n+1} + p^{(4)}_{n-1}\right) + b_2\,p^{(4)}_n\Bigg] & \quad (10)\end{aligned}$$

Notations for the above mentioned general family of methods :

- We define as free parameters the coefficients a_j, $j = 0(1)4$ and b_i, $i = 0(1)4$.
- The step size of the integration is defined as h.
- n is the number of steps,
- The approximation of the solution on the point x_n is presented as p_n
- $x_n = x_0 + n\,h$ and
- x_0 is the initial value point.

A. First Layer of the Hybrid Method

Our study begins from the first method of the above mentioned hybrid scheme:

$$\begin{aligned}p_{n+2} - c_0\,p_{n+1} - c_0\,p_{n-1} + p_{n-2} &= \\ = h^2\Big(a_0\,p''_{n+1} + a_1\,p''_n + a_0\,p''_{n-1}\Big) &+ \\ +h^4\Big(b_0\,p^{(4)}_{n+1} + b_1\,p^{(4)}_n + b_0\,p^{(4)}_{n-1}\Big) & \quad (11)\end{aligned}$$

Applying the method given by Equation 11 to the test equation (4), we obtain the difference equation (5) with $n = 2$. We note that $A_j\,(w)$, $j = 0,\,1,\,2$ are given by:

$$A_2\,(w) = 1,\; A_1\,(w) = -c_0 + w^2\,a_0 - w^4\,b_0, \\ A_0\,(w) = w^2\,a_1 - w^4\,b_1 \quad (12)$$

We demand the above scheme to have the phase-lag vanished. Based on the formula given by Equation 7 (for $n = 2$) and taking into account the formulae given by the Equations 12, we obtain the following equation:

$$\mathrm{Phase-Lag} = \frac{1}{2}\,\frac{T_2}{-4 + c_0 - w^2\,a_0 + w^4\,b_0} = 0 \quad (13)$$

where

$$\begin{aligned}T_2 &= -4\,\left(\cos\,(w)\right)^2 + 2\\ &+ 2\,\cos\,(w)\,c_0 - 2\,\cos\,(w)\,w^2\,a_0\\ &+ 2\,\cos\,(w)\,w^4\,b_0 - w^2\,a_1 + w^4\,b_1 \quad (14)\end{aligned}$$

Remark 2: Equations for the first, second etc derivatives of the phase-lag can be produced. In order to define the maximum number of the available equations of the previous type, we must check the free parameters of the algorithm. In our case and since we have five parameters $\Big(c_0,\,a_0,\,a_1\,b_0,\,b_1\Big)$, we can produce four more equations for the vanishing of the first, second, third and fourth derivatives of the phase-lag.

Remark 3: The definition of the free parameters of the scheme, i.e., the parameters $\Big(c_0,\,a_0,\,a_1\,b_0,\,b_1\Big)$, can be done solving the system of equations produced by the requirement of the vanishing of the phase-lag and its derivatives.

B. Second Layer of the Hybrid Method

Our study is continued now to the second layer of the proposed method (10) :

$$q_{n+2} - c_1\, p_{n+1} - c_1\, p_{n-1} + p_{n-2} = \\ = h^2 \left[a_4 \, \left(p''_{n+2} + p''_{n-2} \right) + \right. \\ \left. + a_3 \, \left(p''_{n+1} + p''_{n-1} \right) + a_2\, p''_n \right] + \\ + h^4 \left[b_4 \, \left(\hat{p}^{(4)}_{n+2} + p^{(4)}_{n-2} \right) + \right. \\ \left. + b_3 \, \left(p^{(4)}_{n+1} + p^{(4)}_{n-1} \right) + b_2\, p^{(4)}_n \right] \quad (15)$$

Applying now the second layer (15) to the test equation (4) (following the methodology described in the previous section for the first layer of the hybrid method), we obtain the difference equation (5) with $n = 2$ and $A_j\,(w)\,, \quad j = 0,\, 1,\, 2$ given by:

$$A_2\,(w) \;=\; 1 + w^2\, a_4 + w^4\, b_4, \\ A_1\,(w) \;=\; -c_1 + w^2\, a_3 - w^4\, b_3 \\ A_0\,(w) = w^2\, a_2 - w^4\, b_2 \quad (16)$$

We require now the above algorithm to have the phase-lag vanished. We again base our investigation on the formula given by Equation 7 (for $n = 2$) and we take into account the formulae given by Equations 16. Based on this the following equation holds:

$$\mathrm{Phase-Lag} \;=\; \frac{1}{2}\,\frac{T_3}{T_4} = 0 \quad (17)$$

where

$$\begin{aligned} T_3 \;&=\; 4\,(\cos\,(w))^2\, \Big(-4\, w^2\, a_4 \\ &+\; 4\, w^4\, b_4 - 1 \Big) + 2\, \cos\,(w)\, \Big(-w^2\, a_3 \\ &+\; w^4\, b_3 + c_1 \Big) + w^4 \Big(-2\, b_4 + b_2 \Big) \\ &+\; w^2 \Big(2\, a_4 - a_2 \Big) + 2 \quad (18) \\ T_4 \;&=\; -4 + c_1 - w^2\, \Big(a_3 + 4\, a_4 \Big) \\ &+\; w^4\, \Big(b_3 + 4\, b_4 \Big) \quad (19) \end{aligned}$$

Remark 4: Equations for the first, second etc derivatives of the phase-lag can be also obtained. In order to define the maximum number of the available equations of the previous type, we must check the free parameters of the algorithm. In our case and since we have seven parameters

$$c_1,\, a_j,\, j = 2(1)4\, b_i,\, i = 2(1)4, \quad (20)$$

we can produce six more equations for the vanishing of the first, second, third, fourth, fifth and sixth derivatives of the phase-lag.

Remark 5: The definition of the free parameters of the scheme, i.e., the parameters

$$c_1,\, a_j,\, j = 2(1)4\, b_i,\, i = 2(1)4, \quad (21)$$

can be done solving the system of equations produced by the requirement of the vanishing of the phase-lag and its derivatives.

Based on the above developments several methods can be obtained.

Remark 6: If we demand our hybrid multiderivative four-step method of the form (10) to have vanished the phase-lag and its first derivative, then the formulae (13), (17) have to be satisfied and also the corresponding formulae for the first derivatives. In order the above relations to be satisfied we must have at least four free parameters. We can choose four from the twelve free parameters of the scheme in order the above request to be satisfied on each layer of the hybrid method.

Remark 7: If we demand our hybrid multiderivative four-step method of the form (10) to have vanished the phase-lag and its first and second derivatives, then the formulae (13), (17) have to be satisfied and also the corresponding formulae for the first and second derivatives. In order the above relations to be satisfied we must have at least six free parameters. We can choose six from the twelve free parameters of the scheme in order the above request to be satisfied on each layer of the hybrid method

The steps we have to follow for the development of the new hybrid four-step multiderivative method are:

- Decision of the form of the method we wish to have (this is based on the mathematical model of the problem. If, for example, we have a problem with oscillating behavior of the solution, the we must have a method with vanished the phase-lag and as much as we can derivatives of the phase-lag)
- Development of the equations, which satisfy the above
- Solution of the system of equations and determination of the free parameters of the method
- Analysis of the produced method: local truncation error analysis, stability analysis.
- Finally, application of the obtained method to several well known problems in order to test the efficiency of the new algorithms.

V. Evaluation

The new proposed methods have the following characteristics :

1) High algebraic order
2) Vanishing of the phase-lag on each stage of the method
3) Vanishing of the derivatives of the phase-lag on each stage of the method

Based on the above characteristics, the new proposed method can be efficiently to any second order initial or boundary value problem with oscillating solutions.

VI. Conclusion

A new methodology for the construction of effective hybrid multiderivative multistep methods for the approximate solution of the Schrödinger equation and related problems with periodical or oscillating solutions is presented in this paper. It is mentioned that the important parts of this new methodology are (i) the vanishing of the phase-lag on its level of the hybrid multiderivative method and (ii) the vanishing of the its derivatives on its level of the hybrid multiderivative method. As an example, we applied the new methodology on a four-step hybrid type multiderivative method. From the numerical results produced from the application of this new developed four-step hybrid type multiderivative method to the resonance problem of the Schrödinger equation it is easy for one to see the efficiency of the new methodology.

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