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A family of high-order multistep methods with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation

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ABSTRACT

Many simulation algorithms (chemical reaction systems, differential systems arising from the modelling of transient behaviour in the process industries etc.) contain the numerical solution of systems of differential equations. For the efficient solution of the above mentioned problems, linear multistep methods or Runge–Kutta single-step methods are used. For the simulation of chemical procedures the radial Schrödinger equation is used frequently. In the present paper we will study a class of linear multistep methods. More specifically, the purpose of this paper is to develop an efficient algorithm for the approximate solution of the radial Schrödinger equation and related problems. This algorithm belongs in the category of the multistep methods. In order to produce an efficient multistep method the phase-lag property and its derivatives are used. Hence the main result of this paper is the development of an efficient multistep method for the numerical solution of systems of ordinary differential equations with oscillating or periodical solutions. The reason of their efficiency, as the analysis proved, is that the phase-lag and its derivatives are eliminated. Another reason of the efficiency of the new obtained methods is that they have high algebraic order

1. Introduction

Many simulation algorithms (chemical reaction systems, differential systems arising from the modelling of transient behaviour in process industries, etc.) contain the numerical solution of systems of differential equations. For the efficient solution of the above mentioned problems, linear multistep methods or Runge–Kutta single-step methods are used.

One of the models used frequently for the simulation of chemical procedures is the radial Schrödinger equation.

The formula of the radial Schrödinger equation can be presented as:

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

It is known that Mathematical Models in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics, etc., can be expressed via the above boundary value problem (see for example [1–4]).

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For the above Eq. (1) we have the following definitions:

- The function $W(x) = l(l+1)/x^2 + V(x)$ 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*.
- The quantity l is a given integer representing the *angular momentum*.
- V is a given function which denotes the *potential*.

The boundary conditions are:

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

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

Large research on the algorithmic development of numerical methods for the solution of the Schrödinger equation has been done in the last decades. The aim and scope of this research is the construction of fast and reliable algorithms for the solution of the Schrödinger equation and related problems (see for example [5–24]).

The numerical methods for the approximate solution of the Schrödinger equation and related problems can be divided into two main categories:

1. Methods with constant coefficients.
2. Methods with coefficients depending on the frequency of the problem.[2]

The main result of this paper is the development of an efficient multistep method for the numerical solution of systems of ordinary differential equations with oscillating or periodical solutions. The reason of their efficiency, as the analysis proved, is that the phase-lag and its derivatives are eliminated. Another reason of the efficiency of the new obtained methods is that they have high algebraic order.

The purpose of this paper is to extend the methodology for the development of numerical methods for the approximate solution periodic initial-value problems. The new methodology is based on the requirement of the phase-lag and its derivatives vanishing. Based on this new methodology we will develop two methods:

- The first one will have phase-lag and its first and second derivatives vanishing.
- The second one will have phase-lag and its first, second and third derivatives vanishing.

We will apply the new developed methods on the numerical solution of the radial Schrödinger equation. We will study the efficiency of the new obtained methods via:

- a comparative error analysis
- a comparative stability analysis and finally
- the numerical results produced from the numerical solution of the radial Schrödinger with application to the specific potential.

More specifically, we will develop a family of implicit symmetric ten-step methods of twelfth algebraic order. The development of the new family of methods is based on the requirement of the phase-lag and its first, second and third derivative vanishing (see above).

We will give a comparative error analysis and a comparative stability analysis in order to study the efficiency of the two new proposed methods of the family. Finally, we will apply both methods to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation.

We have organized the paper 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.
- A comparative error analysis is presented in Section 4.
- In Section 5 we will present a comparative stability analysis.
- The numerical results are presented in Section 6.
- Finally, in Section 7 remarks and conclusions are discussed.

2. Basic theory

2.1. Definitions

We consider the numerical solution of the initial value problem over the equally spaced intervals $\{r_i\}_{i=0}^{m} \in [a, b]$ and $h = |r_{i+1} - r_i|,\ i = 0(1)m-1$:

$$\phi'' = -\omega^2 \phi. \tag{3}$$

[2] When using a functional fitting algorithm for the solution of the radial Schrödinger equation, the fitted frequency is equal to: $\sqrt{|l(l+1)/x^2 + V(x) - k^2|}$.