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A new family of symmetric linear four-step methods for the efficient integration of the Schrödinger equation and related oscillatory problems

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ABSTRACT

In this article we develop a family of three explicit symmetric linear four-step methods. The new methods, with nullified phase-lag, are optimized for the efficient solution of the Schrödinger equation and related oscillatory problems. We perform an analysis of the local truncation error of the methods for the general case and for the special case of the Schrödinger equation, where we show the decrease of the maximum power of the energy in relation to the corresponding classical methods. We also perform a periodicity analysis, where we find that there is a direct relationship between the periodicity intervals of the methods and their local truncation errors. In addition we determine their periodicity regions. We finally compare the new methods to the corresponding classical ones and other known methods from the literature, where we show the high efficiency of the new methods.

1. Introduction

The numerical solution of the Schrödinger equation and related initial value problems with oscillating/periodic solutions has attracted the interest of many researchers during the last decades [1–35]. We consider the one-dimensional time-independent Schrödinger equation, which is given by

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - E\right) y(x), \tag{1}$$

where $\frac{l(l+1)}{x^2}$ is the *centrifugal potential*, $V(x)$ is the *potential*, E is the *energy* and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the *effective potential*. It is valid that $\lim_{x\to\infty} V(x) = 0$ and therefore $\lim_{x\to\infty} W(x) = 0$.

We consider $E > 0$ and divide $[0, x_{max}]$, where x_{max} is the end of the integration interval and depends on the potential used, into subintervals $[a_i, b_i]$, so that on each subinterval $W(x)$ is a constant with value $\overline{W}_i$. Then the problem (1) can be expressed by the approximation

$$y_i'' = (\overline{W}_i - E) y_i, \quad \text{whose solution is } y_i(x) = A_i e^{\sqrt{\overline{W}_i - E}x} + B_i e^{-\sqrt{\overline{W}_i - E}x}, \quad A_i,\ B_i \in \mathbb{R}, \quad \text{and } x \in [a_i, b_i]. \tag{2}$$

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We use the approach above, so that we can use an approximation $\overline{W}_i$ of the potential $W(x)$. This approximation is used in both the numerical integration and the local truncation error analysis of the method, when it is applied to the Schrödinger equation. The error analysis reveals the important relation of the error to the energy, as we can see in Section 3.2.

In this work we produce a family of three explicit symmetric linear four-step methods with fourth algebraic order and zero phase-lag for the numerical solution of the above equation and related oscillatory problems. More specifically, in Section 2 we provide the necessary definitions and theorems. In Section 3 we present the development, truncation error analysis and periodicity analysis of the method. In Section 4 we show the application of the method to the Schrödinger equation and related problems, as well as the comparison to other methods in terms of efficiency. Finally, in Section 5 we give some conclusions on the results of this work.

2. Theory

For the numerical solution of the initial value problem

$$y'' = f(x, y), \tag{3}$$

where f does not contain an explicit form of $y'(x)$, we define a multistep method of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \tag{4}$$

with m steps, which can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)m - 1$. The method is called symmetric if $a_i = a_{m-i}$ and $b_i = b_{m-i}, \ i = 0(1)\lfloor \frac{m}{2} \rfloor$.

Method (4) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i u(x + ih) - h^2 \sum_{i=0}^{m} b_i u''(x + ih), \tag{5}$$

where $u \in C^2$.

Definition 1. The multistep method (4) is called algebraic of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p+1}$.

2.1. Periodicity analysis of multistep methods

Here we will provide the necessary definitions and theorems to perform a periodicity analysis of multistep methods [7].

We apply the linear m-step method (4) to the scalar test equation

$$y'' = -\theta^2 y \tag{6}$$

and then we solve the corresponding characteristic equation, which has m characteristic roots λ_i, $i = 0(1)m - 1$, where λ_0 and λ_1 are the principal roots.

Definition 2 [8]. If the characteristic roots satisfy the conditions $|\lambda_i| \leqslant 1$, $i = 0(1)m - 1$ for all $s = \theta h$, then we say that the method is *unconditionally stable*.

Definition 3 [8]. If the characteristic roots satisfy the conditions $\lambda_0 = e^{I\phi(s)}$, $\lambda_1 = e^{-I\phi(s)}$, and $|\lambda_i| \leqslant 1$, $i = 2(1)m - 1$ for all $s < s_0$, where $s = \theta h$ and $\phi(s)$ is a real function of s, then we say that the method has interval of periodicity $(0, s_0^2)$.

We deliberately use frequency θ for the periodicity analysis that is different from frequency ω used for phase-fitting. In this way we will be able to produce the v–s plane, which gives the periodicity regions of the method.

Definition 4 [12]. A *region of periodicity* for a multistep method is a region of the v–s plane, throughout which the roots of the corresponding characteristic equation satisfy the conditions of Definition 3. If the conditions are valid for the equality only ($|\lambda_i| = 1$, $i = 2(1)m - 1$), then the corresponding curve is called *periodicity boundary*.

If we set $r = \frac{v}{s} = \frac{\omega}{\theta}$, then we can say that the *principal interval of periodicity*is represented by the line segment from the beginning of the axes to the intersection of line $v = rs$ and the periodicity boundary. The *secondary intervals of periodicity* can be defined along the line $v = rs$ further from the beginning of the axes, but they are less important since the method must always be periodic around the area where $h \to 0$.

2.2. Phase-lag analysis of symmetric multistep methods

When a symmetric $2k$-step method is applied to the scalar test equation