A new four-step explicit method with vanished phase-lag and its derivatives for the numerical solution of radial Schrödinger equation

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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 illustrate the accuracy and computational efficiency of the new developed method via numerical examples.

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1 Introduction

The radial time- independent Shorödinger equation can be written as

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

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 $[0, \infty)$ into subintervals $[a_i, b_i)$ so that $W(x)$ is a constant with value $\overline{W}$. After this the problem (1) can be expressed by the approximation: $y_i'' = (\overline{W} - E)y_i$, whose theoretical solution is $y_i = A_i \exp(\sqrt{\overline{W} - E}x) + B_i \exp(\sqrt{\overline{W} - E}\,x)$, where $A_i,\ B_i \in \mathbb{R}$. Many numerical methods have been developed for the efficient solution of the Schrödinger equation and related problems [1 - 5].

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{2}$$

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