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EXPONENTIAL FITTED METHODS FOR THE NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION*

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Abstract

A new sixth-order Runge-Kutta type method is developed for the numerical integration of the radial Schrödinger equation and of the coupled differential equations of the Schrödinger type. The formula developed contains certain free parameters which allows it to be fitted automatically to exponential functions. We give a comparative error analysis with other sixth order exponentially fitted methods. The theoretical and numerical results indicate that the new method is more accurate than the other exponentially fitted methods.

1. Introduction

In recent years the Schrödinger equation has been the subject of great activity, the aim is to achieve a fast and reliable algorithm that generates a numerical solution.

1.1. Radial Schrödinger equation

The one dimensional or radial Schrödinger equation has the form:

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

where one boundary condition is $y(0) = 0$ with the other boundary condition being specified at $x = \infty$. Equations of this type occur very frequently in theoretical physics[5], and there is a real need to be able to solve them both efficiently and reliably by numerical methods. In (**??**) the function $W(x) = l(l+1)/x^2 + V(x)$ is denoted as *the effective potential*, for which $W(x) \to 0$ as $x \to \infty$, and k^2 is a real number denoting *the energy*. The boundary conditions are:

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

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

Boundary value methods based on either collocation or finite differences are not very popular for the solution of (**??**) due to the fact that the problem is posed on an infinite interval. Initial value methods, such as shooting, need to take into account the fact that $\mid y'(x) \mid$ is very large near $x = 0$. So, it is very inappropriate to use

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standard library packages for the numerical solution of (**??**). Also Runge-Kutta and Runge-Kutta-Nyström methods have been proved inefficient for the numerical solution of the Schrödinger equation (see [9] for details).

One of the most popular method for the solution of (**??**) is the **Numerov's method.** This method is only of order four, but in practice it has been found to have a superior performance to higher order four-step method. The reason for this, as proved in [9], is that the Numerov method has the same phase-lag order with the four-step methods but it has a larger interval of periodicity. So, the investigation of linear multistep methods is not a fruitful way to deriving efficient high order methods.

An alternative approach to deriving higher order methods for (**??**) was given by Cash and Raptis[1]. In [1] *a* sixth order Runge-Kutta type method with a large interval of periodicity was derived. This method has a phase-lag of order six (while the Numerov's method has phase-lag of order four) and an interval of periodicity much more larger than the method of Numerov.

Another alternative approach for developing efficient methods for the solution of (**??**) is to use exponential fitting. This approach is appropriate because for large x the solution of (**??**) is *periodic*. Raptis and Allison[6] have derived a Numerov type exponentially fitted method. Numerical results presented in [6] indicate that these fitted methods are much more efficient than Numerov's method for the solution of (**??**). Many authors have investigated the idea of exponential fitting, since Raptis and Allison. Perhaps the most significant work in this general area was that of Ixaru and Rizea[3]. They showed that for the resonance problem defined by (**??**) it is generally more efficient to derive methods which exactly integrate functions of the form:

$$\{1, x, x^2, \ldots, x^p, \exp(\pm wx), x\exp(\pm wx), \ldots, x^m\exp(\pm wx)\} \tag{3}$$

than to use classical exponential fitting methods. A powerful low order method of this type was developed by Raptis[7]. Also Simos[10] has derived a four-step method of this type which gives much more accurate results compared with other four-step methods. Simos[11] has derive a family of four-step methods which gives more efficient results than other four-step methods. Also Raptis and Cash[8] have derived an exponential fitted method and Cash, Raptis and Simos[2] have derived a method fitted to (**??**) with $m = 1$ and $p = 3$.

The purpose of this paper is to derive Runge-Kutta type methods fitted to (**??**) and in particular to derive a method with $m = 3$. We give a comparative error analysis with other sixth order exponentially fitted methods. The theoretical and numerical results indicate that the new method is more accurate than the other exponentially fitted methods.

1.2. Coupled differential equations

The close-coupled equations may be written

$$[\frac{d^2}{dR^2} + k_i^2 - \frac{l_i(l_i+1)}{R^2} - V_{ii}]y_{ij} = \sum_{k=1}^{N}{}_{k\neq i} V_{ik}y_{kj} \tag{4}$$

for $1 \leq i \leq N,\ 1 \leq j \leq N$ and where **V** and **Y** are matrices.