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Closed Newton-Cotes Trigonometrically-Fitted Formulae for the Solution of the Schrödinger Equation

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Abstract

In this paper the connection between closed Newton-Cotes, trigonometrically-fitted differential methods, symplectic integrators and efficient solution of the Schrödinger equation is investigated. Several one step symplectic integrators have been obtained based on symplectic geometry, as one can see from the literature. However, the investigation of multistep symplectic integrators is very poor. Zhu et. al. [1] has presented the well known open Newton-Cotes differential methods as multilayer symplectic integrators. The construction of multistep symplectic integrators based on the open Newton-Cotes integration methods was studied by Chiou and Wu [2]. In this paper we study the closed Newton-Cotes formulae and we write them as symplectic multilayer structures. We also construct trigonometrically-fitted symplectic methods which are based on the closed Newton-Cotes formulae. We apply the symplectic schemes to the well known radial Schrödinger equation in order to investigate the efficiency of the proposed method to these type of problems.

1 Introduction

The radial Schrödinger equation has the form:

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]y(r). \quad (1)$$

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Differential equations of this type, which represent a boundary value problem, occur frequently in theoretical physics and chemistry, (see for example [3] - [6]). In the following we present some notations for (1):

- The function $W(r) = l(l+1)/r^2 + V(r)$ denotes *the effective potential*. This function satisfies $W(r) \to 0$ as $r \to \infty$
- k^2 is a real number denoting *the energy*
- l is a given integer representing *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 r, determined by form of the problem.

We note that recently much work has been done on the numerical solution of ordinary differential equations (see [7] - [21] and references therein). It is also known from the literature that the last decades many numerical methods have been constructed for the approximate solution of the radial Schrödinger equation (see [22] - [51] and references therein). The aim and the scope of the above activity was the development of fast and reliable methods.
The developed methods can be divided into two main categories:

- Methods with constant coefficients
- Methods with coefficients dependent on the frequency of the problem [1].

The organization of the paper is the following:

1. We try to present Closed Newton-Cotes differential methods as multi-layer symplectic integrators.
2. We apply the closed Newton-Cotes methods on the Hamiltonian system:

$$\begin{aligned} \dot{q} &= m\,p \\ \dot{p} &= -m\,q \end{aligned} \tag{3}$$

[1] In the case of the Schrödinger equation the frequency of the problem is equal to: $\sqrt{|l(l+1)/r^2 + V(r) - k^2|}$

which represents the Hamilton's equations of motion which are linear in position p and monentum q (m is a constant scalar or matrix). It is well known that the Equation (3) is a an important one in the field of molecular dynamics. As a result of the above application we will try to prove that the Hamiltonian energy of the system remains almost constant as the integration proceeds.

3. A trigonometrically-fitted method is developed.

The results about symplectic matrices and schemes are presented in section 2. In section 3 Closed Newton-Cotes integral formulae and differential methods are described and the new trigonometrically - fitted methods are developed. The conversion of the closed Newton-Cotes differential methods into multilayer symplectic structures is presented in section 4. Finally in section 5 numerical results are presented.

2 Basic Theory on Symplectic Schemes and Numerical Methods

The following basic theory on symplectic numerical schemes and symplectic matrices is based on that developed by Zhu et. al. [1]. The proposed methods can be used for non-linear differential equations as well as linear ones.
Dividing an interval $[a, b]$ with N points we have

$$x_0 = a,\ x_n = x_0 + nh = b, \quad n = 1, 2, \ldots, N. \tag{4}$$

We note that x is the independent variable and a and b in the equation for x_0 (Eqn (4)) are different than the a and b in Eqn (5).
The above division leads to the following discrete scheme:

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = M_{n+1} \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \quad M_{n+1} = \begin{pmatrix} a_{n+1} & b_{n+1} \\ c_{n+1} & d_{n+1} \end{pmatrix} \tag{5}$$

Based on the above we can write the n-step approximation to the solution as:

$$\begin{aligned} \begin{pmatrix} p_n \\ q_n \end{pmatrix} &= \begin{pmatrix} a_n & b_n \\ c_n & d_n \end{pmatrix} \begin{pmatrix} a_{n-1} & b_{n-1} \\ c_{n-1} & d_{n-1} \end{pmatrix} \cdots \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \\ &= M_n\, M_{n-1} \cdots M_1 \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \end{aligned}$$

Defining

$$S = M_n\, M_{n-1} \cdots M_1 = \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix}$$

the discrete transformation can be written as:

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = S \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}$$

A discrete scheme (5) is a symplectic scheme if the transformation matrix S is symplectic.
A matrix A is symplectic if $A^T JA = J$ where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

The product of symplectic matrices is also symplectic. Hence, if each matrix M_n is symplectic the transformation matrix S is symplectic. Consequently, the discrete scheme (2) is symplectic if each matrix M_n is symplectic.

3 Trigonometrically-Fitted Closed Newton-Cotes Differential Methods

3.1 General Closed Newton-Cotes Formulae

The closed Newton-Cotes integral rules are given by:

$$\int_a^b f(x)dx \approx z\, h \sum_{i=0}^{k} t_i f(x_i)$$

where

$$h = \frac{b-a}{N}, \quad x_i = a + ih, \quad i = 0, 1, 2, \ldots, N$$

The coefficient z as well as the weights t_i are given in the following table

k	z	t_0	t_1	t_2	t_3	t_4
0	1	1				
1	1/2	1	1			
2	1/3	1	4	1		
3	3/8	1	3	3	1	
4	2/45	7	32	12	32	7

Table 1: *Closed Newton-Cotes integral rules.*

From the above Table it is easy to see that the coefficients t_i are symmetric i.e. we have the following relation:

$$t_i \;=\; t_{k-i}, \quad i = 0, 1, \ldots, \frac{k}{2}$$

Closed Newton-Cotes differential methods were produced from the integral rules. For the above Table we have the following differential methods:

$k=1$ $\quad y_{n+1}-y_n=\frac{h}{2}(f_{n+1}+f_n)$

$k=2$ $\quad y_{n+1}-y_{n-1}=\frac{h}{3}(f_{n-1}+4f_n+f_{n+1})$

$k=3$ $\quad y_{n+1}-y_{n-2}=\frac{3h}{8}(f_{n-2}+3f_{n-1}+3f_n+f_{n+1})$

$k=4$ $\quad y_{n+2}-y_{n-2}=\frac{2h}{45}(7f_{n-2}+32f_{n-1}+12f_n+32f_{n+1}+7f_{n+1})$

In the present paper we will investigate the case $k=2$ and we will produce trigonometrically-fitted differential methods.

3.2 Trigonometrically-Fitted Closed Newton-Cotes Differential Method

Requiring the differential scheme:

$$y_{n+1}-y_{n-1}=h\Big(a_0\,f_{n-1}+a_1\,f_n+a_2\,f_{n+1}\Big) \tag{4}$$

to be accurate for the following set of functions (we note that $f_i=y_i'$, $i=n-1,n,n+1$):

$$\{1,\,\cos(\pm wx),\,\sin(\pm wx),\,x\,\cos(\pm wx),\,x\,\sin(\pm wx)\} \tag{5}$$

the following set of equations is obtained:

$$\begin{aligned}
a_0-a_2&=0\\
w\,h\Big[\Big(a_0+a_2\Big)\cos(w\,h)+a_1\Big]&=2\sin(w\,h)\\
-h(-a_0\cos(w\,h)-\cos(w\,h)\,a_2+\sin(w\,h)\,a_0\,w\,x+\sin(w\,h)\,h\,a_2\,w&\\
-a_1-\sin(w\,h)\,a_2\,w\,x+\sin(w\,h)\,h\,a_0\,w)&=2\,h\cos(w\,h)\\
h(a_0\,w\,x\cos(w\,h)-\cos(w\,h)\,h\,a_2\,w+\cos(w\,h)\,a_2\,w\,x+h\,a_0\,w\cos(w\,h)&\\
+\sin(w\,h)\,a_0-\sin(w\,h)\,a_2+a_1\,x\,w)&=2\sin(w\,h)\,x
\end{aligned} \tag{6}$$

The requirement for the accurate integration of functions (5), helps the method to be accurate for all the problems with solution which has behavior of trigonometric functions.

Solving the above system of equations we obtain:

$$a_0 = \frac{-\cos(v)\,v + \sin(v)}{v^2 \sin(v)} = a_2$$
$$a_1 = \frac{-\sin(2\,v) + 2\,v}{v^2 \sin(v)} \tag{7}$$

where $v = w\,h$. For small values of v the above formulae are subject to heavy cancellations. In this case the following Taylor series expansions must be used.

$$\begin{aligned} a_0 = {} & \frac{1}{3} + \frac{1}{45}\,v^2 + \frac{2}{945}\,v^4 + \frac{1}{4725}\,v^6 + \frac{2}{93555}\,v^8 \\ & + \frac{1382}{638512875}\,v^{10} + \frac{4}{18243225}\,v^{12} + \ldots = a_2 \\ a_1 = {} & \frac{4}{3} - \frac{2}{45}\,v^2 + \frac{13}{1890}\,v^4 + \frac{1}{2700}\,v^6 + \frac{647}{14968800}\,v^8 \\ & + \frac{176639}{40864824000}\,v^{10} + \frac{2867}{6538371840}\,v^{12} + \ldots \end{aligned} \tag{8}$$

The Local Truncation Error for the above differential method is given by:

$$L.T.E(h) = -\frac{h^5}{90}\left(y_n^{(5)} + 2\,v^2\,y_n^{(3)} + v^4\,y_n^{(1)}\right) \tag{9}$$

The $L.T.E.$ is obtained expanding the terms $y_{n\pm1}$ and $f_{n\pm1}$ in (4) into Taylor series expansions and substituting the Taylor series expansions of the coefficients of the method.

4 Closed Newton-Cotes can be expressed as symplectic integrators

Theorem 1 *A discrete scheme of the form*

$$\begin{pmatrix} b & -a \\ a & b \end{pmatrix} \begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix} \tag{10}$$

is symplectic.

Proof. We rewrite (3) as

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} b & -a \\ a & b \end{pmatrix}^{-1} \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix}$$

Define

$$M = \begin{pmatrix} b & -a \\ a & b \end{pmatrix}^{-1} \begin{pmatrix} b & a \\ -a & b \end{pmatrix} = \frac{1}{b^2 + a^2} \begin{pmatrix} b^2 - a^2 & 2ab \\ -2ab & b^2 - a^2 \end{pmatrix}$$

and it can easily be verified that

$$M^T J M = J$$

thus the matrix M is symplectic.
In [1] Zhu et al. have proved the symplectic structure of the well-known second-order differential scheme (SOD),

$$y_{n+1} - y_n \;=\; 2h f_n$$

The above method has been produced by the simplest Open Newton-Cotes integral rule.
Based on the paper Chiou et al. [2] we will try to write Closed Newton-Cotes differential schemes as multilayer symplectic structures.
Application of the Newton-Cotes differential formula for $n = 2$ to the linear Hamiltonian system (3) gives

$$\begin{aligned} q_{n+1} - q_{n-1} &= s\left(a_0\, p_{n-1} + a_1\, p_n + a_2\, p_{n+1}\right) \\ p_{n+1} - p_{n-1} &= -s\left(a_0\, q_{n-1} + a_1\, q_n + a_2\, q_{n+1}\right) \end{aligned} \tag{11}$$

where $s = m\,h$, where m is defined in (3).
¿From (11) we have that:

$$\begin{aligned} q_{n+1} - q_{n-1} &= 2\,s\,p_n \\ p_{n+1} - p_{n-1} &= -2\,s\,q_n \end{aligned}$$

Substituting p_n and q_n into (11) we obtain:

$$\begin{aligned} q_{n+1} - q_{n-1} &= s\left(a_0\, p_{n-1} + a_2\, p_{n+1}\right) + \frac{a_1}{2}\left(q_{n+1} - q_{n-1}\right) \\ p_{n+1} - p_{n-1} &= -s\left(a_0\, q_{n-1} + a_2\, q_{n+1}\right) + \frac{a_1}{2}\left(p_{n+1} - p_{n-1}\right) \end{aligned}$$

The above formula in matrix form can be written as:

$$\begin{pmatrix} \left(1 - \frac{a_1}{2}\right) & -s\,a_0 \\ s\,a_0 & \left(1 - \frac{a_1}{2}\right) \end{pmatrix} \begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} \left(1 - \frac{a_1}{2}\right) & s\,a_0 \\ -s\,a_0 & \left(1 - \frac{a_1}{2}\right) \end{pmatrix} \begin{pmatrix} q_{n-1} \\ p_{n-1} \end{pmatrix}$$

which is a discrete scheme of the form (10) and hence it is symplectic.
We note here than in [2] Chiou et al. have re-written Open Newton-Cotes differential schemes as multilayer symplectic structures based on (11).

5 Numerical Illustrations

In this section we present some numerical results to illustrate the performance of our new methods. Consider the numerical integration of the Schrödinger equation (1) using the well-known Woods-Saxon potential (see [1], [4-6], [8]) which is given by

$$V(r) = V_w(r) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{12}$$

with $z = \exp[(r - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$.. In Figure 1 we give a graph of this potential. In the case of negative eigenenergies (i.e. when $E \in [-50, 0]$) we have the well-known **bound-states problem** while in the case of positive eigenenergies (i.e. when $E \in (0, 1000]$) we have the well-known **resonance problem** (see [22], [23] and [32]).

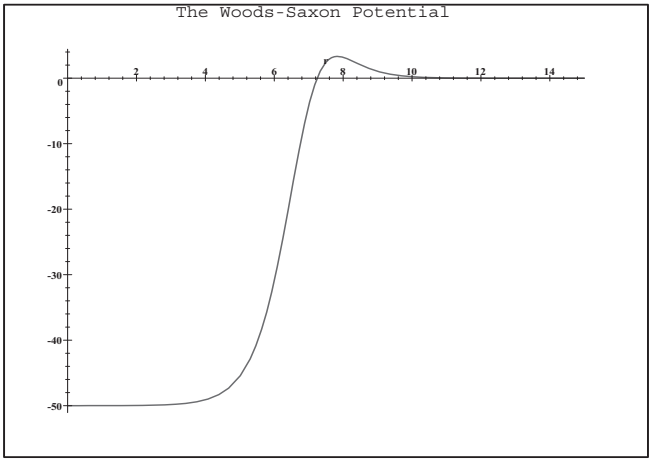

Figure 1: The Woods-Saxon potential.

5.1 Resonance Problem

In the asymptotic region the equation (1) effectively reduces to

$$y''(x) + (k^2 - \frac{l(l+1)}{x^2})y(x) = 0, \tag{13}$$

for x greater than some value X.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx), n_l(kx)$ are the **spherical Bessel and Neumann functions** respectively. Thus the solution of equation (1) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)] \end{aligned} \tag{14}$$

where δ_l is the **phase shift** which may be calculated from the formula

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{15}$$

for x_1 and x_2 distinct points on the asymptotic region (for which we have that x_1 is the right hand end point of the interval of integration and $x_2 = x_1 - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.
Since the problem is treated as an initial-value problem, one needs y_0 and y_1 before starting a two-step method. From the initial condition, $y_0 = 0$. The value y_1 is computed using the Runge-Kutta-Nyström 12(10) method of Dormand et. al. [20]-[21]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l from the above relation.

5.1.1 The Woods-Saxon Potential

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (1) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods-Saxon one (12).
One can investigate the problem considered here, following two procedures. The first procedure consists of finding the **phase shift** $\delta(E) = \delta_l$ for $E \in [1, 1000]$. The second procedure consists of finding those E, for $E \in [1, 1000]$, at which δ equals $\pi/2$. In our case we follow the first procedure i.e. we try to find the phase shifts for given energies. The obtained phase shift is then compared to the analytic value of $\pi/2$.
The above problem is the so-called **resonance problem** when *the positive eigenenergies lie under the potential barrier*. We solve this problem, using the technique fully described in [5].
The boundary conditions for this problem are:

$$\begin{aligned} y(0) &= 0, \\ y(x) &\sim \cos[\sqrt{E}x] \text{ for large } x. \end{aligned}$$

The domain of numerical integration is [0, 15].

For comparison purposes in our numerical illustration we use the following methods:

- The Trigonometrically-Fitted Runge-Kutta Method developed by Anastassi and Simos [49] (which is indicated as Method A)
- The well known Numerov's method (which is indicated as Method B)
- The Explicit Numerov-Type Method developed by Chawla and Rao [19] (which is indicated as Method C)
- The P-stable Exponentially Fitted Method developed by Kalogiratou and Simos [50] (which is indicated as Method D)
- The New Proposed Method (which is indicated as Method E)

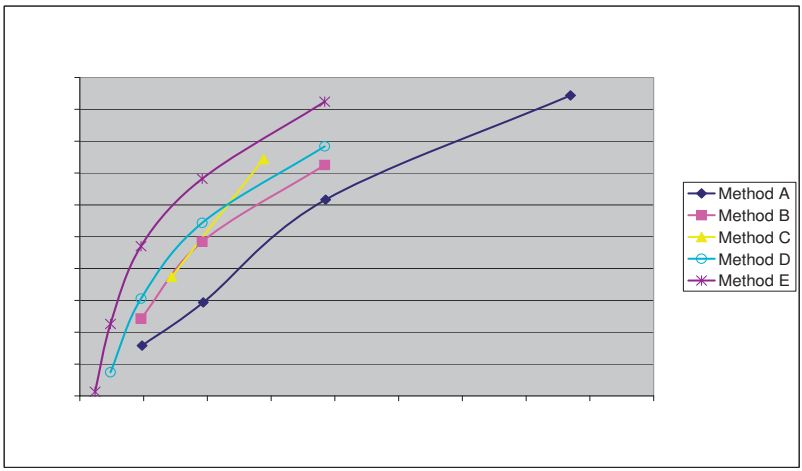

Figure 2: Error $Errmax$ for several values of n for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of $Errmax$ indicates that for this value of n, $Errmax$ is positive.

The numerical results obtained for the four methods, with several number of function evaluations (NFE), were compared with the analytic solution of the Woods-Saxon potential resonance problem, rounded to six decimal places. Figure 2 show the errors $Err = -log_{10}|E_{calculated} - E_{analytical}|$ of the highest eigenenergy $E_3 = 989.701916$ for several values of n.

6 Conclusions

In this paper a new approach for constructing efficient methods for the numerical solution of the Schrödinger type equations is introduced.
¿From the numerical results we have the following remarks:

- The well known Numerov's method has better behavior than the Trigonometrically-Fitted Runge-Kutta Method developed by Anastassi and Simos [49]
- The Explicit Numerov-Type Method developed by Chawla and Rao [19] has better behavior than the well known Numerov's method
- The P-stable Exponentially Fitted Method developed by Kalogiratou and Simos [50] has better behavior than the explicit Numerov-type method with minimal phase-lag of Chawla et. al. [19] for small number of function evaluations
- The New Proposed Method has the better behavior i.e. is the most efficient

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

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