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ORIGINAL PAPER

Closed Newton–Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation

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Abstract In this paper we investigate the connection between (i) closed Newton–Cotes formulae, (ii) trigonometrically-fitted differential methods, (iii) symplectic integrators and (iv) efficient solution of the Schrödinger equation. In the last decades several one step symplectic integrators have been produced based on symplectic geometry, (see the relevant literature and the references here). However, the study of multistep symplectic integrators is very poor. In this paper we investigate the closed Newton–Cotes formulae and we write them as symplectic multilayer structures. We also develop 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.

Keywords Numerical methods · Orbital problems · Closed Newton–Cotes differential methods · Symplectic integrators · Multistep methods · Trigonometric fitting · Energy preservation · Schrödinger equation

Abbreviation

LTE Local truncation error

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1 Introduction

The research area of construction of numerical integration methods for ordinary differential equations that preserve qualitative properties of the analytic solution is of great interest. In this paper we consider Hamilton's equations of motion which are linear in position p and monentum q

$$\begin{aligned} \dot{q} &= m\,p \\ \dot{p} &= -m\,q \end{aligned} \tag{1}$$

where m is a constant scalar or matrix. The Eq. 1 is a an important one in the field of molecular dynamics. It is necessary to use symplectic integrators in order to preserve the characteristics of the Hamiltonian system in the numerical approximation. In the recent years work has been done mainly in the production of one step symplectic integrators (see [1]). Zhu et al. [2] has studied the symplectic integrators and the well known open Newton–Cotes differential methods and as a result has presented the open Newton–Cotes differential methods as multilayer symplectic integrators. The construction of multistep symplectic integrators based on the open Newton–Cotes integration methods was investigated by Chiou and Wu [3].

The last decades much work has been done on exponential—trigonometrically fitting and the numerical solution of periodic initial value problems (see [4–85] and references therein).

In this paper:

- We try to present closed Newton–Cotes differential methods as multilayer symplectic integrators
- We apply the closed Newton–Cotes methods on the Hamiltonian system (1) and we obtain the result that the Hamiltonian energy of the system remains almost constant as the integration proceeds
- The trigonometrically-fitted methods are developed

We note that the aim of this paper is to generate methods that can be used for non-linear differential equations as well as linear ones.

In Sect. 2 the results about symplectic matrices and schemes are presented. In Sect. 3 closed Newton–Cotes integral rules and differential methods are described and the new trigonometrically-fitted methods are developed. In Sect. 4 the conversion of the closed Newton–Cotes differential methods into multilayer symplectic structures is presented. Numerical results are presented in Sect. 5.

2 Basic theory on symplectic schemes and numerical methods

Zhu et al. [2] have developed a theory on symplectic numerical schemes and symplectic matrices in which the following basic theory is based. 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

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

We note that x is the independent variable and a and b in the equation for x_0 (Eq. 2) are different than the a and b in Eq. 3.

The above division leads to the following discrete scheme:

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = M_{n+1} \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \quad M_{n+1} = \begin{pmatrix} a_{n+1} & b_{n+1} \\ c_{n+1} & d_{n+1} \end{pmatrix} \tag{3}$$

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

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

Defining

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

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 (3) is a symplectic scheme if the transformation matrix S is symplectic.
A matrix A is symplectic if $A^T J A = J$ 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:

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

Table 1 Closed Newton–Cotes integral rules

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		
5	5/288	19	75	50	50	75	19	
6	1/140	41	216	27	272	27	216	41

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 (Table 1).

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:

$$\begin{aligned}
&k=1 \quad y_{n+1} - y_n = \tfrac{h}{2}(f_{n+1} + f_n) \\
&k=2 \quad y_{n+1} - y_{n-1} = \tfrac{h}{3}(f_{n-1} + 4f_n + f_{n+1}) \\
&k=3 \quad y_{n+1} - y_{n-2} = \tfrac{3h}{8}(f_{n-2} + 3f_{n-1} + 3f_n + f_{n+1}) \\
&k=4 \quad y_{n+2} - y_{n-2} = \tfrac{2h}{45}(7f_{n-2} + 32f_{n-1} + 12f_n + 32f_{n+1} + 7f_{n+1}) \\
&k=5 \quad y_{n+2} - y_{n-3} = \tfrac{5h}{288}(19f_{n-3} + 75f_{n-2} + \ 50f_{n-1} + 50f_n \\
&\qquad\qquad\qquad\qquad\quad + 75f_{n+1} + 19f_{n+2}) \\
&k=6 \quad y_{n+3} - y_{n-3} = \tfrac{h}{140}(41f_{n-3} + 216f_{n-2} + \ 27f_{n-1} + 272f_n \\
&\qquad\qquad\qquad\qquad\quad + 27f_{n+1} + 216f_{n+2} + 41f_{n+3})
\end{aligned}$$

In the present paper we will investigate the case $k = 6$ and we will produce trigonometrically-fitted differential methods of order 2.

3.2 Trigonometrically-fitted closed Newton–Cotes differential method

Requiring the differential scheme:

$$y_{n+3} - y_{n-3} = h\Big(a_0\, f_{n-3} + a_1\, f_{n-2} + a_2\, f_{n-1} + a_3\, f_n + a_4\, f_{n+1} + a_5\, f_{n+2} + a_6\, f_{n+3}\Big) \tag{4}$$

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

$$\{1,\ x,\ x^2,\ x^3,\ \cos(\pm wx),\ \sin(\pm wx),\ x\ \cos(\pm wx),\ x\ \sin(\pm wx)\} \tag{5}$$

the following set of equations is obtained:

$$\begin{aligned}
a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + a_6 &= 6\\
-6\,a_0 - 4\,a_1 - 2\,a_2 + 2\,a_4 + 4\,a_5 + 6\,a_6 &= 0\\
27\,a_0 + 12\,a_1 + 3\,a_2 + 3\,a_4 + 12\,a_5 + 27\,a_6 &= 54\\
v\,h\sin(v\,h)(-a_0 + a_2 - a_4 + a_6 + 2\,a_1\cos(v\,h)&\\
-\,2\,a_5\cos(v\,h) - 4\,a_6\cos(v\,h)^2 +\ 4\,a_0\cos(v\,h)^2) &= 0\\
2\sin(v\,h)\,(-1 + 4\cos(v\,h)^2) = v\,h(-a_1 + a_3 - a_5 + 4\,a_0\cos(v\,h)^3&\\
+\,2\,a_1\cos(v\,h)^2 - 3\cos(v\,h)\,a_0 - 3\,a_6\cos(v\,h) + a_4\cos(v\,h)&\\
+\,a_2\cos(v\,h) + 4\,a_6\cos(v\,h)^3 + 2\,a_5\cos(v\,h)^2)&\\
6\cos(v\,h)\,h\,(-3 + 4\cos(v\,h)^2) = h(4\,a_6\cos(v\,h)^3 - a_1 + a_3 - a_5&\\
+\,2\,a_1\cos(v\,h)^2 - 3\cos(v\,h)\,a_0 + 2\,a_5\cos(v\,h)^2 - 3\,a_6\cos(v\,h)&\\
-\,4\cos(v\,h)\,h\,a_1\ v\sin(v\,h) - 4\cos(v\,h)\,h\,a_5\ v\sin(v\,h)&\\
-\,2\cos(v\,h)\,a_5\ v\,x\sin(v\,h) + 2\cos(v\,h)\,a_1\ v\,x\sin(v\,h) + a_2\cos(v\,h)&\\
-\,12\sin(v\,h)\,h\,a_0\ v\cos(v\,h)^2 + a_4\cos(v\,h) + 4\,a_0\cos(v\,h)^3&\\
+\,3\sin(v\,h)\,h\,a_0\ v - \sin(v\,h)\,a_0\ v\,x + \sin(v\,h)\,a_2\ v\,x - \sin(v\,h)\,h\,a_2\ v&\\
-\sin(v\,h)\,a_4\ v\,x + \sin(v\,h)\,a_6\ v\,x + 3\sin(v\,h)\,h\,a_6\ v&\\
-\sin(v\,h)\,h\,a_4\ v + 4\sin(v\,h)\,a_0\ v\,x\cos(v\,h)^2&\\
-\,4\sin(v\,h)\,a_6\ v\,x\cos(v\,h)^2 - 12\sin(v\,h)\,h\,a_6\ v\cos(v\,h)^2)&\\
2\sin(v\,h)\,x\,(-1 + 4\cos(v\,h)^2) = h(\sin(v\,h)\,a_0&\\
-\sin(v\,h)\,a_2 - 9\,h\,a_6\ v\cos(v\,h) + a_4\ v\,x\cos(v\,h)&\\
+\cos(v\,h)\,h\,a_4\ v + 2\,a_1\ v\,x\cos(v\,h)^2 + 9\cos(v\,h)\,h\,a_0\ v&\\
+\cos(v\,h)\,a_2\ v\,x + 2\,a_5\ v\,x\cos(v\,h)^2 - 3\cos(v\,h)\,a_6\ v\,x&\\
+\,4\,h\,a_5\ v\cos(v\,h)^2 - 4\,h\,a_1\ v\cos(v\,h)^2 - h\,a_2\ v\cos(v\,h)&\\
-\,3\cos(v\,h)\,a_0\ v\,x - 4\sin(v\,h)\,a_0\cos(v\,h)^2 + 4\sin(v\,h)\,a_6\cos(v\,h)^2&\\
+\,12\,h\,a_6\ v\cos(v\,h)^3 - \sin(v\,h)\,a_6 + \sin(v\,h)\,a_4&
\end{aligned}$$

$$
\begin{aligned}
&- 2\cos(v\,h)\,a_1 \sin(v\,h) + 4\,a_6\,v\,x\cos(v\,h)^3 + 2\cos(v\,h)\,a_5 \sin(v\,h)\\
&\quad + a_3\,x\,v - a_1\,v\,x - a_5\,v\,x - 2\,h\,a_5\,v + 2\,h\,a_1\,v\\
&\quad - 12\,h\,a_0\,v\cos(v\,h)^3 + 4\,a_0\,v\,x\cos(v\,h)^3)
\end{aligned}
\tag{6}
$$

where $v = w\,h$. We note that the first, second and third equations are produced requiring the scheme (4) to be accurate for $x^j,\ j = 0(1)3$, while the fourth, fifth, sixth and seventh equations are obtained requiring the algorithm (4) to be accurate for $\cos(\pm vx),\ \sin(\pm vx),\ x\ \cos(\pm vx),\ x\ \sin(\pm vx)$. 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:

$$
\begin{aligned}
a_0 &= (v\cos(4\,v) + 5\,v\cos(2\,v) - \sin(4\,v) - \sin(2\,v)\\
&\quad - 6\,v\cos(3\,v) + 2\sin(3\,v) - 9\,v^2\sin(2\,v) + 6\,v^2\sin(v))/denom\\
a_1 &= (\sin(5\,v) - 6\sin(3\,v) + \sin(v) + 18\,v\cos(3\,v)\\
&\quad - 6\,v\cos(v) + 2\sin(4\,v) + 2\sin(2\,v)\\
&\quad - 12\,v\cos(2\,v) + 18\,v^2\sin(3\,v) + 18\,v^2\sin(v))/denom\\
a_2 &= (-4\sin(5\,v) + 6\sin(3\,v) - 4\sin(v)\\
&\quad - 9\,v\cos(4\,v) + 3\,v\cos(2\,v) - 18\,v\cos(3\,v)\\
&\quad + 24\,v\cos(v) + \sin(4\,v) + \sin(2\,v)\\
&\quad - 9\,v^2\sin(4\,v) - 45\,v^2\sin(2\,v) - 18\,v^2\sin(3\,v))/denom\\
a_3 &= (6\sin(5\,v) - 4\sin(3\,v) + 6\sin(v) + 16\,v\cos(4\,v)\\
&\quad + 8\,v\cos(2\,v) - 4\sin(4\,v) - 4\sin(2\,v)\\
&\quad + 12\,v^2\sin(4\,v) + 24\,v^2\sin(2\,v) + 12\,v\cos(3\,v)\\
&\quad - 36\,v\cos(v) + 36\,v^2\sin(3\,v) + 36\,v^2\sin(v))/denom\\
a_4 &= a_2,\ a_5 = a_1,\ a_6 = a_0
\end{aligned}
\tag{7}
$$

where $denom = -v^2\sin(4\,v) - 14\,v^2\sin(2\,v) + 6\,v^2\sin(3\,v) + 14\,v^2\sin(v)$.

For small values of v the above formulae are subject to heavy cancellations. In this case the following Taylor series expansions must be used.

$$
\begin{aligned}
a_0 &= \frac{41}{140} + \frac{9}{700}\,v^2 + \frac{3}{3850}\,v^4 + \frac{577}{10510500}\,v^6\\
&\quad + \frac{191}{42042000}\,v^8 + \frac{431}{1021020000}\,v^{10} + \frac{852437}{20532303792000}\,v^{12}\\
&\quad + \frac{2479369}{594356162400000}\,v^{14} + \ldots
\end{aligned}
$$

$$
\begin{aligned}
a_1 = {} & \frac{54}{35} - \frac{27}{350}\,v^2 + \frac{27}{15400}\,v^4 - \frac{2341}{14014000}\,v^6 \\
& - \frac{83}{8624000}\,v^8 - \frac{17247}{19059040000}\,v^{10} - \frac{4663753}{54752810112000}\,v^{12} \\
& - \frac{19482877}{2316465043200000}\,v^{14} + \ldots \\
a_2 = {} & \frac{27}{140} + \frac{27}{140}\,v^2 - \frac{27}{1925}\,v^4 + \frac{61}{350350}\,v^6 \\
& - \frac{67}{28028000}\,v^8 - \frac{171}{952952000}\,v^{10} - \frac{450869}{13688202528000}\,v^{12} \\
& - \frac{5874133}{1505702278080000}\,v^{14} + \ldots \\
a_3 = {} & \frac{68}{35} - \frac{9}{35}\,v^2 + \frac{177}{7700}\,v^4 - \frac{521}{4204200}\,v^6 \\
& + \frac{359}{24024000}\,v^8 + \frac{7573}{5717712000}\,v^{10} + \frac{12582191}{82129215168000}\,v^{12} \\
& + \frac{147083219}{9034213668480000}\,v^{14}
\end{aligned} \tag{8}
$$

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

$$
L.T.E(h) = -\frac{9\,h^9}{1400}\left(y_n^{(9)} + 2\,w^2\,y_n^{(7)} + w^4\,y_n^{(5)}\right) \tag{9}
$$

The $L.T.E.$ is obtained expanding the terms $y_{n\pm j}$ and $f_{n\pm j}$, $j = 1(1)3$ 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 Zhu et al. [2] have proved the symplectic structure of the well-known second-order differential scheme (SOD),

$$\begin{aligned} y_{n+1} - y_{n-1} &= 2hf_n \\ y_{n+2} - y_{n-2} &= 4hf_n \\ y_{n+3} - y_{n-3} &= 6hf_n \end{aligned} \tag{11}$$

The above methods have been produced by the simplest open Newton–Cotes integral formula.

Based on the paper Chiou and Wu [3] the closed Newton–Cotes differential schemes will be written as multilayer symplectic structures.

Application of the Newton–Cotes differential formula for $n = 3$ to the linear Hamiltonian system (1) gives

$$\begin{aligned} q_{n+3} - q_{n-3} = s\ (&a_0\, p_{n-3} + a_1\, p_{n-2} + a_2\, p_{n-1} + a_3\, p_n \\ &+ a_4\, p_{n+1} + a_5\, p_{n+2} + a_6\, p_{n+3}) \\ p_{n+3} - p_{n-3} = -s\ (&a_0\, q_{n-3} + a_1\, q_{n-2} + a_2\, q_{n-1} + a_3\, q_n \\ &+ a_4\, q_{n+1} + a_5\, q_{n+2} + a_6\, q_{n+3}) \end{aligned} \tag{12}$$

where $s = m\, h$, where m is defined in (1).

From (11) we have that:

$$\begin{aligned} q_{n+3} - q_{n-3} &= 6\, s\, p_n \\ p_{n+3} - p_{n-3} &= -6\, s\, q_n \end{aligned} \tag{13}$$

$$\begin{aligned} q_{n+2} - q_{n-2} &= 4\, s\, p_n \\ p_{n+2} - p_{n-2} &= -4\, s\, q_n \end{aligned} \tag{14}$$

$$\begin{aligned} q_{n+1} - q_{n-1} &= 2\, s\, p_n \\ p_{n+1} - p_{n-1} &= -2\, s\, q_n \end{aligned} \tag{15}$$

$$\begin{aligned} q_{n+\frac{3}{2}} - q_{n-\frac{3}{2}} &= 3\, s\, p_n \\ p_{n+\frac{3}{2}} - p_{n-\frac{3}{2}} &= -3\, s\, q_n \end{aligned} \tag{16}$$

$$\begin{aligned} q_{n+\frac{1}{2}} - q_{n-\frac{1}{2}} &= s\, p_n \\ p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}} &= -s\, q_n \end{aligned} \tag{17}$$

Considering the approximation based on the first formula of (17) for $(n+1)$-step gives (taking into account the second formula of (17)):

$$\begin{aligned} q_{n+1} + q_{n-1} &= \left(q_n + s\, p_{n+\frac{1}{2}}\right) + \left(q_n - s\, p_{n-\frac{1}{2}}\right) \\ &= 2\, q_n + s\, \left(p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}}\right) = \left(2 - s^2\right)\, q_n \end{aligned} \tag{18}$$

Similarly we have:

$$\begin{aligned} p_{n+1} + p_{n-1} &= \left(p_n - s\, q_{n+\frac{1}{2}}\right) + \left(p_n + s\, q_{n-\frac{1}{2}}\right) \\ &= 2\, p_n - s\, \left(q_{n+\frac{1}{2}} - q_{n-\frac{1}{2}}\right) = \left(2 - s^2\right)\, p_n \end{aligned} \tag{19}$$

Considering the approximation based on the first formula of (17) for $(n+2)$-step gives (taking into account the second formula of (16) and (19)):

$$\begin{aligned} q_{n+2} + q_{n-2} &= \left(q_{n+1} + s\, p_{n+\frac{3}{2}}\right) + \left(q_{n-1} - s\, p_{n-\frac{3}{2}}\right) \\ &= q_{n+1} + q_{n-1} + s\, \left(p_{n+\frac{3}{2}} - p_{n-\frac{3}{2}}\right) \\ &= \left(2 - s^2\right)\, q_n - 3\, s^2\, q_n = 2\, \left(1 - 2\, s^2\right)\, q_n \end{aligned} \tag{20}$$

Similarly we have:

$$\begin{aligned} p_{n+2} + p_{n-2} &= \left(p_{n+1} - s\, q_{n+\frac{3}{2}}\right) + \left(p_{n-1} + s\, q_{n-\frac{3}{2}}\right) \\ &= p_{n+1} + p_{n-1} - s\, \left(q_{n+\frac{3}{2}} - q_{n-\frac{3}{2}}\right) \\ &= \left(2 - s^2\right)\, p_n - 3\, s^2\, p_n = 2\, \left(1 - 2\, s^2\right)\, p_n \end{aligned} \tag{21}$$

Substituting (18–21) into (12) and considering that $a_0 = a_6$, $a_1 = a_5$ and $a_2 = a_4$ we have:

$$\begin{aligned} q_{n+3} - q_{n-3} &= s\, \left[a_0\, \left(p_{n-3} + p_{n+3}\right) + \left(2\, a_1\, \left(1 - 2\, s^2\right) + a_2\, \left(2 - s^2\right) + a_3\right)\, p_n\right] \\ p_{n+3} - p_{n-3} &= s\, \left[a_0\, \left(q_{n-3} + q_{n+3}\right) + \left(2\, a_1\, \left(1 - 2\, s^2\right) + a_2\, \left(2 - s^2\right) + a_3\right)\, q_n\right] \end{aligned}$$

and with (13) we have

$$
\begin{aligned}
q_{n+3} - q_{n-3} = s\, \Big[& a_0\ (p_{n-3} + p_{n+3}) + \Big(2\,a_1\ \Big(1 - 2\,s^2\Big) \\
& + a_2\ \Big(2 - s^2\Big) + a_3\Big)\ \frac{q_{n+3} - q_{n-3}}{6\,s}\Big] \\
p_{n+3} - p_{n-3} = s\, \Big[& a_0\ (q_{n-3} + q_{n+3}) + \Big(2\,a_1\ \Big(1 - 2\,s^2\Big) \\
& + a_2\ \Big(2 - s^2\Big) + a_3\Big)\ \Big[-\frac{p_{n+3} - p_{n-3}}{6\,s}\Big]\Big]
\end{aligned}
$$

which gives:

$$
\begin{aligned}
(q_{n+3} - q_{n-3}) \left[1 - \frac{2\,a_1\,(1 - 2\,s^2) + a_2\ (2 - s^2) + a_3}{6}\right] &= s\,a_0\ (p_{n-3} + p_{n+3}) \\
(p_{n+3} - p_{n-3}) \left[1 - \frac{2\,a_1\,(1 - 2\,s^2) + a_2\ (2 - s^2) + a_3}{6}\right] &= -s\,a_0\ (q_{n+3} + q_{n-3})
\end{aligned}
$$

The above formula in matrix form can be written as:

$$
\begin{pmatrix} T(s) & -s\,a_0 \\ s\,a_0 & T(s) \end{pmatrix} \begin{pmatrix} q_{n+3} \\ p_{n+3} \end{pmatrix} = \begin{pmatrix} T(s) & s\,a_0 \\ -s\,a_0 & T(s) \end{pmatrix} \begin{pmatrix} q_{n-3} \\ p_{n-3} \end{pmatrix}
$$

where

$$
T(s) = 1 - \frac{2\,a_1\,(1 - 2\,s^2) + a_2\ (2 - s^2) + a_3}{6} \tag{22}
$$

which is a discrete scheme of the form (10) and hence it is symplectic. □

Remark 1 Chiou and Wu in [3] have re-written open Newton–Cotes differential schemes as multilayer symplectic structures based on (11).

5 Numerical example

In this section we present some numerical results to illustrate the performance of our new methods. Consider the numerical integration of the Schrödinger equation:

$$
y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x). \tag{23}
$$

using the well-known Woods–Saxon potential (see [2,4–6,8]) which is given by

$$
V(x) = V_w(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{24}
$$

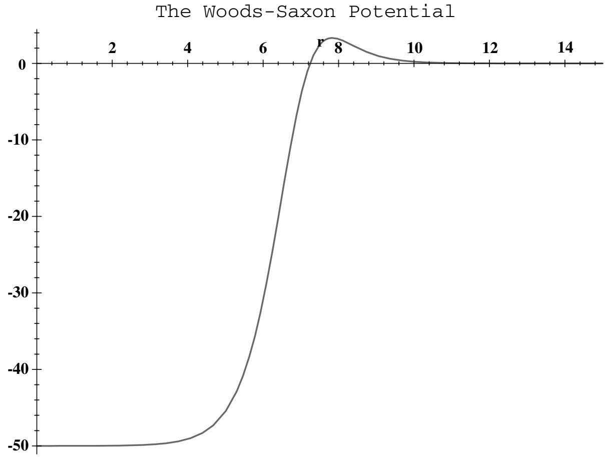

Fig. 1 The Woods–Saxon potential

with $z = \exp[(x - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$. In Fig. 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 [4,5,14]).

Many problems in chemistry, physics, physical chemistry, chemical physics, electronics etc., are expressed by Eq. 23 (see [86–89]).

5.1 Resonance problem

In the asymptotic region the Eq. 23 effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{25}$$

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 Eq. 1 has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)] \end{aligned} \tag{26}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{27}$$

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_i, $i = 1(1)5$ before starting a six-step method. From the initial condition, $y_0 = 0$. The value y_i, $i = 1(1)5$ are computed using the high order Runge–Kutta method of Prince and Dormand [80,81]. 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 (23) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods–Saxon one (24).

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 well known Numerov's method (which is indicated as Method A)
- The Explicit Numerov-Type Method developed by Chawla and Rao [77] (which is indicated as Method B)
- The P-stable Exponentially Fitted Method developed by Kalogiratou and Simos [85] (which is indicated as Method C)
- The four-step method developed by Henrici [90] (which is indicated as Method D)
- The Newton–Cotes Trigonometrically-Fitted Formula developed in [91] (which is indicated as Method E)
- The new proposed method (which is indicated as Method F)

The numerical results obtained for the six 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 NFE, where NFE are the Number of Function Evaluations.

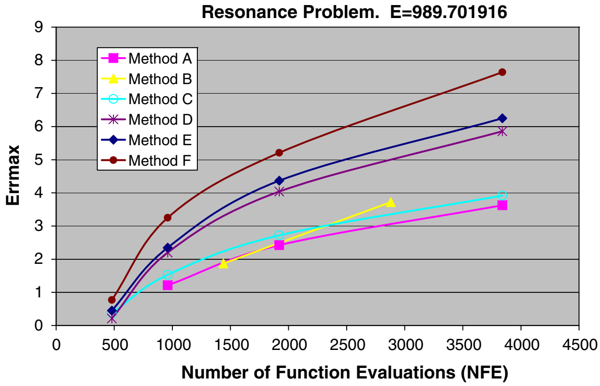

Fig. 2 Error $Errmax$ for several values of n for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of $Errmax$ indicates that for this value of n, $Errmax$ is positive

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 Explicit Numerov-Type Method developed by Chawla and Rao [77] has better behavior than the well known Numerov's method
- The P-stable Exponentially Fitted Method developed by Kalogiratou and Simos [85] has better behavior than the explicit Numerov-type method with minimal phase-lag of Chawla and Rao [77] for small number of function evaluations
- The four-step method developed by Henrici [90] has better behavior than all the previous mentioned methods
- The Newton–Cotes Trigonometrically-Fitted Formula developed in [91] has better behavior than all the above methods
- The new developed method 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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