Iranian Journal of Mathematical Sciences and Informatics
Vol. 13, No. 1 (2018), pp 111-129
DOI: 10.7508/ijmsi.2018.1.011

A New High Order Closed Newton-Cotes Trigonometrically-fitted Formulae for the Numerical Solution of the Schrödinger Equation

Ali Shokri*, Hosein Saadat, Alireza Khodadadi

Department of Mathematics, Faculty of Basic Science, University of Maragheh, P.O. Box 55181-83111, Maragheh, Iran.

E-mail: shokri@maragheh.ac.ir
E-mail: hosein67saadat@yahoo.com
E-mail: ali_reza_khodadadi@yahoo.com

Abstract. In this paper, we investigate the connection between closed Newton-Cotes formulae, trigonometrically-fitted methods, symplectic integrators and efficient integration of the Schrödinger equation. The study of multistep symplectic integrators is very poor although in the last decades several one step symplectic integrators have been produced based on symplectic geometry (see the relevant literature and the references here). In this paper, we study the closed Newton-Cotes formulae and we write them as symplectic multilayer structures. Based on the closed Newton-Cotes formulae, we also develop trigonometrically-fitted symplectic methods. An error analysis for the one-dimensional Schrödinger equation of the new developed methods and a comparison with previous developed methods is also given. We apply the new 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: Phase-lag, Schrödinger equation, Numerical solution, Newton-Cotes formulae, Derivative.

*Corresponding Author

Received 04 October 2015; Accepted 30 April 2016

2000 Mathematics subject classification: 65L05, 65L06, 65L20.

1. Introduction

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

$$\begin{aligned}\dot{q} =& mp \\ \dot{p} =& -mq\end{aligned} \tag{1.1}$$

where m is a constant scalar or matrix. The Eq. (1.1) is an important one in the field of molecular dynamics.

In order to preserve the characteristics of the Hamiltonian system in the numerical approximation, it is necessary to use symplectic integrators. In the recent years work has been done mainly in the production of one step symplectic integrators (see [1]). Zhu et al. [26] have studied the symplectic integrators and the well-known open Newton-Cotes differential methods. They have 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 [2]. The last decades much work has been done on exponential and trigonometrically fitting and the numerical solution of periodic initial value problems (see [3-20] 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.

• An error analysis for the one-dimensional Schrödinger equation of the new developed methods and a comparison with previous developed methods is also given.

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 Section 2 the results about symplectic matrices and schemes are presented. In Section 3 closed Newton-Cotes integral rules and differential methods are described and the new trigonometrically-fitted methods are developed. In Section 4 the conversion of the closed Newton-Cotes differential methods into multilayer symplectic structures is presented. The error analysis for the one-dimensional Schrödinger equation of the new developed methods and a comparison with previous developed methods is presented in Section 5. Finally, numerical results are presented in Section 6.

2. Basic Theory on Symplectic Schemes and Numerical Methods

Zhu et al. [26] have obtained a theory on symplectic numerical schemes and symplectic matrices in which the following basic theory is based.

Dividing an interval $[a, b]$ with N points we have

$$x_0 = a\,, \quad x_n = x_0 + nh = b, \quad n = 1, 2, \cdots, N \tag{2.1}$$

The above division leads to the following discrete scheme:

$$\binom{p_{n+1}}{q_{n+1}} = M_{n+1}\binom{p_n}{q_n}, \quad M_{n+1} = \begin{pmatrix} a_{n+1} & b_{n+1} \\ c_{n+1} & d_{n+1} \end{pmatrix}. \tag{2.2}$$

We note that x is the independent variable and a and b in the equation for x_0 (Eq. (2.1)) are different than the a and b in Eq. (2.2). Based on the above we can write the n-step approximation to the solution as

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

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

$$\binom{p_{n+1}}{q_{n+1}} = S\binom{p_0}{q_0}.$$

A discrete scheme (2.2) 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 (2.1) 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

$$\int_a^b f(x)\,dx \approx z\,h \sum_{i=0}^{k} t_i f(x_i) \tag{3.1}$$

k	z	t_0	t_1	t_2	t_3	t_4	t_5
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
7	7/17280	751	3577	1323	2989	2989	3577
8	4/14175	989	5888	−928	10496	−4540	10496
9	1/89600	25713	141669	9720	174096	52002	52002
10	5/299376	427368	−260550	272400	−48525	106300	16067

TABLE 1. The coefficient z and its weights t_i for $i = 1, 2, \ldots, 5$

k	z	t_6	t_7	t_8	t_9	t_{10}
0	1					
1	1/2					
2	1/3					
3	3/8					
4	2/45					
5	5/288					
6	1/140	41				
7	7/17280	3577	751			
8	4/14175	−928	5888	989		
9	1/89600	174096	9720	141669	25713	
10	5/299376	106300	−48525	272400	−260550	427368

TABLE 2. The coefficient z and its weights t_i for $i = 6, 7, \ldots, 10$

Where

$$h = \frac{b-a}{N}, \quad x_i = a + ih, \quad i = 0, 1, 2, \ldots, N. \tag{3.2}$$

The coefficient z as well as the weights t_i are given in Tables 1,2. From tables 1 and 2 it is easy to see that the coefficients t_i are symmetric, i.e., we have the following relation:

$$t_i = t_{k-i}, \quad i = 0, 1, \ldots, \frac{k}{2}. \tag{3.3}$$

Closed Newton-Cotes differential methods were produced from the integral rules. For Table 1 we have the following differential methods:

$$
\begin{aligned}
&k=1 \qquad y_{n+1}-y_n=\frac{h}{2}(f_{n+1}+f_n)\\
&k=2 \qquad y_{n+1}-y_{n-1}=\frac{h}{3}(f_{n-1}+4f_n+f_{n+1})\\
&k=3 \qquad y_{n+1}-y_{n-2}=\frac{3h}{8}(f_{n-2}+3f_{n-1}+3f_n+f_{n+1})\\
&k=4 \qquad y_{n+2}-y_{n-2}=\frac{2h}{45}(7f_{n-2}+32f_{n-1}+12f_n+32f_{n+1}+f_{n+2})\\
&k=5 \qquad y_{n+2}-y_{n-3}=\frac{h}{140}(19f_{n-3}+75f_{n-2}+50f_{n-1}+50f_n+75f_{n+1}+19f_{n+2})\\
&\quad\vdots \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.4)\\
&k=10 \quad y_{n+5}-y_{n-5} = \frac{5h}{299376}(427368f_n-260550\left(f_{n+1}+f_{n-1}\right)\\
&\qquad\qquad +272400\left(f_{n+2}+f_{n-2}\right)-48525\left(f_{n+3}+f_{n-3}\right)\\
&\qquad\qquad +106300\left(f_{n+4}+f_{n-4}\right)+16067\left(f_{n+5}+f_{n-5}\right))
\end{aligned}
$$

In the present paper we will investigate the case $k = 10$ and we will produce trigonometrically-fitted differential methods of order 12.

3.2. **Trigonometrically-fitted closed Newton-Cotes differential method.** Requiring the differential scheme

$$y_{n+5}-y_{n-5}=h\left(b_0f_n+\sum_{i=1}^{5}b_i\left(f_{n+i}+f_{n-i}\right)\right) \qquad (3.5)$$

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

$$\{1,x,x^2,x^3,x^4,x^5,x^6,x^7,x^8,x^9,\cos(\omega h),\sin(\omega h)\} \qquad (3.6)$$

the following set of equations is obtained:

$$
\begin{aligned}
&2\,b_1+2\,b_2+2\,b_3+2\,b_4+2\,b_5+b_0=10\\
&6\,b_1+24\,b_2+54\,b_3+96\,b_4+150\,b_5=250\\
&2560\,b_4+810\,b_3+160\,b_2+6250\,b_5+10\,b_1=6250\\
&10206\,b_3+57344\,b_4+14\,b_1+218750\,b_5+896\,b_2=156250\\
&118098\,b_3+4608\,b_2+1179648\,b_4+7031250\,b_5+18\,b_1=3906250\\
&-24\,\sin(v)\left(\cos(v)\right)^2+2\sin(v)+32\sin(v)\left(\cos(v)\right)^4-2b_4v-b_0v\\
&-8\left(\cos\left(v\right)\right)^3b_3v-32\,b_5v\left(\cos\left(v\right)\right)^5\\
&-16\,b_4v\left(\cos\left(v\right)\right)^4+40\,\left(\cos\left(v\right)\right)^3b_5v-10\,\cos\left(v\right)b_5v-4\,\left(\cos\left(v\right)\right)^2b_2v\\
&+16\,\left(\cos\left(v\right)\right)^2b_4v+6\,\cos\left(v\right)b_3v-2\,b_1\cos\left(v\right)v+2\,b_2v=0
\end{aligned}
\qquad (3.7)
$$

Solving the above system of equations we obtain

$$b_0 = \frac{1}{2268}\frac{a_0}{T} \qquad b_1 = \frac{1}{4536}\frac{a_1}{T}, \qquad b_2 = \frac{1}{1134}\frac{a_2}{T},$$
$$b_3 = \frac{1}{9072}\frac{a_3}{T}, \qquad b_4 = \frac{1}{9072}\frac{a_4}{T}, \qquad b_5 = \frac{1}{9072}\frac{a_5}{T},$$

where

$$\begin{aligned} a_0 &= 169555v\cos^5(v) + (426400v - 571536\sin(v))\cos^4(v) \\ &\quad -145625v\cos^3(v) + (-344200v + 428652\sin(v))\cos^2(v) \\ &\quad +60275v\cos(v) - 35721\sin(v) + 12200v, \end{aligned}$$

$$\begin{aligned} a_1 &= -275350v\cos^5(v) + (-746875v + 952560\sin(v))(\cos(v))^4 \\ &\quad +315125v(\cos(v))^3 + (501250v - 714420\sin(v))(\cos(v))^2 \\ &\quad -64250v\cos(v) + 59535\sin(v) - 27575v, \end{aligned}$$

$$\begin{aligned} a_2 &= 41675v\cos^5(v) + (95000v - 136080\sin(v))\cos^4(v) \\ &\quad -21625v\cos^3(v) + (-95000v + 102060\sin(v))\cos^2(v) \\ &\quad +20875v\cos(v) - 8505\sin(v) + 1600v, \end{aligned}$$

$$\begin{aligned} a_3 &= -116900v\cos^5(v) + (-325625v + 408240\sin(v))\cos^4(v) \\ &\quad +146125v\cos^3(v) + (203750v - 306180\sin(v))\cos^2(v) \\ &\quad -22000v\cos(v) - 12925v + 25515\sin(v), \end{aligned}$$

$$\begin{aligned} a_4 &= 20225v\cos^5(v) - 45360\sin(v)\cos^4(v) + 56125v\cos^3(v) \\ &\quad + (-95000v + 34020\sin(v))\cos^2(v) + 38625v\cos(v) \\ &\quad -5800v - 2835\sin(v), \end{aligned}$$

$$\begin{aligned} a_5 &= (-20225v + 9072\sin(v))\cos^4(v) + 29225v\cos^3(v) \\ &\quad + (-21450v - 6804\sin(v))\cos^2(v) + 12500v\cos(v) \\ &\quad -2885v + 567\sin(v), \end{aligned}$$

and

$$T = v(\cos(v) - 1)^5.$$

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

$$\begin{aligned} b_0 &= \frac{89035}{12474} - \frac{673175}{648648}v^2 + \frac{19375}{2594592}v^4 + \frac{395515}{264648384}v^6 \\ &\quad + \frac{173704325}{2534272925184}v^8 + \frac{104265059}{557540043540480}v^{10} + \frac{1839935}{115700039110656}v^{12} \\ &\quad - \frac{14814979111}{8401905440137617408}v^{14} - \frac{19367733685}{134430487042201878528}v^{16} + \cdots, \end{aligned}$$

$$
\begin{aligned}
b_1 \quad = \quad & -\frac{24125}{5544} + \frac{3365875}{3891888}v^2 - \frac{96875}{15567552}v^4 - \frac{1977575}{1587890304}v^6 \\
& - \frac{868521625}{15205637551104}v^8 - \frac{521325295}{334524026124288}v^{10} - \frac{9199675}{694200234663936}v^{12} \\
& + \frac{74074895555}{5041143264082570448}v^{14} + \frac{96838668425}{806582922253211271168}v^{16} + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
b_2 \quad = \quad & \frac{28375}{6237} - \frac{3365875}{6810804}v^2 + \frac{96875}{27243216}v^4 + \frac{1977575}{2778808032}v^6 \\
& + \frac{868521625}{26609865714432}v^8 + \frac{521325295}{585417045717504}v^{10} + \frac{9199675}{1214850410661888}v^{12} \\
& - \frac{74074895555}{8822000712144498 2784}v^{14} - \frac{96838668425}{1411520113943119724544}v^{16} + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
b_3 \quad = \quad & -\frac{80875}{99792} + \frac{3365875}{18162144}v^2 - \frac{96875}{72648576}v^4 - \frac{1977575}{7410154752}v^6 \\
& - \frac{868521625}{70959641905152}v^8 - \frac{521325295}{1561112121913344}v^{10} - \frac{9199675}{3239601095098368}v^{12} \\
& + \frac{74074895555}{23525335232385328 7424}v^{14} + \frac{96838668425}{3764053637181652598784}v^{16} + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
b_4 \quad = \quad & \frac{132875}{74844} - \frac{3365875}{81729648}v^2 + \frac{96875}{326918592}v^4 + \frac{1977575}{33345696384}v^6 \\
& + \frac{868521625}{319318388573184}v^8 + \frac{521325295}{7025004548610048}v^{10} + \frac{9199675}{14578204927942656}v^{12} \\
& - \frac{74074895555}{105864008545733979 3408}v^{14} - \frac{96838668425}{16938241367317436694528}v^{16} + \cdots ,
\end{aligned}
$$

$$
\begin{aligned}
b_5 \quad = \quad & \frac{80335}{299376} + \frac{673175}{163459296}v^2 - \frac{19375}{653837184}v^4 - \frac{395515}{66691392768}v^6 \\
& - \frac{173704325}{638636777146368}v^8 - \frac{104265059}{14050009097220096}v^{10} - \frac{1839935}{29156409855885312}v^{12} \\
& + \frac{14814979111}{21172801709146795 86816}v^{14} + \frac{19367733685}{33876482734634873389056}v^{16} + \cdots .
\end{aligned}
$$

The local truncation error for the above differential method is given by

$$
LTE = -\frac{673175}{163459296} \left({y_n}^{(13)} + \omega^2 {y_n}^{(11)} \right) h^{13}. \tag{3.8}
$$

4. Closed Newton-Cotes Can be Expressed as Symplectic Integrators

Theorem 4.1. *A discrete scheme of the form*

$$
\begin{pmatrix} b & -a \\ a & b \end{pmatrix} \begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix}, \tag{4.1}
$$

is symplectic.

FIGURE 1. Behavior of the coefficients b_0 and b_1 of the new method.

FIGURE 2. Behavior of the coefficients b_2 and b_3 of the new method.

FIGURE 3. Behavior of the coefficients b_4 and b_5 of the new method.

Proof. We rewrite (2.3) 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. The symplectic structure of the well-known second order differential scheme (SOD) has been proven in [26] by Zhu et al.

$$y_{n+i} - y_{n-i} = 2ihf_n \quad i = 1(1)5 \tag{4.2}$$

The above methods have been produced by the simplest open Newton-Cotes integral formula. Based on the paper Chiou et al. [2], the closed Newton-Cotes differential schemes will be written as multilayer symplectic structures. If we apply the Newton-Cotes differential formula for $n = 5$ to the linear Hamiltonian system (1.1) we obtain

$$\begin{aligned} q_{n+5} - q_{n-5} =& s\left(b_0 p_n + \sum_{i=1}^{5} b_i \left(p_{n+i} + p_{n-i}\right)\right), \\ p_{n+5} - p_{n-5} =& s\left(b_0 q_n + \sum_{i=1}^{5} b_i \left(q_{n+i} + q_{n-i}\right)\right) \end{aligned} \tag{4.3}$$

where $s = mh$, where m is defined in (1). From (3.4) we have

$$\begin{aligned} q_{n+j} - q_{n-j} =& 2\,j\,s\,p_n\,, \\ p_{n+j} - p_{n-j} =& -2\,j\,s\,q_n\,,\ j = 1(1)5\,,\ \text{or}\ j = \frac{1}{2}(1)\frac{5}{2}. \end{aligned} \tag{4.4}$$

Considering the approximation based on the first formula of (4.1) for $(n+1)$-step gives (taking into account the second formula of (4.1))

$$\begin{aligned} q_{n+i} + q_{n-j} &= \left(q_n + sp_{n+i-\frac{1}{2}}\right) + \left(q_n - sp_{n-i+\frac{1}{2}}\right) \\ &= q_{n+i-1} + q_{n-i+1} + s\left(p_{n+i-\frac{1}{2}} - p_{n-i+\frac{1}{2}}\right) \\ &= (2 - i^2 s^2) q_n. \end{aligned} \tag{4.5}$$

Substituting (4.2)-(4.5) into (3.5) and considering that $b_i = b_{5-i}$, $i = 0(1)4$, we have

$$\begin{aligned} q_{n+5} - q_{n-5} &= s\Big[b_5(p_{n-5} + p_{n+5}) + \big(b_4(2 - 4^2 s^2) + b_3(2 - 3^2 s^2) \\ &\quad + b_2(2 - 2^2 s^2) + b_1(2 - s^2) + b_0\big)p_n\Big], \end{aligned} \tag{4.6}$$

$$
\begin{aligned}
p_{n+5}-p_{n-5} &= s\Big[b_5(q_{n-5}+q_{n+5})+\big(b_4(2-4^2s^2)+b_3(2-3^2s^2)\\
&\quad +b_2(2-2^2s^2)+b_1(2-s^2)+b_0\big)q_n\Big],
\end{aligned}
$$

and with (3.6) we have

$$
\begin{aligned}
q_{n+5}-q_{n-5} &= s\Big[b_5(p_{n-5}+p_{n+5})+\big(b_4(2-4^2s^2)+b_3(2-3^2s^2)\\
&\quad +b_2(2-2^2s^2)+b_1(2-s^2)+b_0\big)\frac{q_{n+5}-q_{n-5}}{10\,s}\Big],\\
p_{n+5}-p_{n-5} &= s\Big[b_5(q_{n-5}+q_{n+5})+\big(b_4(2-4^2s^2)+b_3(2-3^2s^2)\\
&\quad +b_2(2-2^2s^2)+b_1(2-s^2)+b_0\big)\frac{p_{n+5}-p_{n-5}}{10\,s}\Big],
\end{aligned}
$$

which gives

$$
\begin{aligned}
(q_{n+5}-q_{n-5}).A &= s\,b_0(p_{n+5}+p_{n-5}),\\
(p_{n+5}-p_{n-5}).B &= s\,b_0(q_{n+5}+q_{n-5}).
\end{aligned}
$$

where

$$A=1-\frac{b_4(2-4^2s^2)+b_3(2-3^2s^2)+b_2(2-2^2s^2)+b_1(2-s^2)+b_0}{10},$$

and

$$B=1-\frac{b_4(2-4^2s^2)+b_3(2-3^2s^2)+b_2(2-2^2s^2)+b_1(2-s^2)+b_0}{10}.$$

The above formula in matrix form can be written as

$$\begin{pmatrix} T(s) & -s\,b_5\\ s\,b_5 & T(s)\end{pmatrix}\begin{pmatrix} q_{n+5}\\ p_{n+5}\end{pmatrix}=\begin{pmatrix} T(s) & s\,b_5\\ -s\,b_5 & T(s)\end{pmatrix}\begin{pmatrix} q_{n-5}\\ p_{n-5}\end{pmatrix}$$

where

$$T(s)=1-\frac{b_4(2-4^2s^2)+b_3(2-3^2s^2)+b_2(2-2^2s^2)+b_1(2-s^2)+b_0}{10} \tag{4.7}$$

which is a discrete scheme of the form (3.3) and hence it is symplectic. □

5. Error Analysis for the Radial Schrödinger Equation

In this section, we will investigate theoretically the methods constructed in [21, 22, 23, 24, 25] and in this paper. The scope of this investigation is to find a quantitative estimation for the extent of the accuracy gain to be expected from the exponentially-fitted versions.

Definition 5.1. A method is called classical if it has constant coefficients.

Remark 5.2. A trigonometrically-fitted method is not a classical one because it has coefficients which are dependent on the quantity $v=\omega\,h$, where w is the frequency of the problem and h is the step length of the integration.

Consider the radial Schrödinger equation

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - k^2 \right) y(x) = f(x)y(x). \tag{5.1}$$

where $f(x) = U(x) - k^2$ and $U(x) = l(l+1)/x^2 + V(x)$. We write $f(x)$ in (5.1) in the form

$$f(x) = g(x) + d, \tag{5.2}$$

where $g(x) = U(x) - U_c = g$, where U_c is the constant approximation of the potential and $G = v^2 = U_c - E$.

So, $g(x)$ depends on the potential and the constant approximation of the potential while d shows the energy dependence. We will compare the following methods:

- The classical fourth order closed Newton-Cotes formulae (Method I).
- The classical sixth order closed Newton-Cotes formulae (Method II).
- The classical eighth order closed Newton-Cotes formulae (Method III).
- The closed Newton-Cotes formulae developed in [21] (Method IV).
- The closed Newton-Cotes formulae developed in [19] (Method V).
- The closed Newton-Cotes formulae developed in [23] (Method VI).
- The classical tenth order closed Newton-Cotes formulae (Method VII)
- The closed Newton-Cotes formulae developed in the paragraph 3.2, in [22] (Method VIII).
- The closed Newton-Cotes formulae developed in the paragraph 3.3 in [22] (Method IX).
- The closed Newton-Cotes formulae developed in this paper (Method X).

We now present the formulae of the local truncation error (LTE) for the above methods.

For the Method I is equal to:

$$LTE_{MI} = -\frac{h^5}{90} y_n^{(5)}.$$

For the Method II is equal to:

$$LTE_{MII} = -\frac{8h^5}{945} y_n^{(7)}.$$

For the Method III is equal to:

$$LTE_{MIII} = -\frac{9h^9}{1400} y_n^{(9)}.$$

For the Method IV is equal to:

$$LTE_{MIV} = -\frac{8h^9}{945} (y_n^{(7)} + v^2 y_n^{(5)}).$$

For the Method V is equal to:

$$LTE_{MV} = -\frac{h^5}{90} (y_n^{(5)} + v^2 y_n^{(3)}).$$

For the Method VI is equal to:

$$LTE_{MVI} = -\frac{9h^5}{1400}(y_n^{(9)} + 3v^2 y_n^{(7)} + 3v^4 y_n^{(5)} + v^6 y_n^{(3)}).$$

For the Method VII is equal to:

$$LTE_{MVII} = -\frac{2368}{467775} y_n^{(11)} h^{11}.$$

For the Method VIII is equal to:

$$LTE_{MVIII} = -\frac{2368}{467775}\left(y_n^{(11)} + 2\nu^2 y_n^{(9)} + \nu^4 y_n^{(7)}\right) h^{11}.$$

For the Method IX is equal to:

$$LTE_{MIX} = -\frac{2368}{467775}\left(y_n^{(11)} + 5\nu^2 y_n^{(9)} + 4\nu^4 y_n^{(7)}\right) h^{11}.$$

For the new Method (Method X) is equal to:

$$LTE_{MX} = -\frac{673175}{163459296}\left(y_n^{(13)} + v^2 y_n^{(11)}\right) h^{13}.$$

We express, now, the derivatives $y^{(2)}$, $y^{(4)}$, $\ldots$ and $y^{(13)}$ in terms of Eq. (5.1), ie.

$$\begin{aligned}
y_n^{(2)} &= f(x).y(x),\\
y_n^{(3)} &= \left(\frac{d}{dx}g(x)\right)y(x) + (g(x)+d)\frac{d}{dx}y(x)\\
y_n^{(5)} &= \left(\frac{d^3}{dx^3}g(x)\right)y(x) + 3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}y(x),\\
&+3\left(\frac{d}{dx}g(x)\right)\frac{d^2}{dx^2}y(x) + (g(x)+d)\frac{d^3}{dx^3}y(x),
\end{aligned} \tag{5.3}$$

and etc. We note that $g^{(n)} = U^{(n)}(x)$ for the n-th order derivative with respect to x. Introducing the expressions obtained in (5.3) into the Local Truncation Error of the methods mentioned above, we obtain the expressions (as polynomials of d) for local truncation error of the methods. The leading terms (in d) of the above expressions are given by:

For the Method I is equal to:

$$LTE_{MI} = h^5 d^2\left(-\frac{1}{90}\frac{d}{dx}y(x)\right).$$

For the Method II is equal to:

$$LTE_{MII} = h^7 d^3\left(-\frac{8}{945}\frac{d}{dx}y(x)\right).$$

For the Method III is equal to:

$$LTE_{MIII} = h^9 d^4\left(-\frac{9}{1400}\frac{d}{dx}y(x)\right).$$

For the Method IV is equal to:

$$LTE_{MIV} = -\frac{8}{945}\left(g(x)\frac{d}{dx}y(x) + 5\left(\frac{d}{dx}g(x)\right)y(x)\right)h^9 d^2.$$

For the Method V is equal to:

$$LTE_{MV} = -\frac{1}{90}\left(\left(\frac{d}{dx}y(x)\right)g(x) + 3\left(\frac{d}{dx}g(x)\right)y(x)\right)h^9 d.$$

For the Method VI is equal to:

$$\begin{aligned} LTE_{MVI} &= -\frac{9}{700}\left(3\left(\frac{d}{dx}g(x)\right)y(x)g(x) + 8\left(\frac{d^3}{dx^3}g(x)\right)y(x)\right. \\ &\quad \left. +2\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}y(x)\right)h^9 d^2. \end{aligned}$$

For the Method VII is equal to:

$$LTE_{MVII} = h^{11}d^5\left(-\frac{2368}{467775}\frac{d}{dx}y(x)\right).$$

For the Method VIII is equal to:

$$LTE_{MVIII} = h^{11}d^4\left(-\frac{4736}{467775}y(x)\frac{d}{dx}g(x)\right).$$

For the Method IX is equal to:

$$LTE_{MIX} = \frac{2368}{155925}h^{11}d^4\left(\frac{19}{3}\left(\frac{d}{dx}g(x)\right)y(x) + \left(\frac{d}{dx}y(x)\right)g(x)\right).$$

For the Method X is equal to:

$$LTE_{MX} = -\frac{673175}{163459296}\left(g(x)\frac{d}{dx}y(x) + 11\left(\frac{d}{dx}g(x)\right)y(x)\right)h^{13}d^5.$$

From the above equations we have the following theorem:

Theorem 5.3. *For the Closed Newton-Cotes formulae studied in this paper we have:*

- ***Fourth Algebraic Order Methods***

  In the fourth algebraic order method MI the error increases as the second power of d, while in the fourth algebraic order method MV the the error increases as the first power of d. So, for the numerical solution of the time independent radial Schrödinger equation the Method MV is more accurate, especially for large values of d.

- ***Sixth Algebraic Order Methods***

  In the sixth algebraic order method MII the error increases as the third power of d, while in the sixth algebraic order method MIV the the error increases as the second power of d. So, for the numerical solution of the time independent radial Schrödinger equation the Method MIV is more accurate, especially for large values of d.

- ***Eighth Algebraic Order Methods***

  In the eighth algebraic order method MIII the error increases as the fourth power of d, while in the eighth algebraic order method MVI the the error increases as the second power of d. So, for the numerical solution of the time independent radial Schrödinger equation new Method MVI is more accurate, especially for large values of d.

- ***Tenth Algebraic Order Methods***

  In the tenth algebraic order method MVII the error increases as the fifth power of d, while in the tenth algebraic order methods MVIII and MIX the the error increases as the fourth power of d. The coefficient of the fourth power of d in the Method MVIII is much lower than the coefficient of the fourth power of d in the Method MIX. So, for the numerical solution of the time independent radial Schrödinger equation new Methods MVIII is the most accurate one, especially for large values of d.

- ***Twelfth Algebraic Order Methods***

  In the twelfth algebraic order method MX the error increases as the fifth power of d. So, for the numerical solution of the time independent radial Schrödinger equation new Methods MX is the most accurate one, especially for large values of d.

6. Numerical Results

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

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - k^2\right) y(x), \tag{6.1}$$

using the well-known Woods-Saxon potential which is given by

$$V(x) = V_w = \frac{u_0}{1+z} - \frac{u_0 z}{a(1+z)^2}, \tag{6.2}$$

with $z = \exp[(x - R_0)/a]$, $u_0 = -50$, $a = 0.6$, and $R_0 = 7.0$. In Fig. 2, 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. Many problems in chemistry, physics, physical chemistry, chemical physics, electronics etc., are expressed by Eq. (6.1).

6.1. **Resonance problem.** In the case of positive energies, $E = k^2$, the potential dies away faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation

FIGURE 4. The Woods - Saxon potential.

effectively reduces to

$$y''(x) = \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x), \tag{6.3}$$

for x greater than some value X. The last equation has two linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. (6.1) has When $(x \to \infty)$ the solution takes the asymptotic form

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D\,[\sin(k\,x - \pi l/2) + \tan(\delta_{\,l})\cos(kx - \pi l/2)], \end{aligned}$$

where $\delta_{\,l}$ is called *scattering phase shift* that may be calculated from the formula

$$\tan(\delta_{\,l}) = \frac{y(x_{\,i})\,S(x_{\,i+1}) - y(x_{\,i+1})\,S(x_{\,i})}{y(x_{\,i+1})\,C(x_{\,i}) - y(x_{\,i},)\,C(x_{\,i+1})} \tag{6.4}$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right-hand end point of the interval of integration and $x_2 = x_1 - h$)with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need y_0 before starting a eight-step method. From the initial condition we obtain y_0. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l from the above relation.

6.1.1. *The woods-saxon potential.* As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (6.1) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods-Saxon one (6.2). 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 [1]. The boundary conditions for this problem are:

$$y(0) = 0, \quad y(x) \approx \cos(\sqrt{E}x), \quad \text{for large } x. \tag{6.5}$$

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 exponentially-fitted method of Raptis and Allison [11] (which is indicated as Method B).
- The P-stable exponentially-fitted Method developed by Kalogiratou and Simos [6] (which is indicated as Method C)
- The four-step method developed by Henrici [3] (which is indicated as Method D).
- The Newton-Cotes trigonometrically-fitted formula developed in [20] (which is indicated as Method E).
- The Newton-Cotes trigonometrically-fitted formula developed in [23] (which is indicated as Method F).
- The Newton-Cotes trigonometrically-fitted formula developed in [24] (which is indicated as Method G).
- The Newton-Cotes exponentially-fitted method developed in [22] (which is indicated as Method H).
- The Newton-Cotes trigonometrically-fitted method developed in [22] (which is indicated as Method I).
- The new proposed trigonometrically-fitted method (which is indicated as Method J).

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 , 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.

7. Conclusions

In this paper a new high order closed Newton-Cotes differential method for the numerical solution of the Schrödinger type equations is introduced.

From the numerical results we have the following remarks:

FIGURE 5. Error Errmax for several values of n for the eigenvalue $E_1 = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

- The Numerovs method and the exponentially-fitted method of Raptis and Allison [11] have better behavior than the P-stable exponentially-fitted method developed by Kalogiratou and Simos [6].
- The exponentially-fitted method of Raptis and Allison [11] is more efficient than the well known Numerov method.
- The four-step method developed by Henrici [3] has better behavior than all the previous mentioned methods. The Newton-Cotes trigonometrically-fitted formula developed in [20] has better behavior than all the above methods.
- The Newton-Cotes trigonometrically-fitted formula developed in [22] is more efficient than all the above methods. The behavior of the Newton-Cotes trigonometrically-fitted formula developed in [24] is better than all the above methods.
- The new proposed trigonometrically-fitted method is more efficient than all the above methods.
- Finally, the new developed exponentially-fitted method is the most efficient one.

Remark 7.1. As the theoretical and numerical results show us, for the development of numerical methods for the approximate solution of the radial Schrödinger equation, the exponentially-fitted methodology gives much more efficient methods than the trigonometrically-fitted methodology.

Acknowledgments

The authors wish to thank the anonymous referees for their careful reading of the manuscript and their fruitful comments and suggestions.

References

1. Z.A. Anastassi, T.E., Simos, Trigonometrically-fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, **37**(3), (2005), 281-293.
2. J. C. Chiou, S. D. Wu, Open Newton-Cotes differential methods as multilayer symplectic integrators, *Journal of Chemical Physics*, **107**, (1997), 6894-6897.
3. P. Henrici, *Discrete Variable Methods in Ordinary Differential Equations*, Wiley, New York, 1962.
4. M.K. Jain, R.K. Jain, U.A. Krishnaiah, Obrechkoff methods for periodic initial value problems of second order differential equations, *Journal of Mathematical Physics*, **15**, (1981), 239-250.
5. B. Jazbi , M. Moini, Application of Hes homotopy perturbation method for Schrödinger equation, *Iranian Journal of Mathematical Sciences and Informatics*, **3**(2), (2008), 13-19.
6. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation, *Applied Mathematics and Computations*, **112**, (2000), 99-112.
7. J.D. Lambert, *Numerical methods for ordinary differential systems*, The initial value problem, John Wiley and Sons, 1991.
8. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial value problems, *Journal of the Institute of Mathematics and its Applications*, **18**, (1976), 189-202.
9. P. Mokhtary, S.M. Hosseini, Some implementation aspects of the general linear methods withinherent Runge-Kutta stability, *Iranian Journal of Mathematical Sciences and Informatics*, **3**(1), (2008), 63-76.
10. G. D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits, The Astro, *The Astronomical Journal*, **100**(5), (1990), 1694-1700.
11. A. D. Raptis, A. C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation, *Journal of Computer Physics Communications*, **14**, (1978), 1-5.
12. A. Shokri, An explicit trigonometrically fitted ten-step method with phase-lag of order infinity for the numerical solution of radial Schrödinger equation, *Applied and Computational Mathematics*, **14**(1), (2015), 63-74.
13. A. Shokri, The symmetric two-step P-stable nonlinear predictor-corrector methods for the numerical solution of second order initial value problems, *Bulletin of the Iranian Mathematical Society*, **41**(1), (2015), 191-205.
14. A. Shokri, A.A. Shokri, S. Mostafavi, H. Saadat, Trigonometrically fitted two-step Obrechkoff methods for the numerical solution of periodic initial value problems, *Iranian Journal of Mathematical Chemistry*, **6**(2), (2015), 145-161.
15. A. Shokri, H. Saadat, Trigonometrically fitted high-order predictor-corrector method with phase-lag of order infinity for the numerical solution of radial Schrödinger equation, *Journal of Mathematical Chemistry*, **52**(7), (2014), 1870-1894.
16. A. Shokri, H. Saadat, High phase-lag order trigonometrically fitted two-step Obrechkoff methods for the numerical solution of periodic initial value problems, *Numerical Algorithms*, **68**, (2015), 337-354.

17. A. Shokri, A. A. Shokri, The new class of implicit L-stable hybrid Obrechkoff method for the numerical solution of first order initial value problems, *Journal of Computer Physics Communications*, **184**, (2013), 529-531.
18. T. E. Simos, Accurately closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation, *International Journal of Modern Physics C*, **24**(3), (2013).
19. T. E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems, *Revista Mexicana de Astronomia y Astrofysica*, **42**(2), (2006), 167-177.
20. T. E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high-order for long-time integration of orbital problems, *Applied Mathematical Letters*, **22** (10), (2009), 1616-1621.
21. T. E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration, *International Journal of Modern Physics C*, **14** (8), (2003), 1061-1074.
22. T. E. Simos, High order closed Newton-Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation, *Journal of Mathematical Chemistry*, **50** (5), (2012), 1224-1261.
23. T. E. Simos, High-order closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems, *Journal of Computer Physics Communications*, **178**(3), (2008), 199-207.
24. T. E. Simos, High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation, *Applied Mathematics and Computation*, 209 (1), (2009), 137-151.
25. T. E. Simos, New closed Newton-Cotes type formulae as multilayer symplectic integrators, *Journal of Chemical Physics*, **133** (10), (2010), 104-108.
26. W. Zhu, X. Zhao, Y. Tang, Numerical methods with a high order of accuracy in the quantum system, *Journal of Chemical Physics*, **104**, (1996) 2275-2286.