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ORIGINAL PAPER

New open modified trigonometrically-fitted Newton-Cotes type multilayer symplectic integrators for the numerical solution of the Schrödinger equation

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Abstract In this paper we present new modified open Newton Cotes integrators and we develop a new modified trigonometrically-fitted open Newton-Cotes method. We study the connection between the new proposed schemes, the differential methods and the symplectic integrators. although The research on multistep symplectic integrators is very poor, although, much research has been done on one step symplectic integrators and several of then have obtained based on symplectic geometry. In this paper a new open modified numerical algorithm of Newton-Cotes type is produced. We present the new obtained method as symplectic multilayer integrator. The new obtained symplectic schemes are applied for the solution of the resonance problem of the radial Schrödinger Equation. The results show the efficiency of the new proposed algorithm.

Keywords Numerical methods · Open Newton-Cotes differential methods · Symplectic integrators · Multistep methods · Trigonometric fitting · Energy preservation

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1 Introduction

The last decades an extended study on the numerical solution of Ordinary Differential Equations (ODEs) with special properties (see [1–68] and references therein) has been done. More recently the investigation of the development of numerical integration methods for ODEs that preserve qualitative properties of the analytic solution was of great interest (see [69] and references therein).

The development of one step symplectic integrators (see [69]) was the subject of great activity the last decades. On multistep symplectic integrators we refer on Zhu et al. [70] and on Chiou and Wu [71] who obtained multistep symplectic integrators by writing Open Newton-Cotes differential schemes as multilayer symplectic structures. More recently Simos et al. (see [35–41]) have developed classical closed Newton-Cotes of low and high order as multilayer symplectic integrators. Van den Berghe and Van Van Daele [44] have developed exponentially-fitted open Newton-Cotes differential methods and they expressed them as multilayer symplectic structures. Simos [43] has developed a new modified exponentially-fitted closed Newton-Cotes differential method which is much more efficient than the corresponding closed or open Newton-Cotes differential methods and exponentially-fitted Newton-Cotes differential methods. In the same paper Simos has proved that all closed Newton-Cotes differential schemes can be written as multilayer symplectic structures.

In the present paper

1. We will introduce the modified open Newton-Cotes type differential methods. We note that closed forms of these methods are first introduced in [72].
2. We will develop the new modified trigonometrically-fitted open Newton-Cotes method.
3. We will also express the new modified trigonometrically-fitted open Newton-Cotes method as multilayer symplectic integrator and
4. Finally, we will apply the new modified trigonometrically-fitted open Newton-Cotes method to the radial Schrödinger equation in order to examine the efficiency of the new obtained method.

We note that since the new proposed methods are of explicit form, can very easily be applied to non-linear differential equations as well as linear ones.

The paper is constructed as follows:

– The new modified open trigonometrically-fitted Newton-Cotes method is developed in Sect. 2.
– In Sect. 3 results about symplectic matrices and schemes are presented and we present the conversion of the new modified open Newton-Cotes type differential method into multilayer symplectic structure
– Numerical results are presented in Sect. 4.
– Finally, in Sect. 5 conclusions are given.

2 The new modified open Newton-Cotes differential methods

Consider the differential scheme:

$$\varphi_{n+2} - \varphi_{n-2} = h\Big(a_0\,\upsilon_{n-1} + a_1\,\upsilon_n + a_2\,\upsilon_{n+1}\Big) + h^2\Big(b_0\,\vartheta_{n-1} + b_1\,\vartheta_n + b_2\,\vartheta_{n+1}\Big) \tag{1}$$

where $\upsilon_i = \varphi_i'$, $i = n-1, n, n+1$ and $\vartheta_i = \varphi_i''$, $i = n-1, n, n+1$

It is important to be observed that the numerical scheme (1) only can be derived by using an integral rule based on the Hermite interpolation polynomial with equidistant nodes whereas the Newton-Cotes integral rules are obtained by using the Lagrange interpolation polynomial with equidistant nodes whereas.

Requiring the above differential scheme to be accurate for the following set of functions (we note that $\upsilon_i = \varphi_i'$, $i = n-1, n, n+1$ and $\vartheta_i = \varphi_i''$, $i = n-1, n, n+1$):

$$\{1,\ t,\ t^2,\ \cos(w\,t),\ \sin(w\,t),\ x\,\cos(w\,t),\ x\,\sin(w\,t)\} \tag{2}$$

the following set of equations is obtained:

$$\begin{aligned}
0 &= w\,h[-h\,b_2\,w\,\cos(w\,h) - h\,b_1\,w - \cos(w\,h)\,h\,b_0\,w \\
&\quad - \sin(w\,h)\,a_2 + \sin(w\,h)\,a_0] \\
4\,\cos(w\,h)\,\sin(w\,h) &= w\,h\,[a_2\cos(w\,h) + a_1 + \cos(w\,h)\,a_0 \\
&\quad - \sin(w\,h)\,h\,b_2\,w + \sin(w\,h)\,h\,b_0 w] \\
4 &= a_2 + a_1 + a_0 \\
4\,h[2\,(\cos(w\,h))^2 - 1] &= -h[h\,b_1\,t\,w^2 + h\,b_2\,w^2\,t\,\cos(w\,h) \\
&\quad + w^2\,h^2\,b_2\,\cos(w\,h) - w^2\,h^2\,\cos(w\,h)\,b_0 + w\,h\sin(w\,h)\,a_2 \\
&\quad + w\,h\sin(w\,h)\,a_0 - a_2\cos(w\,h) + 2\,\sin(w\,h)\,h\,b_2\,w - 2\,\sin(w\,h)\,h\,b_0\,w \\
&\quad - \cos(w\,h)\,a_0 - a_1 + \cos(w\,h)\,h\,b_0 w^2\,t - \sin(w\,h)\,a_0 w\,t + \sin(w\,h)\,a_2 w\,t] \\
4\,t\,\sin(w\,h)\cos(w\,h) &= -h[\sin(w\,h)\,h\,b_2\,w^2\,t - \sin(w\,h)\,h\,b_0\,w^2\,t \\
&\quad - w\,h\,a_2\,\cos(w\,h) + w\,h\cos(w\,h)\,a_0 + w^2\,h^2\,\sin(w\,h)\,b_2 \\
&\quad + w^2\,h^2\,\sin(w\,h)\,b_0 - \cos(w\,h)\,a_0\,w\,t - 2\,h\,b_2\,w\,\cos(w\,h) \\
&\quad - a_1\,t\,w - 2\,h\,b_1\,w - \sin(w\,h)\,a_2 + \sin(w\,h)\,a_0 \\
&\quad - 2\,\cos(w\,h)\,h\,b_0\,w - a_2 w\,t\,\cos(w\,h)] \\
4 &= a_2 + a_1 + a_0 \\
0 &= 2\,a_2 - 2\,a_0 + 2\,b_2 + 2\,b_1 + 2\,b_0
\end{aligned} \tag{3}$$

We note that the first, second, third and fourth equations are obtained requiring the algorithm (1) to be accurate for $\cos(w\,t)$, $\sin(w\,t)$, $x\,\cos(w\,t)$, $x\,\sin(w\,t)$ while the fifth and sixth equations are produced requiring the scheme (1) to be accurate for t^j, $j = 0(1)2$. The requirement for the accurate integration of functions (2), helps the method to be accurate for all the problems with solution which has behavior of

trigonometric functions. Based on the above requirements the following coefficients are obtained:

$$
\begin{aligned}
a_0 &= \frac{-2\cos(v)+2\cos(3v)+v\sin(3v)+v\sin(v)+4\cos(v)v^2}{-2v^2-v\sin(2v)+2v\sin(v)+2\cos(v)v^2}\\
a_1 &= \frac{4\cos(v)-4\cos(3v)-2v\sin(3v)+6v\sin(v)-8v^2-4v\sin(2v)}{-2v^2-v\sin(2v)+2v\sin(v)+2\cos(v)v^2}\\
b_0 &= \frac{T_0}{-2v^3-v^2\sin(2v)+2v^2\sin(v)+2v^3\cos(v)}\\
b_1 &= 0,\ a_2 = a_0,\ b_2 = -b_0
\end{aligned}
\tag{4}
$$

where $T_0 = -v\cos(3v) - 3v\cos(v) + 4v\cos(2v) + 4v^2\sin(v) + \sin(3v) + \sin(v) - 2\sin(2v)$ and $v = wh$.

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

$$
\begin{aligned}
a_0 &= -\frac{16}{15}+\frac{856}{1575}v^2-\frac{391}{7875}v^4+\frac{35557}{18191250}v^6-\frac{3372917}{85135050000}v^8\\
&\quad+\frac{2529073}{5959453500000}v^{10}-\frac{2315387}{552603870000000}v^{12}\\
&\quad+\frac{661553441}{266791622397300000000}v^{14}-\frac{12325988501}{21343329791784000000000}v^{16}+\cdots\\
a_1 &= \frac{92}{15}-\frac{1712}{1575}v^2+\frac{782}{7875}v^4-\frac{35557}{9095625}v^6+\frac{3372917}{42567525000}v^8\\
&\quad-\frac{2529073}{2979726750000}v^{10}+\frac{2315387}{276301935000000}v^{12}\\
&\quad-\frac{661553441}{133395811198650000000}v^{14}+\frac{12325988501}{106716648958920000000000}v^{16}+\cdots\\
b_0 &= -\frac{28}{15}+\frac{428}{1575}v^2-\frac{319}{23625}v^4+\frac{6421}{18191250}v^6-\frac{415351}{85135050000}v^8\\
&\quad+\frac{847607}{17878360500000}v^{10}-\frac{143261}{552603870000000}v^{12}\\
&\quad+\frac{693406873}{266791622397300000000}v^{14}+\frac{490004843}{174627243750960000000000}v^{16}+\cdots
\end{aligned}
\tag{5}
$$

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

$$
L.T.E(h) = -\frac{107\,h^7}{4725}\left(y_n^{(7)} + 2\,w^2\,y_n^{(5)} + w^4\,y_n^{(3)}\right) \tag{6}
$$

The $L.T.E.$ is obtained expanding the terms $y_{n\pm i},\ j = 0, 1, 2,\ f_{n\pm j}$ and $g_{n\pm j},\ j = 0, 1$ in (1) into Taylor series expansions and substituting the Taylor series expansions of the coefficients of the method.

So, based on the above we, have the following theorem.

Theorem 1 *The method* (1) *with coefficients* a_i, b_i, $i = 0(1)2$ *mentioned in* (4) *and* (5) *is a trigonometrically-fitted explicit method which is accurate for the set of functions* (2) *and is of sixth algebraic order.*

3 Comparative error analysis

We will study the following methods:

- The classical open Newton-Cotes differential method of order four which is indicated as **METH I**
- The classical open Newton-Cotes differential method of order six which is indicated as **METH II**
- The trigonometrically fitted fourth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] which is indicated as **METH III**
- The trigonometrically fitted sixth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] which is indicated as **METH IV**
- The classical method[1] of the new sixth algebraic order modified open Newton-Cotes family of differential algorithms presented in this paper which is indicated as **METH V**
- The new trigonometrically fitted sixth algebraic order modified open Newton-Cotes differential method developed in this paper which is indicated as **METH VI**

The error analysis is based on the following steps:

- The one-dimensional time independent Schrödinger equation is of the form

$$y''(x) = f(x)\, y(x) \tag{7}$$

- The function $f(x)$ is written in the form (based on the paper of Ixaru and Rizea [67]):

$$f(x) = g(x) + G \tag{8}$$

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

- Our analysis is based also on the expression of the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the equation (7). The expressions are presented as polynomials of G.
- Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae.

[1] Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

Based on the procedure mentioned above and on the formulae:

$$
\begin{aligned}
y_n^{(2)} &= (\mathrm{V}(x) - V_c + G)\,\mathrm{y}(x) \\
y_n^{(4)} &= \left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\mathrm{y}(x) + 2\left(\frac{d}{dx}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right) \\
&\quad +(\mathrm{V}(x) - V_c + G)\left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right) \\
y_n^{(6)} &= \left(\frac{d^4}{dx^4}\,\mathrm{V}(x)\right)\mathrm{y}(x) + 4\left(\frac{d^3}{dx^3}\,\mathrm{V}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right) \\
&\quad +3\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right) \\
&\quad +4\left(\frac{d}{dx}\,\mathrm{V}(x)\right)^2\mathrm{y}(x) \\
&\quad +6\,(\mathrm{V}(x) - V_c + G)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d}{dx}\,\mathrm{V}(x)\right) \\
&\quad +4\,(\mathrm{U}(x) - V_c + G)\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\,\mathrm{V}(x)\right) \\
&\quad +(\mathrm{V}(x) - V_c + G)^2\left(\frac{d^2}{dx^2}\,\mathrm{y}(x)\right)\ldots
\end{aligned}
$$

we obtain the expressions mentioned below.

We consider two cases in terms of the value of E:

- The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. Thus for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G, are the same for the cases of the classical method and of the new developed methods.
- $G \gg 0$ or $G \ll 0$. Then $\mid G \mid$ is a large number.
  So, we have the following asymptotic expansions of the equations produced from the Local Truncation errors and based on the above procedure.

The classical open Newton-Cotes differential method of order four

$$
\mathrm{LTE}_{\mathrm{METHI}} = \frac{14\,h^5}{45}\,\frac{d}{dx}\mathrm{y}\,(x)\;G^2 + \cdots \tag{9}
$$

The classical open Newton-Cotes differential method of order six

$$
\mathrm{LTE}_{\mathrm{METHII}} = \frac{41\,h^7}{140}\,\frac{d}{dx}y\,(x)\;G^3 + \cdots \tag{10}
$$

Table 1 Comparative error analysis for the methods mentioned in Sect. 3

Method	Algebraic order	Order of G	CFAE
METH I	4	2	$-\frac{14}{45}$
METH II	6	3	$-\frac{41}{140}$
METH III	4	1	$-\frac{14}{45}$
METH IV	6	2	$-\frac{41}{140}$
METH V	6	3	$-\frac{107}{4725}$
METH VI	6	2	$-\frac{214}{4725}$

We note that *CFAE* is the coefficient of the maximum power of G in the asymptotic expansion and order of G is the order of G in the asymptotic expansion of the local truncation error

The trigonometrically fitted fourth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44]

$$\mathrm{LTE}_{\mathrm{METHIII}} = h^5 \left[\left(\frac{14}{15} \left(\frac{d}{dx} g\left(x\right) \right) y\left(x\right) + \frac{14}{45} g\left(x\right) \frac{d}{dx} y\left(x\right) \right) G + \cdots \right] \quad (11)$$

The trigonometrically fitted sixth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44]

$$\mathrm{LTE}_{\mathrm{METHIV}} = h^7 \left[\left(\frac{41}{28} \left(\frac{d}{dx} g\left(x\right) \right) y\left(x\right) + \frac{41}{140} g\left(x\right) \frac{d}{dx} y\left(x\right) \right) G^2 + \cdots \right] \quad (12)$$

The classical method[2] of the new sixth algebraic order modified open Newton-Cotes family of differential algorithms presented in this paper

$$\mathrm{LTE}_{\mathrm{METHV}} = h^7 \left(\frac{107}{4725} \frac{d}{dx} y\left(x\right) \; G^3 + \cdots \right) \quad (13)$$

The new trigonometrically fitted sixth algebraic order modified open Newton-Cotes differential method developed in this paper

$$\mathrm{LTE}_{\mathrm{METHVI}} = h^7 \left(\frac{214}{4725} \left(\frac{d}{dx} g\left(x\right) \right) y\left(x\right) \; G^2 + \cdots \right) \quad (14)$$

From the above equations and Table 1 we have the following theorem:

[2] Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

Theorem 2

- *For the classical well known open Newton-Cotes fourth algebraic order method (METH I) the error increases as the second power of G*
- *For the classical well known open Newton-Cotes sixth algebraic order method (METH II) the error increases as the third power of G*
- *For the trigonometrically fitted fourth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] (METH III) the error increases as the first power of G*
- *For the trigonometrically fitted sixth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] (METH IV) the error increases as the second power of G*
- *For the classical method*[3] *of the new sixth algebraic order modified open Newton-Cotes family of differential algorithms presented in this paper (METH V) the error increases as the third power of G*
- *For the new trigonometrically fitted sixth algebraic order modified open Newton-Cotes differential method developed in this paper the error increases as the second power of G*

So, for the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper (Sect. 2—METH IV) is the most accurate Method , especially for large values of $\mid G \mid = \mid V_c - E \mid$*, since it is of a sixth algebraic order method for which the error increases as the second power of G and has absolute minimal coefficient of the maximum power (*CFAE*).*

4 Symplectic schemes and numerical methods

4.1 Basic theory

Dividing an interval $[a, b]$ with N points we have (see Zhu et. al. [70] and references therein)

$$t_0 = a,\ t_n = x_0 + n\,h,\ t_N = x_0 + N\,h = b, \quad n = 1, 2, \ldots, N, \tag{15}$$

where t is the independent variable.

The above division leads to the following discrete scheme:

$$\begin{pmatrix} \psi_{n+1} \\ \phi_{n+1} \end{pmatrix} = M_{n+1} \begin{pmatrix} \psi_n \\ \phi_n \end{pmatrix}, \quad M_{n+1} = \begin{pmatrix} p_{n+1} & q_{n+1} \\ r_{n+1} & s_{n+1} \end{pmatrix} \tag{16}$$

where $p,\ q,\ r,\ s \in \Re$. Based on the above we can write the n-step approximation to the solution as:

$$\begin{pmatrix} \psi_n \\ \phi_n \end{pmatrix} = \begin{pmatrix} p_n & q_n \\ r_n & s_n \end{pmatrix} \begin{pmatrix} p_{n-1} & q_{n-1} \\ r_{n-1} & s_{n-1} \end{pmatrix} \cdots \begin{pmatrix} p_1 & q_1 \\ r_1 & s_1 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \phi_0 \end{pmatrix}$$

$$= M_n\, M_{n-1}\, \cdots\, M_1 \begin{pmatrix} \psi_0 \\ \phi_0 \end{pmatrix}$$

[3] Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

Defining

$$S = M_n M_{n-1} \cdots M_1 = \begin{pmatrix} P_n & Q_n \\ R_n & S_n \end{pmatrix}$$

the discrete transformation can be written as:

$$\begin{pmatrix} \psi_n \\ \phi_n \end{pmatrix} = S \begin{pmatrix} \psi_0 \\ \phi_0 \end{pmatrix}$$

Definition 1 A discrete scheme (16) is a symplectic scheme if the transformation matrix S is symplectic.

Definition 2 A matrix S is symplectic if $S^T J S = J$ where

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

Remark 1 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.

The proposed methods can be used for non-linear differential equations as well as linear ones.

Theorem 3 *A discrete scheme of the form*

$$\begin{pmatrix} b & -a \\ a & b \end{pmatrix} \begin{pmatrix} \phi_{n+1} \\ \psi_{n+1} \end{pmatrix} = \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} \phi_{n-1} \\ \psi_{n-1} \end{pmatrix} \tag{17}$$

is symplectic.

Proof We rewrite (17) as

$$\begin{pmatrix} \phi_{n+1} \\ \psi_{n+1} \end{pmatrix} = \begin{pmatrix} b & -a \\ a & b \end{pmatrix}^{-1} \begin{pmatrix} b & a \\ -a & b \end{pmatrix} \begin{pmatrix} \phi_{n-1} \\ \psi_{n-1} \end{pmatrix}$$

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. □

Theorem 4 *A discrete scheme of the form*

$$\begin{pmatrix} k-w & d \\ -d & k-w \end{pmatrix}\begin{pmatrix} \phi_{n+1} \\ \psi_{n+1} \end{pmatrix} = \begin{pmatrix} k+w & -d \\ d & k+w \end{pmatrix}\begin{pmatrix} \phi_{n-1} \\ \psi_{n-1} \end{pmatrix} \tag{18}$$

is symplectic if $w = 0$ *(for any* $k,\ d \in \mathbb{R}$ *and* $k \neq 0$*).*

Proof We rewrite (18) as

$$\begin{pmatrix} \phi_{n+1} \\ \psi_{n+1} \end{pmatrix} = \begin{pmatrix} k-w & d \\ -d & k-w \end{pmatrix}^{-1}\begin{pmatrix} k+w & -d \\ d & k+w \end{pmatrix}\begin{pmatrix} \phi_{n-1} \\ \psi_{n-1} \end{pmatrix}$$

Define

$$\begin{aligned} M &= \begin{pmatrix} k-w & d \\ -d & k-w \end{pmatrix}^{-1}\begin{pmatrix} k+w & -d \\ d & k+w \end{pmatrix} \\ &= \frac{1}{k^2-2\,k\,w+w^2+d^2}\begin{pmatrix} k^2-w^2-d^2 & -2\,k\,d \\ 2\,k\,d & k^2-w^2-d^2 \end{pmatrix} \end{aligned}$$

and it can easily be verified that

$$M^T J M = \begin{pmatrix} 0 & T_1 \\ -T_1 & 0 \end{pmatrix}$$

where $T_1 = \frac{k^2+2\,k\,w+w^2+d^2}{k^2-2\,k\,w+w^2+d^2}$.

It can be easily seen that in order the matrix M to be symplectic the following relation must hold, for any $k,\ d \in \mathbb{R}$:

$$T_1 = \frac{k^2+2\,k\,w+w^2+d^2}{k^2-2\,k\,w+w^2+d^2} = 1 \Leftrightarrow 4\,k\,w = 0 \Leftrightarrow w = 0 \tag{19}$$

for any $k \neq 0$. □

4.2 The new modified open Newton-Cotes can be expressed as symplectic integrators

In the literature it has proved the symplectic structure of the following second-order differential scheme (SOD) [70],

$$y_{n+1} - y_{n-1} = 2hf_n \tag{20}$$

Based on the papers of Zhu et al. [70] and Chiou et al. [71] we will prove the multilayer symplectic structure of the new proposed modified Open Newton-Cotes differential schemes.

An application of the new Newton-Cotes differential formula (1) with the coefficients given by (4) to the linear Hamiltonian system

$$\begin{aligned}\dot{\phi} &= s\,\psi \\ \dot{\psi} &= -s\,\phi \end{aligned} \tag{21}$$

(where ϕ is the position, ψ is the monentum and s is a constant scalar or matrix) leads to:

$$\begin{aligned}\phi_{n+2} - \phi_{n-2} &= s\ (a_0\,\psi_{n-1} + a_1\,\psi_n + a_2\,\psi_{n+1}) \\ &\quad -s^2\ (b_0\,\phi_{n-1} + b_1\,\phi_n + b_2\,\phi_{n+1}) \\ \psi_{n+2} - \psi_{n-2} &= -s\ (a_0\,\phi_{n-1} + a_1\,\phi_n + a_2\,\phi_{n+1}) \\ &\quad -s^2\ (b_0\,\psi_{n-1} + b_1\,\psi_n + b_2\,\psi_{n+1}) \end{aligned} \tag{22}$$

where $s = m\,h$, where m is defined in (21).

From (20) we have that:

$$\phi_{n+1} - \phi_{n-1} = 2\,s\,\psi_n \tag{23}$$
$$\psi_{n+1} - \psi_{n-1} = -2\,s\,\phi_n \tag{24}$$
$$\phi_{n+2} - \phi_{n-2} = 4\,s\,\psi_n \tag{25}$$
$$\psi_{n+2} - \psi_{n-2} = -4\,s\,\phi_n \tag{26}$$
$$\phi_{n+\frac{1}{2}} - \phi_{n-\frac{1}{2}} = s\,\psi_n \tag{27}$$
$$\psi_{n+\frac{1}{2}} - \psi_{n-\frac{1}{2}} = -\,s\,\phi_n \tag{28}$$
$$\phi_{n+\frac{3}{2}} - \phi_{n-\frac{3}{2}} = 3\,s\,\psi_n \tag{29}$$
$$\psi_{n+\frac{3}{2}} - \psi_{n-\frac{3}{2}} = -\,3\,s\,\phi_n \tag{30}$$

Considering the approximation based on the formulae (27) and (28) for the $n+1$-step and for the n-step gives:

$$\phi_{n+1} - \phi_n = s\,\psi_{n+\frac{1}{2}} \tag{31}$$
$$\phi_n - \phi_{n-1} = s\,\psi_{n-\frac{1}{2}} \tag{32}$$
$$\psi_{n+1} - \psi_n = -\,s\,\phi_{n+\frac{1}{2}} \tag{33}$$
$$\psi_n - \psi_{n-1} = -\,s\,\phi_{n-\frac{1}{2}} \tag{34}$$
$$\tag{35}$$

From (31), (32) and (33), (34) we have:

$$\phi_{n+1} + \phi_{n-1} = 2\,\phi_n + s\left(\psi_{n+\frac{1}{2}} - \psi_{n-\frac{1}{2}}\right) \tag{36}$$
$$\psi_{n+1} + \psi_{n-1} = 2\,\psi_n - s\left(\phi_{n+\frac{1}{2}} - \phi_{n-\frac{1}{2}}\right) \tag{37}$$

The formulae (36) and (37) can be written as (taking into account the formula (28) and (27) respectively):

$$\phi_{n+1} + \phi_{n-1} = 2\,\phi_n - s^2\,\phi_n = \left(2 - s^2\right)\phi_n \tag{38}$$

$$\psi_{n+1} + \psi_{n-1} = 2\,\psi_n - s^2\,\psi_n = \left(2 - s^2\right)\psi_n \tag{39}$$

Considering, now, the approximation based on the formula (29) and (30) for the $n+2$-step and for the $n+1$-step gives:

$$\phi_{n+2} - \phi_{n-1} = 3\,s\,\psi_{n+\frac{1}{2}} \tag{40}$$
$$\phi_{n+1} - \phi_{n-2} = 3\,s\,\psi_{n-\frac{1}{2}} \tag{41}$$
$$\psi_{n+2} - \psi_{n-1} = -3\,s\,\phi_{n+\frac{1}{2}} \tag{42}$$
$$\psi_n - \psi_{n-1} = -3\,s\,\phi_{n-\frac{1}{2}} \tag{43}$$
$$\tag{44}$$

From (40), (41) and (42), (43) we have:

$$\phi_{n+2} + \phi_{n-2} = \phi_{n+1} + \phi_{n-1} + 3\,s\left(\psi_{n+\frac{1}{2}} - \psi_{n-\frac{1}{2}}\right) \tag{45}$$
$$\psi_{n+2} + \psi_{n-2} = \psi_{n+1} + \psi_{n-1} - 3\,s\left(\phi_{n+\frac{1}{2}} - \phi_{n-\frac{1}{2}}\right) \tag{46}$$

The formulae (45) and (46) can be written as (taking into account the formula (38) and (38) respectively and (28) and (27) respectively):

$$\phi_{n+2} + \phi_{n-2} = \left(2 - s^2\right)\phi_n - 3\,s^2\,\phi_n = \left(2 - 4\,s^2\right)\phi_n \tag{47}$$
$$\psi_{n+1} + \psi_{n-1} = \left(2 - s^2\right)\psi_n - 3\,s^2\,\psi_n = \left(2 - 4\,s^2\right)\psi_n \tag{48}$$

From (22) using the relations $a_2 = a_0$ and $b_2 = -b_0$ we have:

$$\begin{aligned}
\phi_{n+2} - \phi_{n-2} &= s\left[a_0\,(\psi_{n-1} + \psi_{n+1}) + a_1\,\psi_n\right] \\
&\quad - s^2\left[b_0\,(\phi_{n-1} - \phi_{n+1}) + b_1\,\phi_n\right] \\
\psi_{n+2} - \psi_{n-2} &= -s\left[a_0\,(\phi_{n-1} + \phi_{n+1}) + a_1\,\phi_n\right] \\
&\quad -s^2\left[b_0\,(\psi_{n-1} - \psi_{n+1}) + b_1\,\psi_n\right]
\end{aligned} \tag{49}$$

Using (38), (39) and (23), (24), the formula (49) gives:

$$\begin{aligned}
\phi_{n+2} - \phi_{n-2} &= s\left[a_0\left(2 - s^2\right) + a_1\right]\psi_n - s^2\left[b_0\,(2\,s\,\psi_n) + b_1\,\phi_n\right] \\
\psi_{n+2} - \psi_{n-2} &= -s\left[a_0\left(2 - s^2\right) + a_1\right]\phi_n - s^2\left[b_0\,(-2\,s\,\phi_n) + b_1\,\psi_n\right]
\end{aligned} \tag{50}$$

The above formulae (50) lead to:

$$\begin{aligned}
\phi_{n+2} - \phi_{n-2} &= \left[s\left[a_0\left(2 - s^2\right) + a_1\right] + 2\,s^3\,b_0\right]\psi_n - s^2\,b_1\,\phi_n \\
\psi_{n+2} - \psi_{n-2} &= \left[-s\left[a_0\left(2 - s^2\right) + a_1\right] - 2\,s^3\,b_0\right]\phi_n - s^2\,b_1\,\psi_n
\end{aligned} \tag{51}$$

Solving (47) and (48) we found that:

$$\begin{aligned}\phi_n &= -\frac{1}{2}\,\frac{\phi_{n+2}+\phi_{n-2}}{-1+2\,s^2}\\ \psi_n &= -\frac{1}{2}\,\frac{\psi_{n+2}+\psi_{n-2}}{-1+2\,s^2}\end{aligned} \tag{52}$$

Substituting ψ_n and ϕ_n into (51) we obtain:

$$\begin{aligned}\phi_{n+2}-\phi_{n-2} &= \left[s\left[a_0\left(2-s^2\right)+a_1\right]+2\,s^3\,b_0\right]\\ &\quad\left(-\frac{1}{2}\,\frac{\psi_{n+2}+\psi_{n-2}}{-1+2\,s^2}\right)-s^2\,b_1\left(-\frac{1}{2}\,\frac{\phi_{n+2}+\phi_{n-2}}{-1+2\,s^2}\right)\\ \psi_{n+2}-\psi_{n-2} &= \left[-s\left[a_0\left(2-s^2\right)+a_1\right]-2\,s^3\,b_0\right]\\ &\quad\left(-\frac{1}{2}\,\frac{\phi_{n+2}+\phi_{n-2}}{-1+2\,s^2}\right)-s^2\,b_1\left(-\frac{1}{2}\,\frac{\psi_{n+2}+\psi_{n-2}}{-1+2\,s^2}\right)\end{aligned} \tag{53}$$

or equivalently:

$$\begin{aligned}&\left(1-\frac{1}{2}\,\frac{s^2b_1}{-1+2\,s^2}\right)\phi_{n+2}+\frac{1}{2}\,\frac{\left(s\left(a_0\left(2-s^2\right)+a_1\right)+2\,s^3\,b_0\right)\psi_{n+2}}{-1+2\,s^2}\\ &=-\left(-1-\frac{1}{2}\,\frac{s^2\,b_1}{-1+2\,s^2}\right)\phi_{n-2}-\frac{1}{2}\,\frac{\left(s\left(a_0\left(2-s^2\right)+a_1\right)+2\,s^3\,b_0\right)\psi_{n-2}}{-1+2\,s^2}\\ &\frac{1}{2}\,\frac{\left(-s\left(a_0\left(2-s^2\right)+a_1\right)-2\,s^3\,b_0\right)\phi_{n+2}}{-1+2\,s^2}+\left(1-\frac{1}{2}\,\frac{s^2\,b_1}{-1+2\,s^2}\right)\psi_{n+2}\\ &=-\frac{1}{2}\,\frac{\left(-s\left(a_0\left(2-s^2\right)+a_1\right)-2\,s^3\,b_0\right)\phi_{n-2}}{-1+2\,s^2}-\left(-1-\frac{1}{2}\,\frac{s^2\,b_1}{-1+2\,s^2}\right)\psi_{n-2}\end{aligned} \tag{54}$$

The above formula in matrix form can be written as:

$$\begin{aligned}&\begin{pmatrix}1-\frac{1}{2}\,\frac{s^2b_1}{-1+2\,s^2} & T_0\\ -T_0 & 1-\frac{1}{2}\,\frac{s^2b_1}{-1+2\,s^2}\end{pmatrix}\begin{pmatrix}\phi_{n+2}\\ \psi_{n+2}\end{pmatrix}\\ &=\begin{pmatrix}1+\frac{1}{2}\,\frac{s^2b_1}{-1+2\,s^2} & -T_0\\ T_0 & 1+\frac{1}{2}\,\frac{s^2b_1}{-1+2\,s^2}\end{pmatrix}\begin{pmatrix}\phi_{n-2}\\ \psi_{n-2}\end{pmatrix}\end{aligned} \tag{55}$$

where

$$T_0=\frac{1}{2}\,\frac{s\left(a_0\left(2-s^2\right)+a_1\right)+2\,s^3\,b_0}{-1+2\,s^2}$$

The equation (55) can be written as:

$$\begin{pmatrix} \phi_{n+2} \\ \psi_{n+2} \end{pmatrix} = M \begin{pmatrix} \phi_{n-2} \\ \psi_{n-2} \end{pmatrix} \tag{56}$$

where

$$M = \begin{pmatrix} 1 - \frac{1}{2}\frac{s^2 b_1}{-1+2s^2} & T_0 \\ -T_0 & 1 - \frac{1}{2}\frac{s^2 b_1}{-1+2s^2} \end{pmatrix}^{-1} \begin{pmatrix} 1 + \frac{1}{2}\frac{s^2 b_1}{-1+2s^2} & -T_0 \\ T_0 & 1 + \frac{1}{2}\frac{s^2 b_1}{-1+2s^2} \end{pmatrix} \tag{57}$$

Based on Theorem 3, the discrete scheme (56) is symplectic and the matrix M is symplectic, since $b_1 = 0$ (see 4).

So, based on the above, we have the following theorem.

Theorem 5 *An application of the new modified open Newton-Cotes differential formula* (1) *with the coefficients given by* (4) *to the linear Hamiltonian system leads to the discrete scheme* (55) *which is symplectic.*

5 Numerical examples

In order to illustrate the efficiency of the new proposed method obtained in Sect. 2 we apply it to the radial time independent Schrödinger equation.

In order to apply the new method to the one-dimensional Schrödinger equation the value of parameter w is needed. For every problem of the radial Schrödinger equation given by

$$y''(x) = [l(l+1)/x^2 + V(x) - E]y(x). \tag{58}$$

the parameter w is given by

$$w = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{59}$$

where $V(x)$ is the potential and E is the energy.

5.1 Woods-Saxon potential

In our example the well known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{60}$$

is used, with $z = exp\,[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

The behavior of Woods-Saxon potential is shown in the Fig. 1.

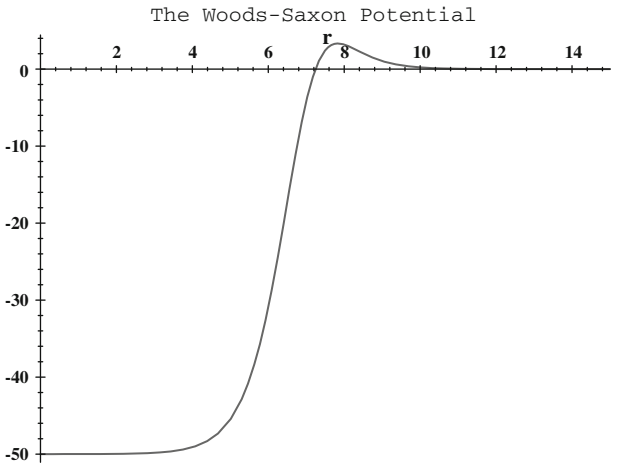

Fig. 1 The Woods-Saxon potential

It is well known that for some potentials, such as the Woods-Saxon potential, the definition of parameter w is not given as a function of x but it is based on some critical points which have been defined from the investigation of the appropriate potential (see for details [50]).

For the purpose of obtaining our numerical results it is appropriate to choose w as follows (see for details [50]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5-h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5+h \\ \sqrt{E}, & \text{for } x \in [6.5+2h, 15] \end{cases} \tag{61}$$

5.2 Radial Schrödinger equation: the resonance problem

We consider the numerical solution of the one-dimensional time independent Schrödinger equation (58) in the well-known case of the Woods-Saxon potential (60). For the numerical solution of the above problem we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical example we take the domain of integration as $x \in [0, 15]$. We consider equation (58) in a rather large domain of energies, i.e. $E \in [1, 1000]$.

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 effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{62}$$

for x greater than some value X.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$ where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. (58) (when $x \to \infty$) has the asymptotic form

$$y(x) \simeq Akxj_l(kx) - Bkxn_l(kx)$$
$$\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \tag{63}$$

where δ_l is the phase shift, that is calculated from the formula

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{64}$$

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 $y_0, y_i,\ i = 1(1)9$ before starting a four-step method. From the initial condition we obtain y_0. The other values can be obtained using the Runge-Kutta-Nyström methods of Dormand et al. (see [9]). With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l.

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$. We actually solve the latter problem, known as *the resonance problem* when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0,\ \ y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{65}$$

We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using:

- The classical open Newton-Cotes differential method of order four which is indicated as **METH I**
- The classical open Newton-Cotes differential method of order six which is indicated as **METH II**
- The trigonometrically fitted fourth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] which is indicated as **METH III**
- The trigonometrically fitted sixth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] which is indicated as **METH IV**
- The classical method[4] of the new sixth algebraic order modified open Newton-Cotes family of differential algorithms presented in this paper which is indicated as **METH V**

[4] Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

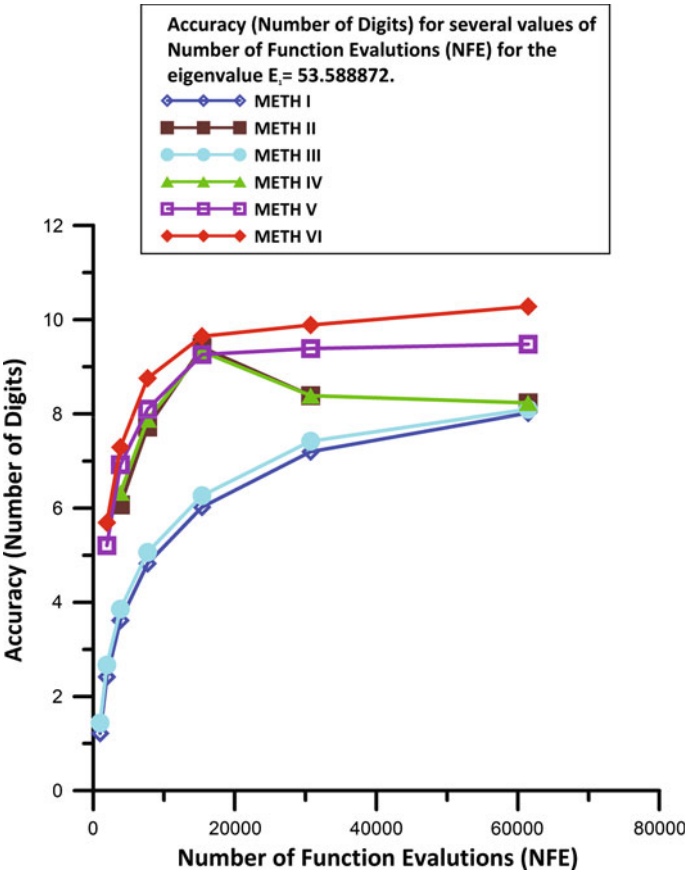

Fig. 2 Accuracy (number of digits) for several values of *NFE* for the eigenvalue $E_1 = 53.58872$. The nonexistence of a value of accuracy indicates that for this value of *NFE*, accuracy is positive

– The new trigonometrically fitted sixth algebraic order modified open Newton-Cotes differential method developed in this paper which is indicated as **METH VI**

The computed eigenenergies are compared with exact ones. In Figs. 2, 3, 4, 5 we present the Accuracy (Number of Digits) of the eigenenergies E_i, $i = 1(1)4$, for several values of *NFE* = Number of Function Evaluations.

6 Remarks–conclusions–summaries

6.1 Remarks and conclusions

The purpose of this paper was the introduction of a new modified open Newton Cotes integrators and the development of a new modified open trigonometrically-fitted Newton-Cotes method. We investigate the connection between the new proposed schemes, the differential methods and the symplectic integrators.

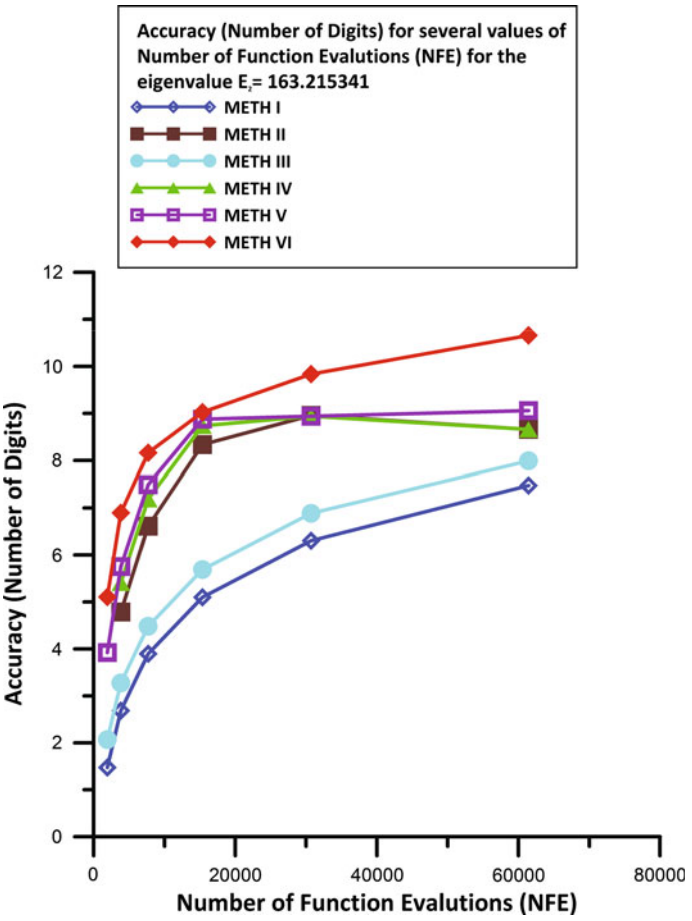

Fig. 3 Accuracy (number of digits) for several values of *NFE* for the eigenvalue $E_2 = 163.215341$. The nonexistence of a value of accuracy indicates that for this value of *NFE*, accuracy is positive

We have applied the new methods to the resonance problem of the one-dimensional Schrödinger equation.

Based on the results presented above we have the following conclusions:

- The trigonometrically fitted fourth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] (METH III)is more efficient than the classical open Newton-Cotes differential method of order four (METH I)
- The classical open Newton-Cotes differential method of order six (METH II) is more efficient than the trigonometrically fitted fourth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] (METH III) and the classical open Newton-Cotes differential method of order four (METH I)

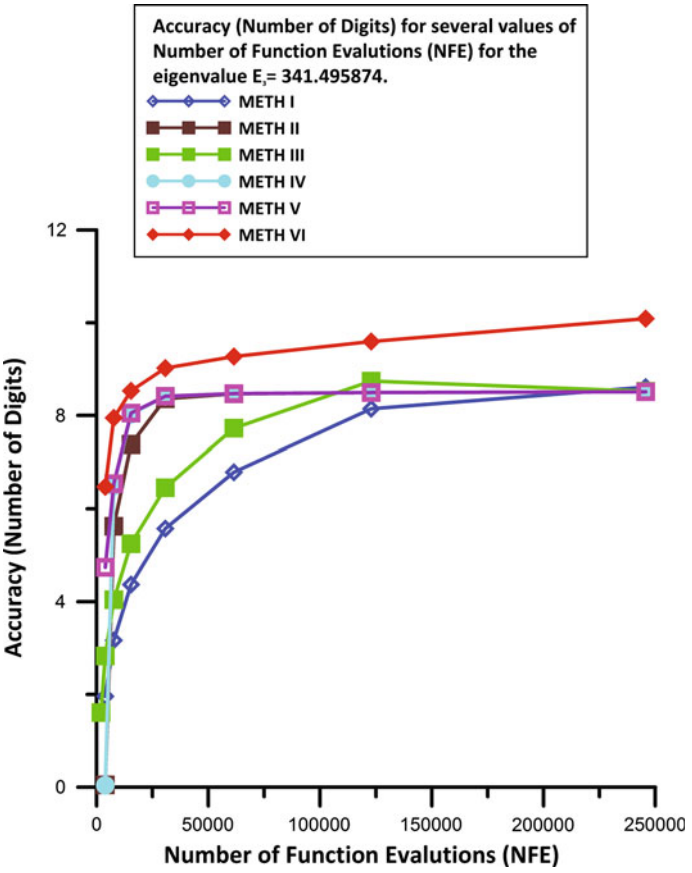

Fig. 4 Accuracy (number of digits) for several values of *NFE* for the eigenvalue $E_3 = 341.495874$. The nonexistence of a value of accuracy indicates that for this value of *NFE*, accuracy is positive

- The trigonometrically fitted sixth algebraic order open Newton-Cotes differential method developed by Vanden Berghe and Van Daele [44] (METH IV) is more efficient than the classical open Newton-Cotes differential method of order six (METH II)
- The classical method[5] of the new sixth algebraic order modified open Newton-Cotes family of differential algorithms presented in this paper (METH V) is more efficient than all the methods mentioned above.
- Finally, the new trigonometrically fitted sixth algebraic order modified open Newton-Cotes differential method developed in this paper (METH VI) is much more efficient than all the other methods.

[5] Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

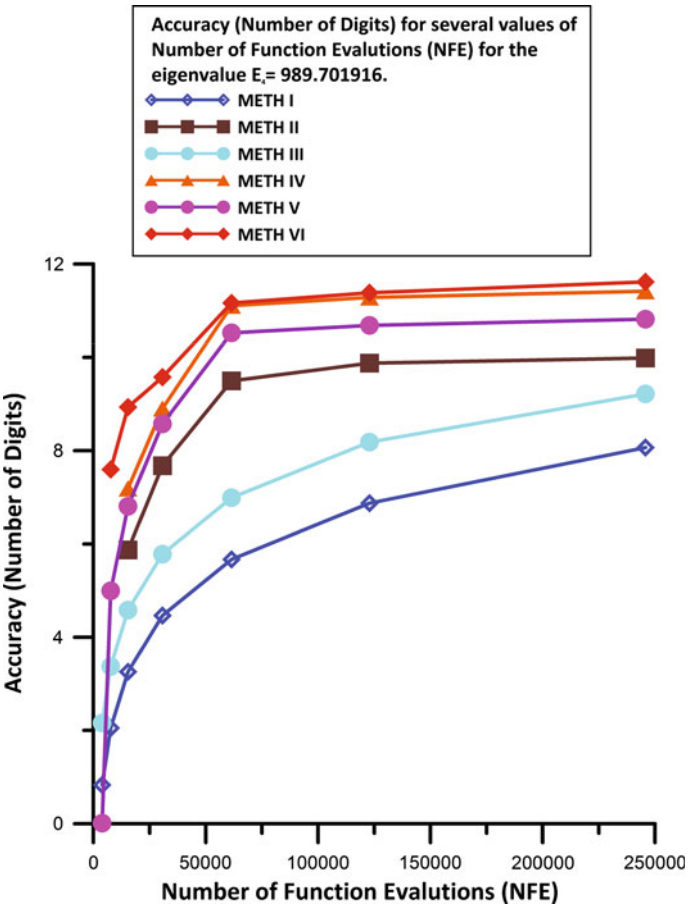

Fig. 5 Accuracy (number of digits) for several values of *NFE* for the eigenvalue $E_4 = 989.701916$. The nonexistence of a value of accuracy indicates that for this value of *NFE*, accuracy is positive

6.2 Summaries on the properties of the numerical methods

From the analysis presented above (comparative error analysis and comparative stability analysis) and from the numerical results presented above, the following summaries on the importance of the properties of the numerical methods are excluded:

- The dependence of the Algebraic Order of a Numerical Method and the parameter $G = V_c - E$ (where V_c is the constant approximation of the potential). For the same algebraic order it is important to have the minimal possible power of the parameter G. This is because in this case we have the minimal Local Truncation Error.
- The Symplectic property is an important property for the efficient solution of the radial Schrödinger equation.

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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