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ORIGINAL PAPER

High order closed Newton-Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation

T. E. Simos

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Abstract In this paper we study the connection between: (i) closed Newton-Cotes formulae of high order, (ii) trigonometrically-fitted and exponentially-fitted differential methods, (iii) symplectic integrators. Several one step symplectic integrators have been produced based on symplectic geometry during the last decades (see the relevant literature and the references here). However, the study of multistep symplectic integrators is very poor. In this paper we investigate the High Order Closed Newton-Cotes Formulae and we write them as symplectic multilayer structures. We develop trigonometrically-fitted and exponentially-fitted symplectic methods which are based on the closed Newton-Cotes formulae. We apply the symplectic schemes in order to solve the resonance problem of the radial Schrödinger equation. Based on the theoretical and numerical results, conclusions on the efficiency of the new obtained methods are given.

Highly Cited Researcher (http://isihighlycited.com/). Active Member of the European Academy of Sciences and Arts. Active Member of the European Academy of Sciences. Corresponding Member of European Academy of Arts, Sciences and Humanities.

T. E. Simos
Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia

T. E. Simos
Laboratory of Computational Sciences, Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, 221 00 Tripolis, Greece

T. E. Simos (✉)
10 Konitsis Street, Amfithea-Paleon Faliron, 175 64 Athens, Greece
e-mail: tsimos.conf@gmail.com

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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 [3]). Zhu et. al. [1] 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 [2].

The last decades much work has been done on exponential–trigonometrically fitting and the numerical solution of periodic initial value problems (see [4–118] 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.
- The exponentially-fitted methods are developed.
- We present a comparative error analysis
- We apply the new developed method to the resonance problem of the radial Schrödinger equation.
- Conclusions on the efficiency of the produced methods are given.

The construction of the papers is as follows:

- 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. The new exponentially-fitted and trigonometrically-fitted methods are also obtained.
- In Sect. 4 the conversion of the closed Newton-Cotes differential methods into multilayer symplectic structures is presented.
- A comparative error analysis is presented in Sect. 5
- Numerical results are presented in Sect. 6
- Finally conclusions are described in Sect. 7

2 Brief presentation of the literature on the subject

Large research on the algorithmic development of numerical methods for the solution of the Schrödinger equation has been done the last decades. The aim and scope of this research is the construction of fast and reliable algorithms for the solution of the Schrödinger equation and related problems (see for example [4–127]).

More specifically the last years:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been developed in [17–33]. The research on this subject has as a scope the production of numerical methods of Runge-Kutta and Runge-Kutta Nyström type which have vanished the phase-lag and/or the amplification factor. More recently this research has also as a subject the vanishing of the derivatives of the phase-lag and/or the amplification factor of the above mentioned methods.
- In [4–6] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are obtained. The main scope of this research subject is the development of numerical methods of Runge-Kutta and Runge-Kutta Nyström type which integrate exactly any linear combination of the functions:

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

  or the functions:

$$\{1, x, x^2, x^3, x^m, \ldots, \cos(w\, x), \sin(w\, x), x\ \cos(w\, x),\\ x\ \sin(w\, x), x^2 \cos(w\, x), x^2 \sin(w\, x), \ldots, x^p\ \cos(w\, x),\ x^p\ \sin(w\, x), \} \tag{3}$$

- Multistep phase-fitted methods and multistep methods with minimal phase-lag are developed in [34–53]. The research on this subject has as a scope the production of numerical nultistep methods of several type (linear, predictor–corrector, hybrid etc) which have vanished the phase-lag. More recently this research has also as a subject the vanishing of the derivatives of the phase-lag of the above mentioned methods. Recently also some techniques which can optimize these methods are also obtained.
- Symplectic integrators are studied in [54–80]. The research on this subject has as a scope the production of numerical methods (Runge-Kutta and Runge-Kutta

Nyström, Partitioned Runge-Kutta, differential schemes based on well known integration formulae etc) which satisfy the symplectic properties.
- Exponentially and trigonometrically multistep methods have been developed in [54–80]. The main scope of this research subject is the development of numerical multistep methods of several type (linear, predictor–corrector, hybrid etc) which integrate exactly any linear combination of the functions (2) or (3). We note here that recently [107] an exponentially-fitted method for the time dependent Schrödinger equation was obtained.
- Several pseudospectral methods have been studied and developed [108]
- New function fitting methods [109]
- Review papers have been written and Special Issues have been published in [110–118]

3 Basic theory on symplectic schemes and numerical methods

Zhu et al. [1] 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

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

We note that x is the independent variable and a and b in the equation for x_0 (Eq. 4) are different than the a and b in Eq. (5).

The above division leads to the following discrete scheme:

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

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

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

Defining

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

the discrete transformation can be written as:

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

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

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

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

4 Trigonometrically-fitted closed Newton-Cotes differential methods

4.1 General closed Newton-Cotes formulae

The closed Newton-Cotes integral rules are given by:

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

where

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

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

From the Table 1 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 Table 1 we have the following differential methods:

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

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

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

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

$$k = 5 y_{n+2} - y_{n-3} = \frac{5h}{288}(19 f_{n-3} + 75 f_{n-2} + 50 f_{n-1} + 50 f_n \\ +75 f_{n+1} + 19 f_{n+2})$$

Table 1 Closed Newton-Cotes integral rules

k	z	t_0	t_1	t_2	t_3	t_4	t_5	t_6	t_7	t_8
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		
7	7/17280	751	3577	1323	2989	2989	1323	3577	751	
8	4/14175	989	5888	−928	10496	−4540	10496	−928	5888	989

$$
\begin{aligned}
k = 6 y_{n+3} - y_{n-3} &= \frac{h}{140}(41 f_{n-3} + 216 f_{n-2} + 27 f_{n-1} + 272 f_n \\
&\quad + 27 f_{n+1} + 216 f_{n+2} + 41 f_{n+3}) \\
k = 7 y_{n+3} - y_{n-4} &= \frac{7h}{17280}(751 f_{n-4} + 3577 f_{n-3} + 1323 f_{n-2} + 2989 f_{n-1} \\
&\quad + 2989 f_n + 1323 f_{n+1} + 3577 f_{n+2} + 751 f_{n+3}) \\
k = 8 y_{n+4} - y_{n-4} &= \frac{4h}{14175}(989 f_{n-4} + 5888 f_{n-3} - 928 f_{n-2} + 10496 f_{n-1} \\
&\quad - 4540 f_n + 10496 f_{n+1} - 928 f_{n+2} + 5888 f_{n+3} + 989 f_{n+4})
\end{aligned}
$$

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

4.2 Exponentially-fitted closed Newton-Cotes differential method

Requiring the differential scheme:

$$
\begin{aligned}
y_{n+4} - y_{n-4} = h(&a_0\, f_{n-4} + a_1\, f_{n-3} + a_2\, f_{n-2} + a_3\, f_{n-1} + a_4\, f_n \\
&+ a_5\, f_{n+1} + a_6\, f_{n+2} + a_7\, f_{n+3} + a_8\, f_{n+4})
\end{aligned} \tag{6}
$$

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

$$
\{1, x, x^2, x^3, x^4, x^5, \cos(w\,x), \sin(w\,x), x\ \cos(w\,x), x\ \sin(w\,x)\} \tag{7}
$$

the set of equations mentioned in the Appendix A is obtained

Solving the above system of equations we obtain:

$$
\begin{aligned}
a_0 = (&-45\,w\cos(5\,w) - 315\,w\cos(3\,w) + 45\sin(5\,w) \\
&+ 45\sin(3\,w) + 360\,w\cos(4\,w) - 90\sin(4\,w)
\end{aligned}
$$

$$
\begin{aligned}
&+ 688\, w^2 \sin(3\, w) + 680\, w^2 \sin(w) - 832\, w^2 \sin(2\, w))/\mathrm{denom} \\
a_1 =\ & (360\, w \cos(2\, w) + 2304\, w^2 \sin(w) - 45 \sin(2\, w) \\
&- 180 \sin(5\, w) - 180 \sin(3\, w) - 45 \sin(6\, w) \\
&- 1800\, w \cos(4\, w) - 128\, w^2 \sin(3\, w) - 2528\, w^2 \sin(2\, w) \\
&+ 1440\, w \cos(3\, w) + 450 \sin(4\, w) - 1376\, w^2 \sin(4\, w))/\mathrm{denom} \\
a_2 =\ & (-2160\, w \cos(2\, w) + 1472\, w^2 \sin(w) + 270 \sin(2\, w) \\
&+ 180 \sin(5\, w) + 180 \sin(3\, w) + 270 \sin(6\, w) \\
&+ 3600\, w \cos(4\, w) + 5584\, w^2 \sin(3\, w) - 1216\, w^2 \sin(2\, w) \\
&- 2340\, w \cos(3\, w) + 900\, w \cos(5\, w) - 900 \sin(4\, w) \\
&+ 2752\, w^2 \sin(4\, w) + 688\, w^2 \sin(5\, w))/\mathrm{denom} \\
a_3 =\ & (5400\, w \cos(2\, w) + 2816\, w^2 \sin(w) - 675 \sin(2\, w) \\
&+ 180 \sin(5\, w) + 180 \sin(3\, w) - 675 \sin(6\, w) \\
&- 3960\, w \cos(4\, w) - 6272\, w^2 \sin(3\, w) - 5152\, w^2 \sin(2\, w) \\
&+ 1440\, w \cos(3\, w) - 2880\, w \cos(5\, w) + 990 \sin(4\, w) \\
&- 6304\, w^2 \sin(4\, w) - 1792\, w^2 \sin(5\, w))/\mathrm{denom} \\
a_4 =\ & (-7200\, w \cos(2\, w) + 576\, w^2 \sin(w) + 900 \sin(2\, w) \\
&- 450 \sin(5\, w) - 450 \sin(3\, w) + 900 \sin(6\, w) \\
&+ 3600\, w \cos(4\, w) + 9976\, w^2 \sin(3\, w) + 2176\, w^2 \sin(2\, w) \\
&- 450\, w \cos(3\, w) + 4050\, w \cos(5\, w) - 900 \sin(4\, w) \\
&+ 6976\, w^2 \sin(4\, w) + 2568\, w^2 \sin(5\, w))/\mathrm{denom} \\
a_5 =\ & a_3,\ a_6 = a_2,\ a_7 = a_1,\ a_8 = a_0 \qquad (8)
\end{aligned}
$$

where $w = v\, h$ and $\mathrm{denom} = 1215\, w^2 \sin(3\, w) + 1890\, w^2 \sin(w) - 360\, w^2 \sin(4\, w) - 2160\, w^2 \sin(2\, w) + 45\, w^2 \sin(5\, w)$.

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

$$
\begin{aligned}
a_0 =\ & \frac{3956}{14175} + \frac{4736}{467775}\, w^2 + \frac{286928}{638512875}\, w^4 + \frac{14024}{638512875}\, w^6 \\
&+ \frac{100297}{69780335625}\, w^8 + \frac{9966841}{77958590960250}\, w^{10} + \frac{4045453}{311834363841000}\, w^{12} \\
&+ \frac{1447489963}{1075828555251450000}\, w^{14} + \frac{1131270600283}{8161801645692895200000}\, w^{16} + \cdots \\
a_1 =\ & \frac{23552}{14175} - \frac{37888}{467775}\, w^2 + \frac{936896}{638512875}\, w^4 - \frac{20096}{127702575}\, w^6 \\
&- \frac{468836}{69780335625}\, w^8 - \frac{504652}{881884513125}\, w^{10} - \frac{4138919}{77958590960250}\, w^{12} \\
&- \frac{3975264586}{739632131735371875}\, w^{14} - \frac{21399079708469}{38768557817041252200000}\, w^{16} + \cdots \\
a_2 =\ & -\frac{3712}{14175} + \frac{18944}{66825}\, w^2 - \frac{1622848}{91216125}\, w^4 + \frac{992}{1964655}\, w^6
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{807076}{69780335625}\, w^8 + \frac{2218526}{2531123083125}\, w^{10} + \frac{4606249}{77958590960250}\, w^{12} \\
&+ \frac{118754903}{22244575390537500}\, w^{14} + \frac{2989110174847}{553836540243446460000 0}\, w^{16} + \cdots \\
a_3 &= \frac{41984}{14175} - \frac{37888}{66825}\, w^2 + \frac{661568}{13030875}\, w^4 - \frac{55424}{58046625}\, w^6 \\
&- \frac{613532}{69780335625}\, w^8 - \frac{2235052}{5568470782875}\, w^{10} + \frac{2643463}{77958590960250}\, w^{12} \\
&+ \frac{580084226}{105661733105053125}\, w^{14} + \frac{27060291451}{457716148961526000 00}\, w^{16} + \cdots \\
a_4 &= -\frac{3632}{2835} + \frac{9472}{13365}\, w^2 - \frac{115744}{1658475}\, w^4 + \frac{149488}{127702575}\, w^6 \\
&+ \frac{69998}{13956067125}\, w^8 - \frac{342211}{5568470782875}\, w^{10} - \frac{131909}{1247337455364}\, w^{12} \\
&- \frac{459801131}{33811754593617000}\, w^{14} - \frac{3179233568663}{221534616097378584000 0}\, w^{16} + \cdots
\end{aligned}
\tag{9}
$$

The behavior of the coefficients is given in the following Fig. 1.
The Local Truncation Error for the above differential method is given by:

$$
L.T.E(h) = -\frac{2368\, h^{11}}{467775} \left(y_n^{(11)} + 2\, v^2\, y_n^{(9)} + v^4\, y_n^{(7)} \right) \tag{10}
$$

The $L.T.E.$ is obtained expanding the terms $y_{n\pm j}$ and $f_{n\pm j}$, $j = 1(1)4$ in (6) into Taylor series expansions and substituting the Taylor series expansions of the coefficients of the method.

4.3 Trigonometrically-fitted closed Newton-Cotes differential method

Requiring the differential scheme (6) to be accurate for the following set of functions (we note that $f_i = y_i'$, $i = n-1, n, n+1$):

$$
\{1, x, x^2, x^3, x^4, x^5, \cos(w\,x), \sin(w\,x), \cos(2\,w\,x), \sin(2\,w\,x)\} \tag{11}
$$

the set of equations mentioned in the Appendix B is obtained. Solving the above system of equations we obtain:

$$
\begin{aligned}
a_0 &= (-3288\, w - 1376\, w \cos(5\, w) - 5872\, w \cos(w) \\
&\quad + 1800 \sin(4\, w) + 90 \sin(7\, w) + 540 \sin(6\, w) \\
&\quad + 90 \sin(w) + 1350 \sin(5\, w) - 3296\, w \cos(4\, w) \\
&\quad - 4576\, w \cos(2\, w) + 540 \sin(2\, w) + 1350 \sin(3\, w) \\
&\quad - 4272\, w \cos(3\, w) - 45 \sin(8\, w))/\text{denom} \\
a_1 &= -(-20720\, w - 11152\, w \cos(5\, w) - 1376\, w \cos(7\, w) \\
&\quad - 43824\, w \cos(w) + 11880 \sin(4\, w) + 1845 \sin(7\, w)
\end{aligned}
$$

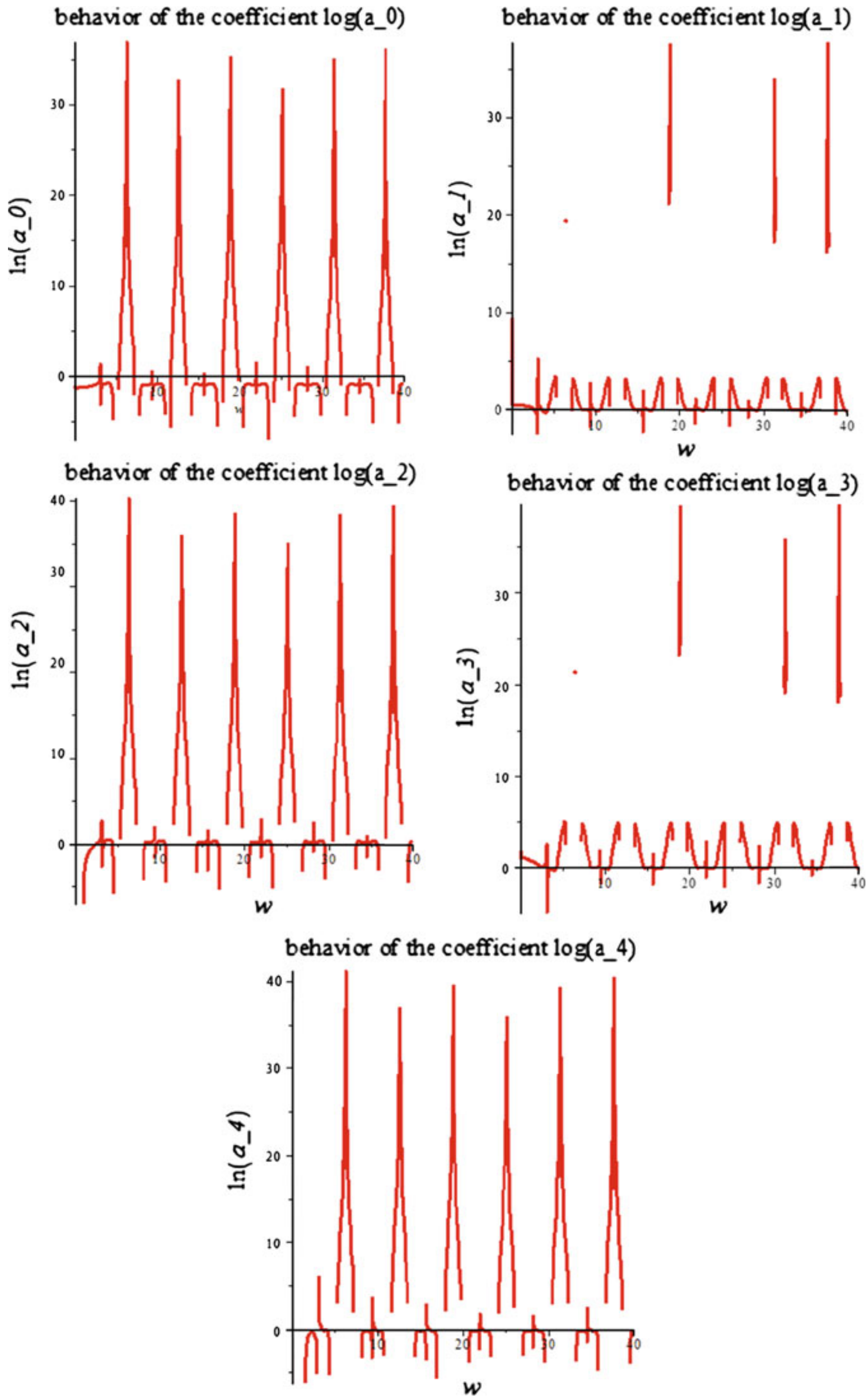

Fig. 1 Behavior of the coefficients of the new proposed method given by (8) for several values of w

$$
\begin{aligned}
&+5040\sin(6\,w)-4672\,w\cos(6\,w)+1800\sin(w)\\
&+9540\sin(5\,w)-20768\,w\cos(4\,w)-43840\,w\cos(2\,w)\\
&+5040\sin(2\,w)+9540\sin(3\,w)+45\sin(9\,w)\\
&-35088\,w\cos(3\,w)+270\sin(8\,w))/\text{denom}\\
a_2 =& -2\,(39600\,w+23136\,w\cos(5\,w)+3440\,w\cos(7\,w)\\
&+76192\,w\cos(w)-17640\sin(4\,w)-4635\sin(7\,w)\\
&-9720\sin(6\,w)+9888\,w\cos(6\,w)-4500\sin(w)\\
&-15120\sin(5\,w)+40352\,w\cos(4\,w)+67872\,w\cos(2\,w)\\
&-9720\sin(2\,w)-15120\sin(3\,w)+688\,w\cos(8\,w)\\
&-135\sin(9\,w)+56352\,w\cos(3\,w)-1260\sin(8\,w))/\text{denom}\\
a_3 =& -(-154128\,w-97136\,w\cos(5\,w)-17056\,w\cos(7\,w)\\
&-299472\,w\cos(w)+63000\sin(4\,w)+21915\sin(7\,w)\\
&+41040\sin(6\,w)-48576\,w\cos(6\,w)+21240\sin(w)\\
&+56700\sin(5\,w)-157920\,w\cos(4\,w)-271552\,w\cos(2\,w)\\
&+41040\sin(2\,w)+56700\sin(3\,w)-3584\,w\cos(8\,w)\\
&+675\sin(9\,w)-220656\,w\cos(3\,w)+6930\sin(8\,w))/\text{denom}\\
a_4 =& \,2\,(-97760\,w-62440\,w\cos(5\,w)-11192\,w\cos(7\,w)\\
&-186840\,w\cos(w)+37800\sin(4\,w)+14400\sin(7\,w)\\
&+26100\sin(6\,w)-31312\,w\cos(6\,w)+13950\sin(w)\\
&+34650\sin(5\,w)-100448\,w\cos(4\,w)-165712\,w\cos(2\,w)\\
&+26100\sin(2\,w)+34650\sin(3\,w)-2568\,w\cos(8\,w)\\
&+450\sin(9\,w)-135528\,w\cos(3\,w)+4725\sin(8\,w))/\text{denom}\\
a_5 =& \,a_3,\ a_6=a_2,\ a_7=a_1,\ a_8=a_0
\end{aligned}
\tag{12}
$$

where $w = v\,h$ and denom $= -1440\,w\cos(4\,w) - 90\,w\cos(8\,w) + 90\,w\cos(7\,w) - 1350\,w - 450\,w\cos(w) + 810\,w\cos(3\,w) + 2340\,w\cos(2\,w) - 450\,w\cos(5\,w) + 540\,w\cos(6\,w)$

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

$$
\begin{aligned}
a_0 =& \frac{3956}{14175}+\frac{2368}{93555}\,w^2+\frac{171488}{91216125}\,w^4-\frac{128}{5108103}\,w^6\\
&-\frac{4555108}{97692469875}\,w^8-\frac{69645922}{5568470782875}\,w^{10}-\frac{41841892}{16119257529375}\,w^{12}\\
&-\frac{73522153976}{147926426347074375}\,w^{14}-\frac{522534555282743}{5538365402434464600000}\,w^{16}+\cdots\\
a_1 =& \frac{23552}{14175}-\frac{18944}{93555}\,w^2+\frac{475136}{91216125}\,w^4+\frac{49024}{127702575}\,w^6\\
&+\frac{24788384}{97692469875}\,w^8+\frac{331785728}{5568470782875}\,w^{10}+\frac{3673343864}{306265893058125}\,w^{12}
\end{aligned}
$$

$$+\frac{67905861416}{29585285269414875}\,w^{14}+\frac{305737725924023}{6922956753043080750000}\,w^{16}+\cdots$$

$$\begin{aligned}
a_2 &= -\frac{3712}{14175}+\frac{9472}{13365}\,w^2-\frac{6280576}{91216125}\,w^4-\frac{230144}{127702575}\,w^6\\
&\quad-\frac{8232592}{13956067125}\,w^8-\frac{597795928}{5568470782875}\,w^{10}-\frac{6140144224}{306265893058125}\,w^{12}\\
&\quad-\frac{1245566512}{325113024938625}\,w^{14}-\frac{1056179934674561}{1384591350608616150000}\,w^{16}+\cdots\\
a_3 &= \frac{41984}{14175}-\frac{18944}{13365}\,w^2+\frac{18102272}{91216125}\,w^4+\frac{106112}{25540515}\,w^6\\
&\quad+\frac{1638752}{1993723875}\,w^8+\frac{519446912}{5568470782875}\,w^{10}+\frac{4220417288}{306265893058125}\,w^{12}\\
&\quad+\frac{55360250248}{21132346621010625}\,w^{14}+\frac{405789446598401}{6922956753043080750000}\,w^{16}+\cdots\\
a_4 &= -\frac{3632}{2835}+\frac{4736}{2673}\,w^2-\frac{4987328}{18243225}\,w^4-\frac{138496}{25540515}\,w^6\\
&\quad-\frac{2451656}{2791213425}\,w^8-\frac{73516316}{1113694156575}\,w^{10}-\frac{383448392}{61253178611625}\,w^{12}\\
&\quad-\frac{4959779536}{4226469324202125}\,w^{14}-\frac{188992617239681}{5538365402434464600000}\,w^{16}+\cdots
\end{aligned}\tag{13}$$

The behavior of the coefficients is given in the following Figure 2.

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

$$L.T.E(h)=-\frac{2368\,h^{11}}{467775}\left(y_n^{(11)}+5\,v^2\,y_n^{(9)}+4\,v^4\,y_n^{(7)}\right)\tag{14}$$

The $L.T.E.$ is obtained expanding the terms $y_{n\pm j}$ and $f_{n\pm j}$, $j=1(1)4$ in (6) into Taylor series expansions and substituting the Taylor series expansions of the coefficients of the method.

5 Closed Newton-Cotes can be expressed as symplectic integrators

Theorem 1 *A discrete scheme of the form*

$$\begin{pmatrix} b & -a\\ a & b\end{pmatrix}\begin{pmatrix} q_{n+1}\\ p_{n+1}\end{pmatrix}=\begin{pmatrix} b & a\\ -a & b\end{pmatrix}\begin{pmatrix} q_n\\ p_n\end{pmatrix}\tag{15}$$

is symplectic.

Proof We rewrite (3) as

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

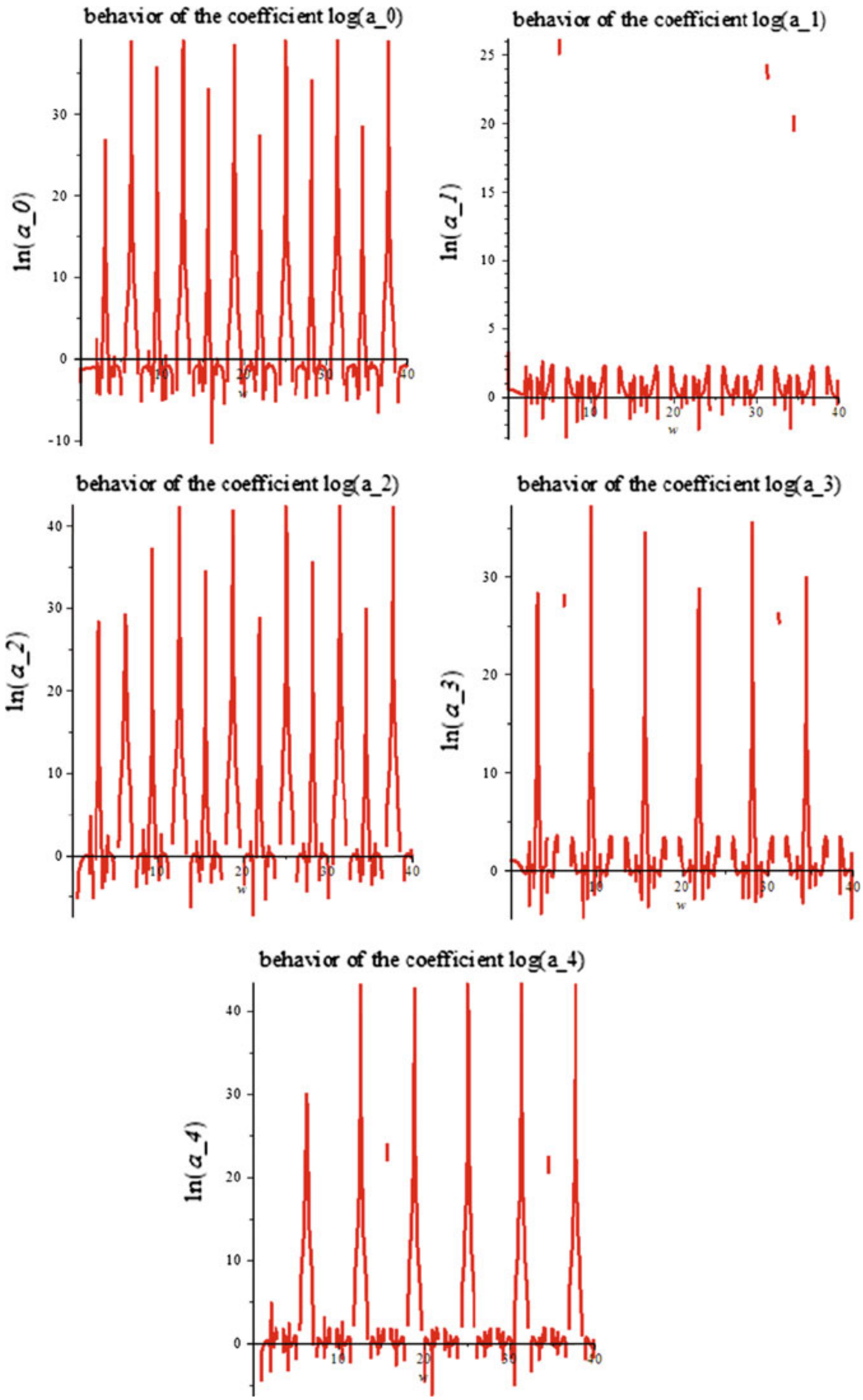

Fig. 2 Behavior of the coefficients of the new proposed method given by (12) for several values of w

Define

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

and it can easily be verified that

$$M^T J M = J$$

thus the matrix M is symplectic.

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

$$y_{n+i} - y_{n-i} = 2\, i\, h\, f_n,\ i = 1(1)4 \tag{16}$$

The above methods have been produced by the simplest Open Newton-Cotes integral formula.

Based on [2] the Closed Newton-Cotes differential schemes will be written as multilayer symplectic structures.

Application of the Newton-Cotes differential formula for $n = 4$ to the linear Hamiltonian system (1) gives

$$\begin{aligned} q_{n+4} - q_{n-4} &= s\ (a_0\, p_{n-4} + a_1\, p_{n-3} + a_2\, p_{n-2} + a_3\, p_{n-1} + a_4\, p_n \\ &\quad + a_5\, p_{n+1} + a_6\, p_{n+2} + a_7\, p_{n+3} + a_8\, p_{n+4}) \\ p_{n+4} - p_{n-4} &= -s\ (a_0\, q_{n-4} + a_1\, q_{n-3} + a_2\, q_{n-2} + a_3\, q_{n-1} + a_4\, q_n \\ &\quad + a_5\, q_{n+1} + a_6\, q_{n+2} + a_7\, q_{n+3} + a_8\, q_{n+4}) \end{aligned} \tag{17}$$

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

From (16) we have that:

$$\begin{aligned} q_{n+i} - q_{n-i} &= 2\, i\, s\, p_n \\ p_{n+i} - p_{n-i} &= -2\, i\, s\, q_n,\ i = 1(1)4 \text{ or } i = \frac{1}{2}(1)\frac{5}{2} \end{aligned} \tag{18}$$

Considering the approximation based on the first formula of (18) for $(n+1)$-step gives (taking into account the second formula of 18) :

$$\begin{aligned} q_{n+i} + q_{n-i} &= (q_n + s\, p_{n+i-\frac{1}{2}}) + (q_n - s\, p_{n-i+\frac{1}{2}}) \\ &= q_{n+i-1} + q_{n-i+1} + s\, (p_{n+i-\frac{1}{2}} - p_{n-i+\frac{1}{2}}) \\ &= (2 - i^2\, s^2)\, q_n,\ \ i = 1(1)3 \end{aligned} \tag{19}$$

Substituting (19) into (17) and considering that $a_0 = a_8$, $a_1 = a_7$, $a_2 = a_6$ and $a_3 = a_5$ we have:

$$\begin{aligned} q_{n+4} - q_{n-4} &= s\,[a_0\,(p_{n-4} + p_{n+4}) + (a_1\,(2 - 9\,s^2) \\ &\quad + 2\,a_2\,(1 - 2\,s^2) + a_3\,(2 - s^2) + a_4)\,p_n] \\ p_{n+4} - p_{n-4} &= s\,[a_0\,(p_{n-3} + p_{n+3}) + (a_1\,(2 - 9\,s^2) \\ &\quad + 2\,a_2\,(1 - 2\,s^2) + a_3\,(2 - s^2) + a_4)\,q_n] \end{aligned}$$

and with (18) we have

$$\begin{aligned} q_{n+4} - q_{n-4} &= s\,\Big[a_0\,(p_{n-4} + p_{n+4}) + (a_1\,(2 - 9\,s^2) + 2\,a_2\,(1 - 2\,s^2) \\ &\quad + a_3\,(2 - s^2) + a_4)\,\frac{q_{n+4} - q_{n-4}}{8\,s}\Big] \\ p_{n+4} - p_{n-4} &= s\,\Big[a_0\,(q_{n-3} + q_{n+3}) + (a_1\,(2 - 9\,s^2) + 2\,a_2\,(1 - 2\,s^2) \\ &\quad + a_3\,(2 - s^2) + a_4)\,\Big[-\frac{p_{n+4} - p_{n-4}}{8\,s}\Big]\Big] \end{aligned}$$

which gives:

$$\begin{aligned} &(q_{n+4} - q_{n-4})\left[1 - \frac{a_1\,(2 - 9\,s^2) + 2\,a_2\,(1 - 2\,s^2) + a_3\,(2 - s^2) + a_4}{8}\right] \\ &= s\,a_0\,(p_{n+4} + p_{n-4}) \\ &(p_{n+4} - p_{n-4})\left[1 - \frac{a_1\,(2 - 9\,s^2) + 2\,a_2\,(1 - 2\,s^2) + a_3\,(2 - s^2) + a_4}{8}\right] \\ &= -s\,a_0\,(q_{n+4} + q_{n-4}) \end{aligned}$$

The above formula in matrix form can be written as:

$$\begin{pmatrix} T(s) & -s\,a_0 \\ s\,a_0 & T(s) \end{pmatrix} \begin{pmatrix} q_{n+4} \\ p_{n+4} \end{pmatrix} = \begin{pmatrix} T(s) & s\,a_0 \\ -s\,a_0 & T(s) \end{pmatrix} \begin{pmatrix} q_{n-4} \\ p_{n-4} \end{pmatrix}$$

where

$$T(s) = 1 - \frac{a_1\,(2 - 9\,s^2) + 2\,a_2\,(1 - 2\,s^2) + a_3\,(2 - s^2) + a_4}{8} \tag{20}$$

which is a discrete scheme of the form (15) and hence it is symplectic. □

6 Comparative error analysis for the radial Schrödinger equation

In this section we will investigate theoretically several differential methods produced by closed Newton-Cotes formulae. 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 1 A method is called classical if it has constant coefficients

Remark 1 A trigonometrically-fitted method is not a classical one because it has coefficients which are dependent on the quantity $v = w\,h$, where w is the frequency of the problem and h is the step length of the integration.

Consider the radial Schrödinger equation:

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x) = f(x)\,y(x) \tag{21}$$

where $f(x) = U(x) - k^2$ and $U(x) = l(l+1)/x^2 + V(x)$.

We write $f(x)$ in (21) in the form

$$f(x) = g(x) + d \tag{22}$$

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

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 [69] (Method IV)
- The closed Newton-Cotes formulae developed in [68] (Method V)
- The closed Newton-Cotes formulae developed in [66] (Method VI)
- The classical tenth order closed Newton-Cotes formulae (Method VII)
- The closed Newton-Cotes Exponentially Fitted formulae developed in the paragraph 3.2 (Method VIII)
-
- The closed Newton-Cotes Trigonometrically Fitted formulae developed in the paragraph 3.3 (Method IX)

We, now, present the formulae of the Local Truncation Error (L.T.E.) for the above methods.

For the Method I is equal to:

$$L.T.E(h)_{MI} = -\frac{h^5}{90} y_n^{(5)} \tag{23}$$

For the Method II is equal to:

$$L.T.E(h)_{MII} = -\frac{8\,h^5}{945} y_n^{(7)} \tag{24}$$

For the Method III is equal to:

$$L.T.E(h)_{MIII} = -\frac{9\,h^9}{1400}\,y_n^{(9)} \tag{25}$$

For the Method IV is equal to:

$$L.T.E(h)_{MIV} = -\frac{8\,h^9}{945}\left(y_n^{(7)} + v^2\,y_n^{(5)}\right) \tag{26}$$

For the Method V is equal to:

$$L.T.E(h)_{MV} = -\frac{h^5}{90}\left(y_n^{(5)} + v^2\,y_n^{(3)}\right) \tag{27}$$

For the Method VI is equal to:

$$L.T.E(h)_{MVI} = -\frac{9\,h^9}{1400}\left(y_n^{(9)} + 3\,v^2\,y_n^{(7)} + 3\,v^4\,y_n^{(5)} + v^6\,y_n^{(3)}\right) \tag{28}$$

For the Method VII is equal to:

$$L.T.E(h)_{MethodVII} = -\frac{2368\,h^{11}}{467775}\,y_n^{(11)} \tag{29}$$

For the Method VIII is equal to:

$$L.T.E(h)_{MethodVIII} = -\frac{2368\,h^{11}}{467775}\left(y_n^{(11)} + 2\,v^2\,y_n^{(9)} + v^4\,y_n^{(7)}\right) \tag{30}$$

For the Method IX is equal to:

$$L.T.E(h)_{MethodIX} = -\frac{2368\,h^{11}}{467775}\left(y_n^{(11)} + 5\,v^2\,y_n^{(9)} + 4\,v^4\,y_n^{(7)}\right) \tag{31}$$

We express, now, the derivatives $y_n^{(9)},\ y_n^{(7)},\ y_n^{(5)}, y_n^{(3)}$ in terms of Eq. (21), i.e.

$$\begin{aligned} y_n^{(2)} &= f(x)\,y(x),\ y_n^{(3)} = \left(\frac{d}{dx}\,g(x)\right)y(x) + (g(x)+d)\left(\frac{d}{dx}\,y(x)\right), \\ y_n^{(5)} &= \left(\frac{d^3}{dx^3}\,g(x)\right)\,y(x) + 3\,\left(\frac{d^2}{dx^2}\,g(x)\right)\,\left(\frac{d}{dx}\,y(x)\right) \\ &\quad + 2\,\left(\frac{d}{dx}\,g(x)\right)\,\left(\frac{d^2}{dx^2}\,y(x)\right) + 2\,(g(x)+d)\,y(x)\,\left(\frac{d}{dx}\,g(x)\right) \\ &\quad + (g(x)+d)^2\,\left(\frac{d}{dx}\,y(x)\right) \end{aligned} \tag{32}$$

etc. We note that $g^{(n)}(x) = U^{(n)}(x)$ for the n-th order derivative with respect to x.

Introducing the expressions obtained in (32) into the Local Truncation Error of the methods mentioned above (see relations (23)–(31)), we obtain the expressions (as polynomials of d) for Local Truncation Error of the methods mentioned in the Appendix C.

The leading terms (in d) of the above expressions are given by:

$$L.T.E(h)_{MI} = h^5\, d^2 \left(-\frac{1}{90}\left(\frac{d}{dx}\, y(x)\right)\right) \tag{33}$$

$$L.T.E(h)_{MII} = h^7\, d^3 \left(-\frac{8}{945}\left(\frac{d}{dx}\, y(x)\right)\right) \tag{34}$$

$$L.T.E(h)_{MIII} = h^9\, d^4 \left(-\frac{9}{1400}\left(\frac{d}{dx}\, y(x)\right)\right) \tag{35}$$

$$\begin{aligned} L.T.E(h)_{MIV} = h^7\, d^2 \Bigg(&-\frac{8}{189}\left(\frac{d}{dx}\, g(x)\right) y(x) \\ &- \frac{8}{945}\left(\frac{d}{dx}\, y(x)\right) g(x)\Bigg) \end{aligned} \tag{36}$$

$$\begin{aligned} L.T.E(h)_{MV} = h^5\, d \Bigg(&-\frac{1}{30}\left(\frac{d}{dx}\, g(x)\right) y(x) \\ &- \frac{1}{90}\left(\frac{d}{dx}\, y(x)\right) g(x)\Bigg) \end{aligned} \tag{37}$$

$$\begin{aligned} L.T.E(h)_{MVI} = h^9\, d^2 \Bigg(&-\frac{18}{175}\left(\frac{d^3}{dx^3}\, g(x)\right) y(x) \\ &- \frac{9}{350}\left(\frac{d^2}{dx^2}\, g(x)\right)\left(\frac{d}{dx}\, y(x)\right) \\ &- \frac{27}{700}\, y(x)\left(\frac{d}{dx}\, g(x)\right) g(x)\Bigg) \end{aligned} \tag{38}$$

$$L.T.E(h)_{MVII} = -\frac{2368}{467775}\, h^{11}\, \frac{d}{dx}\, y(x)\, d^5 \tag{39}$$

$$L.T.E(h)_{MVIII} = -\frac{4736}{467775}\, h^{11}\, y(x)\, \frac{d}{dx}\, g(x)\, d^4 \tag{40}$$

$$\begin{aligned} L.T.E(h)_{MIX} = h^{11} \Bigg[&\frac{2368}{155925}\, g(x)\left(\frac{d}{dx}\, y(x)\right) \\ &+ \frac{44992}{467775}\left(\frac{d}{dx}\, g(x)\right) y(x)\Bigg] d^4 \end{aligned} \tag{41}$$

From the above equations we have the following theorem:

Theorem 2 *For the Closed Newton-Cotes formulae studied in this paper we have:*

- **Fourth Algebraic Order Methods**
  In the Fourth Algebraic Order Method MI the 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 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 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 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.

7 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:

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x). \tag{42}$$

using the well-known Woods-Saxon potential (see [1,4–6,8]) which is given by

$$V(x) = V_w(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{43}$$

with $z = \exp[(x - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$. In Fig. 3 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 [119–122,128,129,132,134–137]).

Many problems in chemistry, physics, physical chemistry, chemical physics, electronics etc., are expressed by Eq. (42) (see [134–137]).

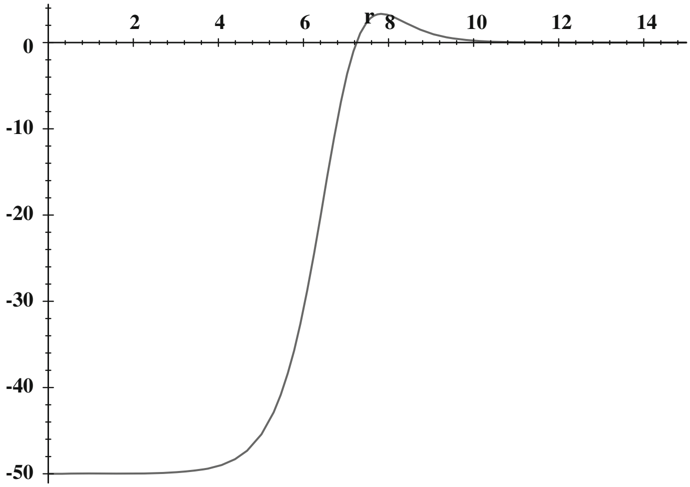

Fig. 3 The Woods-Saxon potential

7.1 Resonance problem

In the asymptotic region the Eq. (42) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{44}$$

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 $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bn_l(kx) \\ &\simeq D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)] \end{aligned} \tag{45}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \tag{46}$$

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 [130,131]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l from the above relation.

7.1.1 The Woods-Saxon potential

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (42) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods-Saxon one (43).

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:

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

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 [14] (which is indicated as Method B)
- The P-stable Exponentially Fitted Method developed by Kalogiratou and Simos [16] (which is indicated as Method C)
- The four-step method developed by Henrici [133] (which is indicated as Method D)
- The Newton-Cotes Trigonometrically-Fitted Formula developed in [67] (which is indicated as Method E)
- The Newton-Cotes Trigonometrically-Fitted Formula developed in [66] (which is indicated as Method F)
- The Newton-Cotes Trigonometrically-Fitted Formula developed in [63] (which is indicated as Method G)
- The new proposed exponentially-fitted method (which is indicated as Method H)
- The new proposed trigonometrically-fitted method (which is indicated as Method I)

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 4 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.

8 Conclusions

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

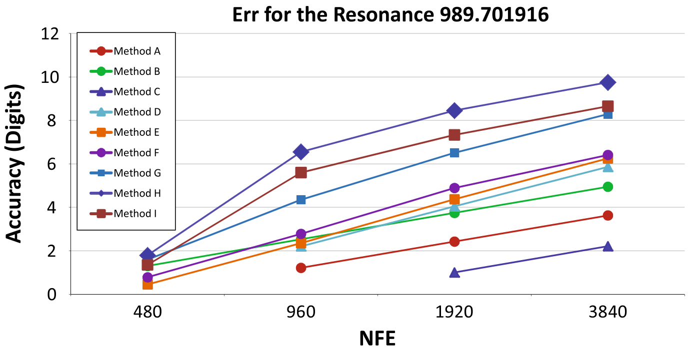

Fig. 4 Accuracy (Digits) for several values of NFE for the eigenvalue $E_3 = 989.701916$. The non-existence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0

From the numerical results we have the following remarks:

– The Numerov's Method and the Exponentially-Fitted Method of Raptis and Allison [14] have better behavior than the P-stable Exponentially Fitted Method developed by Kalogiratou and Simos [16]
– The Exponentially-Fitted Method of Raptis and Allison [14] is more efficient than the well known Numerov's method.
– The four-step method developed by Henrici [133] has better behavior than all the previous mentioned methods
– The Newton-Cotes Trigonometrically-Fitted Formula developed in [67] has better behavior than all the above methods.
– The Newton-Cotes Trigonometrically-Fitted Formula developed in [66] is more efficient than all the above methods.
– The behavior of the Newton-Cotes Trigonometrically-Fitted Formula developed in [63] 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 2 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.

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

Appendix A

$$a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7 + a_8 = 8$$
$$-8\,a_0 - 6\,a_1 - 4\,a_2 - 2\,a_3 + 2\,a_5 + 4\,a_6 + 6\,a_7 + 8\,a_8 = 0$$

$$48\,a_0 + 27\,a_1 + 12\,a_2 + 3\,a_3 + 3\,a_5 + 12\,a_6 + 27\,a_7 + 48\,a_8 = 128$$

$$-256\,a_0 - 108\,a_1 - 32\,a_2 - 4\,a_3 + 4\,a_5 + 32\,a_6 + 108\,a_7 + 256\,a_8 = 0$$

$$\begin{aligned}
&80\,a_2 + 405\,a_1 + 405\,a_7 + 1280\,a_8 + 1280\,a_0\\
&+5\,a_3 + 80\,a_6 + 5\,a_5 = 2048
\end{aligned}$$

$$\begin{aligned}
&v\,h\sin(v\,h)(-a_1 + a_3 - a_5 + a_7 + 4\,a_8\cos(v\,h)\\
&+2\,a_2\cos(v\,h) - 4\,a_7\cos(v\,h)^2 - 8\,a_8\cos(v\,h)^3\\
&-2\,a_6\cos(v\,h) + 8\,a_0\cos(v\,h)^3 - 4\cos(v\,h)\,a_0 + 4\,a_1\cos(v\,h)^2) = 0
\end{aligned}$$

$$\begin{aligned}
&v\,h(-3\,a_1\cos(v\,h) + 8\,a_0\cos(v\,h)^4 + a_0 - a_2 + a_4\\
&-a_6 + a_8 - 8\,a_0\cos(v\,h)^2 + 4\,a_1\cos(v\,h)^3\\
&+8\,a_8\cos(v\,h)^4 + a_3\cos(v\,h)\\
&-8\,a_8\cos(v\,h)^2 - 3\,a_7\cos(v\,h) + 4\,a_7\cos(v\,h)^3\\
&+a_5\cos(v\,h) + 2\,a_6\cos(v\,h)^2\\
&+2\,a_2\cos(v\,h)^2) = 8\cos(v\,h)\sin(v\,h)\,(2\cos(v\,h)^2 - 1)
\end{aligned}$$

$$\begin{aligned}
&h\,(8\,a_8\cos(v\,h)^4 + a_3\cos(v\,h) - 8\,a_8\,v\,x\cos(v\,h)^3\sin(v\,h)\\
&+2\,a_2\,v\,x\cos(v\,h)\sin(v\,h) + 4\,a_8\,v\,x\cos(v\,h)\sin(v\,h)\\
&+8\cos(v\,h)^3\sin(v\,h)\,a_0\,v\,x - 32\cos(v\,h)^3\sin(v\,h)\,h\,a_0\,v\\
&-12\,h\,a_1\,v\sin(v\,h)\cos(v\,h)^2 + 16\cos(v\,h)\sin(v\,h)\,h\,a_0\,v\\
&-4\,a_7\,v\,x\sin(v\,h)\cos(v\,h)^2 - 12\,h\,a_7\,v\cos(v\,h)^2\sin(v\,h)\\
&-32\,h\,a_8\,v\cos(v\,h)^3\sin(v\,h) + 16\,h\,a_8\,v\cos(v\,h)\sin(v\,h)\\
&-2\,a_6\,v\,x\cos(v\,h)\sin(v\,h) + a_0 - a_2 + a_4\\
&-a_6 + a_8 - 4\,h\,a_6\,v\cos(v\,h)\sin(v\,h)\\
&-8\,a_0\cos(v\,h)^2 + 4\,a_1\cos(v\,h)^3\\
&+4\,a_1\,v\,x\sin(v\,h)\cos(v\,h)^2 - a_5\,v\,x\sin(v\,h)\\
&+3\,h\,a_1\,v\sin(v\,h) - a_1\,v\,x\sin(v\,h)\\
&+3\,h\,a_7\,v\sin(v\,h) - h\,a_5\,v\sin(v\,h)\\
&-h\,a_3\,v\sin(v\,h) + 8\,a_0\cos(v\,h)^4 + a_7\,v\,x\sin(v\,h)\\
&+a_3\,v\,x\sin(v\,h) - 8\,a_8\cos(v\,h)^2\\
&-3\,a_7\cos(v\,h) + 4\,a_7\cos(v\,h)^3 + a_5\cos(v\,h)\\
&+2\,a_6\cos(v\,h)^2 - 3\,a_1\cos(v\,h)\\
&+2\,a_2\cos(v\,h)^2 - 4\,h\,a_2\,v\cos(v\,h)\sin(v\,h)\\
&-4\cos(v\,h)\sin(v\,h)\,a_0\,v\,x) = 8\,h\,(1 - 8\cos(v\,h)^2 + 8\cos(v\,h)^4)\\
&-h(-a_1\sin(v\,h) + a_7\sin(v\,h) + a_3\sin(v\,h)\\
&-a_5\sin(v\,h) - 4\,a_0\cos(v\,h)\sin(v\,h) + a_6\,v\,x + 8\,a_0\,v\,x\cos(v\,h)^2\\
&+12\,h\,a_1\,v\cos(v\,h)^3 - 4\,a_1\,v\,x\cos(v\,h)^3 - 32\,h\,a_0\,v\cos(v\,h)^2\\
&-4\,h\,a_8\,v + a_2\,v\,x + 32\,h\,a_0\,v\cos(v\,h)^4 - 8\,a_0\,v\,x\cos(v\,h)^4\\
&-12\,h\,a_7\,v\cos(v\,h)^3 - h\,a_5\,v\cos(v\,h) + 8\,a_8\,v\,x\cos(v\,h)^2\\
&-a_5\,v\,x\cos(v\,h) - 2\,a_2\,v\,x\cos(v\,h)^2 + 32\,h\,a_8\,v\cos(v\,h)^2
\end{aligned}$$

$$\begin{aligned}
&-32\,h\,a_8\,v\cos(v\,h)^4-a_3\,v\,x\cos(v\,h)+9\,h\,a_7\,v\cos(v\,h)\\
&-8\,a_8\,v\,x\cos(v\,h)^4-a_8\,v\,x+4\,h\,a_0\,v-a_0\,v\,x\\
&-a_4\,x\,v+4\,a_1\sin(v\,h)\cos(v\,h)^2-8\,a_8\cos(v\,h)^3\sin(v\,h)\\
&+4\,a_8\cos(v\,h)\sin(v\,h)+2\,a_2\cos(v\,h)\sin(v\,h)\\
&+h\,a_3\,v\cos(v\,h)-2\,a_6\,v\,x\cos(v\,h)^2\\
&+3\,a_7\,v\,x\cos(v\,h)-4\,h\,a_6\,v\cos(v\,h)^2\\
&+4\,h\,a_2\,v\cos(v\,h)^2-9\,h\,a_1\,v\cos(v\,h)+3\,a_1\,v\,x\cos(v\,h)\\
&-4\,a_7\,v\,x\cos(v\,h)^3+2\,h\,a_6\,v+8\,a_0\cos(v\,h)^3\sin(v\,h)\\
&-2\,h\,a_2\,v-4\,a_7\sin(v\,h)\cos(v\,h)^2-2\,a_6\cos(v\,h)\sin(v\,h))=\\
&\quad=8\cos(v\,h)\sin(v\,h)\,x\,(2\cos(v\,h)^2-1) \qquad (47)
\end{aligned}$$

We note that the first, second, third, fourth and fifth equations are produced requiring the scheme (6) to be accurate for x^j, $j = 0(1)5$, while the sixth, seventh, eighth and ninth equations are obtained requiring the algorithm (6) to be accurate for $\cos(vx)$, $\sin(vx)$, $x\ \cos(vx)$, $x\ \sin(vx)$). The requirement for the accurate integration of functions (7), helps the method to be accurate for all the problems with solution which has behavior of trigonometric functions.

Appendix B

$$\begin{aligned}
&a_0+a_1+a_2+a_3+a_4+a_5+a_6+a_7+a_8=8\\
&-8\,a_0-6\,a_1-4\,a_2-2\,a_3+2\,a_5+4\,a_6+6\,a_7+8\,a_8=0\\
&\quad 48\,a_0+27\,a_1+12\,a_2+3\,a_3+3\,a_5+12\,a_6+27\,a_7+48\,a_8=128\\
&-256\,a_0-108\,a_1-32\,a_2-4\,a_3+4\,a_5+\ 32\,a_6+108\,a_7+256\,a_8=0\\
&\quad 80\,a_2+405\,a_1+405\,a_7+1280\,a_8+1280a_0+5a_3+80\,a_6+5\,a_5=2048\\
&\quad v\,h\sin(v\,h)(-a_1+a_3-a_5+a_7+4\,a_1\cos(v\,h)^2\\
&-4\cos(v\,h)\,a_0+4\,a_8\cos(v\,h)-8\,a_8\cos(v\,h)^3+2\,a_2\cos(v\,h)\\
&-4\,a_7\cos(v\,h)^2-2\,a_6\cos(v\,h)+8\,a_0\cos(v\,h)^3)=0\\
&\quad v\,h(a_0-a_2+a_4-a_6+a_8+a_3\cos(v\,h)\\
&+4\,a_7\cos(v\,h)^3-3\,a_1\cos(v\,h)-8\,a_0\cos(v\,h)^2\\
&+2\,a_2\cos(v\,h)^2+8\,a_8\cos(v\,h)^4+a_5\cos(v\,h)-8\,a_8\cos(v\,h)^2\\
&+2\,a_6\cos(v\,h)^2-3\,a_7\cos(v\,h)+8\,a_0\cos(v\,h)^4\\
&+4\,a_1\cos(v\,h)^3)=8\cos(v\,h)\sin(v\,h)\,(2\cos(v\,h)^2-1)\\
&\quad 4\,v\,h\sin(v\,h)\cos(v\,h)(-4\,a_0+3\,a_1-2\,a_2+a_3\\
&-a_5+2\,a_6-3\,a_7+4\,a_8+40\,a_0\cos(v\,h)^2\\
&-64\,a_8\cos(v\,h)^6-4\,a_6\cos(v\,h)^2+96\,a_8\cos(v\,h)^4\\
&-40\,a_8\cos(v\,h)^2+4\,a_2\cos(v\,h)^2-96\,a_0\cos(v\,h)^4\\
&+64\,a_0\cos(v\,h)^6-16\,a_1\cos(v\,h)^2+16\,a_7\cos(v\,h)^2
\end{aligned}$$

$$
\begin{aligned}
&- 16\, a_7 \cos(v\, h)^4 + 16\, a_1 \cos(v\, h)^4) = 0\\
&2\, v\, h(a_0 - a_1 + a_2 - a_3 + a_4 - a_5 + a_6 - a_7 + a_8\\
&+ 18\, a_7 \cos(v\, h)^2 + 32\, a_1 \cos(v\, h)^6 + 2\, a_3 \cos(v\, h)^2\\
&+ 32\, a_7 \cos(v\, h)^6 - 48\, a_7 \cos(v\, h)^4\\
&+ 128\, a_0 \cos(v\, h)^8 + 18\, a_1 \cos(v\, h)^2\\
&- 8\, a_2 \cos(v\, h)^2 + 160\, a_8 \cos(v\, h)^4\\
&+ 8\, a_6 \cos(v\, h)^4 - 32\, a_8 \cos(v\, h)^2\\
&- 256\, a_8 \cos(v\, h)^6 - 8\, a_6 \cos(v\, h)^2\\
&+ 128\, a_8 \cos(v\, h)^8 + 160\, a_0 \cos(v\, h)^4\\
&+ 8\, a_2 \cos(v\, h)^4 - 32\, a_0 \cos(v\, h)^2\\
&- 256\, a_0 \cos(v\, h)^6 - 48\, a_1 \cos(v\, h)^4\\
&+ 2\, a_5 \cos(v\, h)^2) = 16 \sin(v\, h) \cos(v\, h)\\
&(-1 - 24 \cos(v\, h)^4 + 10 \cos(v\, h)^2 + 16 \cos(v\, h)^6) \qquad (48)
\end{aligned}
$$

We note that the first, second, third, fourth and fifth equations are produced requiring the scheme (6) to be accurate for x^j, $j = 0(1)5$, while the sixth, seventh, eighth and ninth equations are obtained requiring the algorithm (6) to be accurate for $\cos(v\, x)$, $\sin(v\, x)$, $\cos(2\, v\, x)$, $\sin(2\, v\, x))$. The requirement for the accurate integration of functions (11), helps the method to be accurate for all the problems with solution which has behavior of trigonometric functions.

Appendix C

Expressions of the local truncation errors

$$
\begin{aligned}
L.T.E(h)_{MI} = h^5\Big(&- \frac{1}{90}\left(\frac{d^3}{dx^3}\, g(x)\right) y(x) - \frac{1}{30}\left(\frac{d^2}{dx^2}\, g(x)\right)\left(\frac{d}{dx}\, y(x)\right)\\
&- \frac{2}{45}\, y(x)\left(\frac{d}{dx}\, g(x)\right) g(x) - \frac{2}{45}\, y(x)\left(\frac{d}{dx}\, g(x)\right) d\\
&- \frac{1}{90}\left(\frac{d}{dx}\, y(x)\right) g(x)^2 - \frac{1}{45}\left(\frac{d}{dx}\, y(x)\right) g(x)\, d\\
&- \frac{1}{90}\left(\frac{d}{dx}\, y(x)\right) d^2\Big) \qquad (49)
\end{aligned}
$$

$$
\begin{aligned}
L.T.E(h)_{MII} = h^7\Big(&- \frac{8}{945}\left(\frac{d^5}{dx^5}\, g(x)\right) y(x)\\
&- \frac{8}{189}\left(\frac{d^4}{dx^4}\, g(x)\right)\left(\frac{d}{dx}\, y(x)\right)\\
&- \frac{88}{945}\, y(x)\left(\frac{d^3}{dx^3}\, g(x)\right) g(x) - \frac{88}{945}\, y(x)\left(\frac{d^3}{dx^3}\, g(x)\right) d\\
&- \frac{8}{63}\left(\frac{d}{dx} g(x)\right) y(x)\left(\frac{d^2}{dx^2} g(x)\right) - \frac{104}{945}\left(\frac{d}{dx}\, y(x)\right)\left(\frac{d^2}{dx^2}\, g(x)\right) g(x)
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{104}{945}\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)d-\frac{16}{189}\left(\frac{d}{dx}\,g(x)\right)^2\left(\frac{d}{dx}\,y(x)\right)\\
&-\frac{8}{105}\,y(x)\left(\frac{d}{dx}\,g(x)\right)g(x)^2-\frac{16}{105}\,y(x)\left(\frac{d}{dx}\,g(x)\right)g(x)\,d\\
&-\frac{8}{105}\,y(x)\left(\frac{d}{dx}\,g(x)\right)d^2-\frac{8}{945}\left(\frac{d}{dx}\,y(x)\right)g(x)^3\\
&-\frac{8}{315}\left(\frac{d}{dx}\,y(x)\right)g(x)^2\,d-\frac{8}{315}\left(\frac{d}{dx}\,y(x)\right)g(x)\,d^2\\
&-\frac{8}{945}\left(\frac{d}{dx}\,y(x)\right)d^3\Big)
\end{aligned}
\tag{50}
$$

$$
\begin{aligned}
L.T.E(h)_{MIII}=h^9\Big(&-\frac{18}{175}\,(g(x)+d)^3\,y(x)\left(\frac{d}{dx}\,g(x)\right)\\
&-\frac{27}{100}\left(\frac{d}{dx}\,g(x)\right)y(x)\left(\frac{d^4}{dx^4}\,g(x)\right)\\
&-\frac{9}{35}\,(g(x)+d)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^4}{dx^4}\,g(x)\right)\\
&-\frac{99}{700}\,(g(x)+d)\,y(x)\left(\frac{d^5}{dx^5}\,g(x)\right)\\
&-\frac{9}{25}\left(\frac{d^2}{dx^2}\,g(x)\right)y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)\\
&-\frac{63}{100}\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^3}{dx^3}\,g(x)\right)\\
&-\frac{207}{700}\,(g(x)+d)^2\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)\\
&-\frac{333}{350}(g(x)+d)y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)\left(\frac{d}{dx}\,g(x)\right)\\
&-\frac{153}{700}\,(g(x)+d)^2\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)-\frac{9}{50}\left(\frac{d}{dx}\,g(x)\right)^3y(x)\\
&-\frac{117}{350}\,(g(x)+d)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d}{dx}\,g(x)\right)^2-\frac{9}{1400}\left(\frac{d^7}{dx^7}\,g(x)\right)y(x)\\
&-\frac{9}{200}\left(\frac{d^6}{dx^6}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)-\frac{81}{200}\left(\frac{d^2}{dx^2}\,g(x)\right)^2\left(\frac{d}{dx}\,y(x)\right)\\
&-\frac{9}{1400}\,(g(x)+d)^4\left(\frac{d}{dx}\,y(x)\right)\Big)
\end{aligned}
\tag{51}
$$

$$
\begin{aligned}
L.T.E(h)_{MIV}=h^7\Big(&-\frac{8}{945}\left(\frac{d^5}{dx^5}\,g(x)\right)y(x)\\
&-\frac{8}{189}\left(\frac{d^4}{dx^4}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\\
&-\frac{88}{945}\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)g(x)-\frac{16}{189}\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)d\\
&-\frac{8}{63}\left(\frac{d}{dx}\,g(x)\right)y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{104}{945}\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)g(x)\\
&-\frac{16}{189}\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)d-\frac{16}{189}\left(\frac{d}{dx}\,g(x)\right)^2\left(\frac{d}{dx}\,y(x)\right)\\
&-\frac{8}{105}\,y(x)\left(\frac{d}{dx}\,g(x)\right)g(x)^2-\frac{16}{135}\,y(x)\left(\frac{d}{dx}\,g(x)\right)g(x)\,d\\
&-\frac{8}{189}\,y(x)\left(\frac{d}{dx}\,g(x)\right)d^2-\frac{8}{945}\left(\frac{d}{dx}\,y(x)\right)g(x)^3\\
&-\frac{16}{945}\left(\frac{d}{dx}\,y(x)\right)g(x)^2\,d-\frac{8}{945}\left(\frac{d}{dx}\,y(x)\right)g(x)\,d^2\Big)
\end{aligned} \tag{52}
$$

$$
\begin{aligned}
L.T.E(h)_{MV}=h^5\Big(&-\frac{1}{90}\left(\frac{d^3}{dx^3}\,g(x)\right)y(x)-\frac{1}{30}\left(\frac{d^2}{dx^2}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\\
&-\frac{2}{45}\,y(x)\left(\frac{d}{dx}\,g(x)\right)g(x)-\frac{1}{30}\,y(x)\left(\frac{d}{dx}\,g(x)\right)d\\
&-\frac{1}{90}\left(\frac{d}{dx}\,y(x)\right)g(x)^2-\frac{1}{90}\left(\frac{d}{dx}\,y(x)\right)g(x)\,d\Big)
\end{aligned} \tag{53}
$$

$$
\begin{aligned}
L.T.E(h)_{MVI}=h^9\Big(&-\frac{9}{50}\left(\frac{d}{dx}\,g(x)\right)^3y(x)-\frac{9}{1400}\left(\frac{d}{dx}\,y(x)\right)g(x)^3\,d\\
&-\frac{63}{100}\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^3}{dx^3}\,g(x)\right)\\
&-\frac{27}{100}\left(\frac{d}{dx}\,g(x)\right)y(x)\left(\frac{d^4}{dx^4}\,g(x)\right)\\
&-\frac{9}{25}\left(\frac{d^2}{dx^2}\,g(x)\right)y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)-\frac{9}{200}\left(\frac{d^6}{dx^6}\,g(x)\right)\left(\frac{d}{dx}y(x)\right)\\
&-\frac{81}{200}\left(\frac{d^2}{dx^2}\,g(x)\right)^2\left(\frac{d}{dx}\,y(x)\right)-\frac{9}{35}\left(\frac{d^4}{dx^4}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)g(x)\\
&-\frac{9}{56}\left(\frac{d^4}{dx^4}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)d-\frac{99}{700}\left(\frac{d^5}{dx^5}\,g(x)\right)y(x)\,g(x)\\
&-\frac{171}{1400}\left(\frac{d^5}{dx^5}\,g(x)\right)y(x)\,d-\frac{207}{700}\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)g(x)^2\\
&-\frac{18}{175}\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)d^2-\frac{531}{1400}\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)g(x)\,d\\
&-\frac{333}{350}\left(\frac{d}{dx}\,g(x)\right)y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)g(x)\\
&-\frac{927}{1400}\left(\frac{d}{dx}\,g(x)\right)y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)d\\
&-\frac{261}{1400}\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)g(x)\,d\\
&-\frac{153}{700}\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)g(x)^2
\end{aligned}
$$

$$- \frac{9}{350} \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^2}{dx^2}\, g(x)\right) d^2 - \frac{27}{200}\, y(x) \left(\frac{d}{dx}\, g(x)\right) g(x)^2\, d$$
$$- \frac{27}{700}\, y(x)\, (\frac{d}{dx}\, g(x)\Big)\, g(x)\, d^2 - \frac{9}{1400} \left(\frac{d^7}{dx^7}\, g(x)\right) y(x)$$
$$- \frac{9}{1400} \left(\frac{d}{dx}\, y(x)\right) g(x)^4 - \frac{18}{175}\, y(x) \left(\frac{d}{dx}\, g(x)\right) g(x)^3$$
$$- \frac{117}{350} \left(\frac{d}{dx}\, g(x)\right)^2 \left(\frac{d}{dx}\, y(x)\right) g(x)$$
$$- \frac{99}{700} \left(\frac{d}{dx}\, g(x)\right)^2 \left(\frac{d}{dx}\, y(x)\right) d\Big) \tag{54}$$

$L.T.E(h)_{MVII}$

$$= -\frac{2368}{467775}\, h^{11} \left[\frac{d}{dx}\, y(x)\right] d^5$$
$$- \frac{2368}{467775}\, h^{11} \left[25 \left(\frac{d}{dx}\, g(x)\right) y(x) + 5\, g(x) \left(\frac{d}{dx}\, y(x)\right)\right] d^4$$
$$- \frac{2368}{467775} h^{11} \Bigg[100\, g(x)\, y(x) \left(\frac{d}{dx}\, g(x)\right) + 130 \left(\frac{d^3}{dx^3}\, g(x)\right) y(x)$$
$$+70 \left(\frac{d^2}{dx^2}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right) + 10\, g(x)^2 \left(\frac{d}{dx}\, y(x)\right)\Bigg] d^3$$
$$- \frac{2368}{467775} h^{11} \Bigg[148 \left(\frac{d^5}{dx^5}\, g(x)\right) y(x) + 160 \left(\frac{d}{dx}\, g(x)\right)^2 \left(\frac{d}{dx}\, y(x)\right)$$
$$+ 210\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^2}{dx^2}\, g(x)\right) + 390\, g(x)\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)$$
$$+ 150\, g(x)^2\, y(x) \left(\frac{d}{dx}\, g(x)\right) + 10\, g(x)^3 \left(\frac{d}{dx}\, y(x)\right)$$
$$+166 \left(\frac{d^4}{dx^4}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right) + 670 \left(\frac{d}{dx}\, g(x)\right) y(x) \left(\frac{d^2}{dx^2}\, g(x)\right)\Bigg] d^2$$
$$- \frac{2368}{467775} h^{11} \Bigg[390\, g(x)^2\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)$$
$$+ 690 \left(\frac{d}{dx}\, g(x)\right) y(x) \left(\frac{d^4}{dx^4}\, g(x)\right) + 296\, g(x)\, y(x) \left(\frac{d^5}{dx^5}\, g(x)\right)$$
$$+ 37 \left(\frac{d^7}{dx^7}\, g(x)\right) y(x) + 5\, g(x)^4 \left(\frac{d}{dx}\, y(x)\right)$$
$$+ 280 \left(\frac{d}{dx}\, g(x)\right)^3 y(x) + 320\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d}{dx}\, g(x)\right)^2$$
$$+ 91 \left(\frac{d^6}{dx^6}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right) + 332\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^4}{dx^4}\, g(x)\right)$$

$$+1340\,g(x)\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\left(\frac{d}{dx}\,g(x)\right)+100\,g(x)^3\,y(x)\,\left(\frac{d}{dx}\,g(x)\right)$$
$$+210\,g(x)^2\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)+531\left(\frac{d^2}{dx^2}\,g(x)\right)^2\left(\frac{d}{dx}\,y(x)\right)$$
$$+818\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^3}{dx^3}\,g(x)\right)+1040\left(\frac{d^2}{dx^2}\right.$$
$$\left.g(x)\right)\,y(x)\,\left(\frac{d^3}{dx^3}\,g(x)\right)\Bigg]d-\frac{2368}{467775}h^{11}\Bigg[25\,g(x)^4\,y(x)\,\left(\frac{d}{dx}\,g(x)\right)$$
$$+160\,g(x)^2\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d}{dx}\,g(x)\right)^2+336\left(\frac{d^3}{dx^3}\,g(x)\right)^2\left(\frac{d}{dx}\,y(x)\right)$$
$$+9\left(\frac{d^8}{dx^8}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)+\left(\frac{d^9}{dx^9}\,g(x)\right)\,y(x)$$
$$+570\left(\frac{d}{dx}\,g(x)\right)^2\,y(x)\left(\frac{d^3}{dx^3}\,g(x)\right)+675\left(\frac{d}{dx}\,g(x)\right)$$
$$y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)^2+210\left(\frac{d^3}{dx^3}\,g(x)\right)\,y(x)\,\left(\frac{d^4}{dx^4}\,g(x)\right)$$
$$+558\left(\frac{d^2}{dx^2}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^4}{dx^4}\,g(x)\right)$$
$$+162\left(\frac{d^2}{dx^2}\,g(x)\right)\,y(x)\,\left(\frac{d^5}{dx^5}\,g(x)\right)+93\left(\frac{d}{dx}\,g(x)\right)\,y(x)\,\left(\frac{d^6}{dx^6}\,g(x)\right)$$
$$+306\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^5}{dx^5}\,g(x)\right)+792\left(\frac{d}{dx}\,g(x)\right)^2$$
$$\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)+280\,g(x)\,y(x)\,\left(\frac{d}{dx}\,g(x)\right)^3$$
$$+g(x)^5\left(\frac{d}{dx}\,y(x)\right)+70\,g(x)^3\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)$$
$$+166\,g(x)^2\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^4}{dx^4}\,g(x)\right)+531\,g(x)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)^2$$
$$+130\,g(x)^3\,y(x)\,\left(\frac{d^3}{dx^3}\,g(x)\right)+148\,g(x)^2\,y(x)\,\left(\frac{d^5}{dx^5}\,g(x)\right)$$
$$+37\,g(x)\,y(x)\,\left(\frac{d^7}{dx^7}\,g(x)\right)+91\,g(x)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^6}{dx^6}\,g(x)\right)$$
$$+1040\,g(x)\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\left(\frac{d^3}{dx^3}\,g(x)\right)$$
$$+818\,g(x)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^3}{dx^3}\,g(x)\right)\left(\frac{d}{dx}\,g(x)\right)$$

$$+690\,g(x)\,y(x)\left(\frac{d^4}{dx^4}g(x)\right)\left(\frac{d}{dx}g(x)\right)$$

$$+670\,g(x)^2\,y(x)\left(\frac{d^2}{dx^2}g(x)\right)\left(\frac{d}{dx}g(x)\right)\Bigg] \tag{55}$$

$$L.T.E\,(h)_{MVIII}$$

$$= -\frac{4736}{467775}\,h^{11}\,y(x)\left[\frac{d}{dx}g(x)\right]d^4$$

$$+h^{11}\Bigg[-\frac{4736}{42525}\,g(x)\,y(x)\left(\frac{d}{dx}g(x)\right)-\frac{16576}{66825}\left(\frac{d^3}{dx^3}g(x)\right)y(x)$$

$$-\frac{2368}{31185}\left(\frac{d^2}{dx^2}g(x)\right)\left(\frac{d}{dx}y(x)\right)-\frac{2368}{467775}\,g(x)^2\left(\frac{d}{dx}y(x)\right)\Bigg]d^3$$

$$+h^{11}\Bigg[-\frac{2368}{4455}\left(\frac{d^5}{dx^5}g(x)\right)y(x)-\frac{68672}{155925}\,g(x)\left(\frac{d}{dx}y(x)\right)\left(\frac{d^2}{dx^2}g(x)\right)$$

$$-\frac{73408}{66825}\,g(x)\,y(x)\left(\frac{d^3}{dx^3}g(x)\right)-\frac{2368}{7425}\,g(x)^2\,y(x)\left(\frac{d}{dx}g(x)\right)$$

$$-\frac{2368}{155925}\,g(x)^3\left(\frac{d}{dx}y(x)\right)-\frac{30784}{66825}\left(\frac{d^4}{dx^4}g(x)\right)\left(\frac{d}{dx}y(x)\right)$$

$$-\frac{921152}{467775}\left(\frac{d}{dx}g(x)\right)y(x)\left(\frac{d^2}{dx^2}g(x)\right)$$

$$-\frac{4736}{14175}\left(\frac{d}{dx}g(x)\right)^2\left(\frac{d}{dx}y(x)\right)\Bigg]d^2$$

$$+h^{11}\Bigg[-\frac{478336}{155925}\left(\frac{d}{dx}g(x)\right)y(x)\left(\frac{d^4}{dx^4}g(x)\right)-\frac{1472896}{467775}\left(\frac{d}{dx}g(x)\right)$$

$$\left(\frac{d}{dx}y(x)\right)\left(\frac{d^3}{dx^3}g(x)\right)-\frac{2197504}{467775}\left(\frac{d^2}{dx^2}g(x)\right)y(x)\left(\frac{d^3}{dx^3}g(x)\right)$$

$$-\frac{705664}{467775}\,g(x)^2\,y(x)\left(\frac{d^3}{dx^3}g(x)\right)-\frac{75776}{66825}\left(\frac{d}{dx}g(x)\right)^3y(x)$$

$$-\frac{2368}{6075}\left(\frac{d^6}{dx^6}g(x)\right)\left(\frac{d}{dx}y(x)\right)-\frac{274688}{51975}\,g(x)$$

$$y(x)\left(\frac{d^2}{dx^2}g(x)\right)\left(\frac{d}{dx}g(x)\right)-\frac{2368}{13365}\left(\frac{d^7}{dx^7}g(x)\right)y(x)$$

$$-\frac{9472}{7425}\,g(x)\left(\frac{d}{dx}y(x)\right)\left(\frac{d^4}{dx^4}g(x)\right)-\frac{9472}{7425}\,g(x)\,y(x)$$

$$\left(\frac{d^5}{dx^5}g(x)\right)-\frac{336256}{467775}\,g(x)^2\left(\frac{d}{dx}y(x)\right)\left(\frac{d^2}{dx^2}g(x)\right)$$

$$- \frac{18944}{17325} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right)^2 - \frac{161024}{467775} g(x)^3 y(x) \left(\frac{d}{dx} g(x)\right)$$

$$- \frac{2368}{1155} \left(\frac{d^2}{dx^2} g(x)\right)^2 \left(\frac{d}{dx} y(x)\right) - \frac{2368}{155925} g(x)^4 \left(\frac{d}{dx} y(x)\right)\Bigg] d$$

$$+ h^{11} \Bigg[- \frac{2368}{18711} g(x)^4 y(x) \left(\frac{d}{dx} g(x)\right) - \frac{75776}{93555} g(x)^2$$

$$\left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right)^2 - \frac{37888}{22275} \left(\frac{d^3}{dx^3} g(x)\right)^2 \left(\frac{d}{dx} y(x)\right)$$

$$- \frac{2368}{51975} \left(\frac{d^8}{dx^8} g(x)\right) \left(\frac{d}{dx} y(x)\right) - \frac{2368}{467775} \left(\frac{d^9}{dx^9} g(x)\right) y(x)$$

$$- \frac{89984}{31185} \left(\frac{d}{dx} g(x)\right)^2 y(x) \left(\frac{d^3}{dx^3} g(x)\right) - \frac{2368}{693} \left(\frac{d}{dx} g(x)\right)$$

$$y(x) \left(\frac{d^2}{dx^2} g(x)\right)^2 - \frac{4736}{4455} \left(\frac{d^3}{dx^3} g(x)\right) y(x) \left(\frac{d^4}{dx^4} g(x)\right)$$

$$- \frac{146816}{51975} \left(\frac{d^2}{dx^2} g(x)\right) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^4}{dx^4} g(x)\right)$$

$$- \frac{4736}{5775} \left(\frac{d^2}{dx^2} g(x)\right) y(x) \left(\frac{d^5}{dx^5} g(x)\right)$$

$$- \frac{73408}{155925} \left(\frac{d}{dx} g(x)\right) y(x) \left(\frac{d^6}{dx^6} g(x)\right)$$

$$- \frac{80512}{51975} \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^5}{dx^5} g(x)\right)$$

$$- \frac{18944}{4725} \left(\frac{d}{dx} g(x)\right)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)$$

$$- \frac{18944}{13365} g(x) y(x) \left(\frac{d}{dx} g(x)\right)^3 - \frac{2368}{467775} g(x)^5 \left(\frac{d}{dx} y(x)\right)$$

$$- \frac{4736}{13365} g(x)^3 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)$$

$$- \frac{393088}{467775} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^4}{dx^4} g(x)\right)$$

$$- \frac{139712}{51975} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)^2$$

$$- \frac{61568}{93555} g(x)^3 y(x) \left(\frac{d^3}{dx^3} g(x)\right) - \frac{350464}{467775} g(x)^2 y(x) \left(\frac{d^5}{dx^5} g(x)\right)$$

$$- \frac{87616}{467775} g(x) y(x) \left(\frac{d^7}{dx^7} g(x)\right) - \frac{30784}{66825} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^6}{dx^6} g(x)\right)$$

$$- \frac{492544}{93555}\, g(x)\, y(x) \left(\frac{d^2}{dx^2}\, g(x)\right) \left(\frac{d^3}{dx^3}\, g(x)\right)$$
$$- \frac{1937024}{467775}\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^3}{dx^3}\, g(x)\right) \left(\frac{d}{dx}\, g(x)\right)$$
$$- \frac{108928}{31185}\, g(x)\, y(x) \left(\frac{d^4}{dx^4}\, g(x)\right) \left(\frac{d}{dx}\, g(x)\right)$$
$$- \frac{317312}{93555}\, g(x)^2\, y(x) \left(\frac{d^2}{dx^2}\, g(x)\right) \left(\frac{d}{dx}\, g(x)\right)\Bigg] \tag{56}$$

$$L.T.E\,(h)_{MIX} = h^{11} \left[\frac{2368}{155925}\, g(x) \left(\frac{d}{dx}\, y(x)\right)\right.$$
$$\left. + \frac{44992}{467775} \left(\frac{d}{dx}\, g(x)\right) y(x)\right] d^4 + h^{11} \left[\frac{18944}{467775}\, g(x)^2 \left(\frac{d}{dx}\, y(x)\right)\right.$$
$$+ \frac{37888}{155925} \left(\frac{d^2}{dx^2}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right) + \frac{161024}{467775}\, g(x)\, y(x) \left(\frac{d}{dx}\, g(x)\right)$$
$$\left. + \frac{18944}{66825} \left(\frac{d^3}{dx^3}\, g(x)\right) y(x)\right] d^3 + h^{11} \left[\frac{4736}{155925}\, g(x)^3 \left(\frac{d}{dx}\, y(x)\right)\right.$$
$$+ \frac{4736}{93555} \left(\frac{d}{dx}\, g(x)\right) y(x) \left(\frac{d^2}{dx^2}\, g(x)\right)$$
$$+ \frac{61568}{155925}\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^2}{dx^2}\, g(x)\right)$$
$$+ \frac{4736}{17325}\, g(x)^2\, y(x) \left(\frac{d}{dx}\, g(x)\right) + \frac{4736}{66825} \left(\frac{d^4}{dx^4}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right)$$
$$- \frac{4736}{22275} \left(\frac{d^5}{dx^5}\, g(x)\right) y(x) + \frac{9472}{31185} \left(\frac{d}{dx}\, g(x)\right)^2 \left(\frac{d}{dx}\, y(x)\right)$$
$$\left. + \frac{61568}{467775}\, g(x)\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)\right] d^2$$
$$+h^{11} \left[- \frac{9472}{14175}\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^4}{dx^4}\, g(x)\right) - \frac{9472}{93555}\, g(x)^3\, y(x) \left(\frac{d}{dx}\, g(x)\right)\right.$$
$$- \frac{18944}{6237}\, g(x)\, y(x) \left(\frac{d}{dx}\, g(x)\right) \left(\frac{d^2}{dx^2}\, g(x)\right)$$
$$- \frac{18944}{17325} \left(\frac{d^2}{dx^2}\, g(x)\right)^2 \left(\frac{d}{dx}\, y(x)\right)$$
$$- \frac{146816}{155925}\, g(x)\, y(x) \left(\frac{d^5}{dx^5}\, g(x)\right) - \frac{75776}{93555}\, g(x)^2\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)$$
$$- \frac{75776}{467775} \left(\frac{d^7}{dx^7}\, g(x)\right) y(x) - \frac{18944}{66825} \left(\frac{d^6}{dx^6}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right)$$

$$- \frac{9472}{31185} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right)^2 - \frac{9472}{13365} \left(\frac{d}{dx} g(x)\right)^3 y(x)$$
$$- \frac{18944}{93555} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)$$
$$- \frac{776704}{467775} \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^3}{dx^3} g(x)\right)$$
$$- \frac{75776}{31185} \left(\frac{d}{dx} g(x)\right) y(x) \left(\frac{d^4}{dx^4} g(x)\right)$$
$$- \frac{359936}{93555} \left(\frac{d^2}{dx^2} g(x)\right) y(x) \left(\frac{d^3}{dx^3} g(x)\right)\Bigg] d$$
$$+h^{11} \Bigg[- \frac{2368}{693} \left(\frac{d}{dx} g(x)\right) y(x) \left(\frac{d^2}{dx^2} g(x)\right)^2 - \frac{2368}{18711} g(x)^4 y(x) \left(\frac{d}{dx} g(x)\right)$$
$$- \frac{2368}{467775} \left(\frac{d^9}{dx^9} g(x)\right) y(x) - \frac{2368}{51975} \left(\frac{d^8}{dx^8} g(x)\right) \left(\frac{d}{dx} y(x)\right)$$
$$- \frac{37888}{22275} \left(\frac{d^3}{dx^3} g(x)\right)^2 \left(\frac{d}{dx} y(x)\right) - \frac{350464}{467775} g(x)^2 y(x) \left(\frac{d^5}{dx^5} g(x)\right)$$
$$- \frac{80512}{51975} \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^5}{dx^5} g(x)\right) - \frac{89984}{31185} \left(\frac{d}{dx} g(x)\right)^2$$
$$y(x) \left(\frac{d^3}{dx^3} g(x)\right) - \frac{146816}{51975} \left(\frac{d^2}{dx^2} g(x)\right) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^4}{dx^4} g(x)\right)$$
$$- \frac{4736}{5775} \left(\frac{d^2}{dx^2} g(x)\right) y(x) \left(\frac{d^5}{dx^5} g(x)\right)$$
$$- \frac{4736}{4455} \left(\frac{d^3}{dx^3} g(x)\right) y(x) \left(\frac{d^4}{dx^4} g(x)\right)$$
$$- \frac{73408}{155925} \left(\frac{d}{dx} g(x)\right) y(x) \left(\frac{d^6}{dx^6} g(x)\right)$$
$$- \frac{18944}{4725} \left(\frac{d}{dx} g(x)\right)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)$$
$$- \frac{75776}{93555} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right)^2$$
$$- \frac{317312}{93555} g(x)^2 y(x) \left(\frac{d}{dx} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)$$
$$- \frac{1937024}{467775} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \left(\frac{d}{dx} g(x)\right)$$
$$- \frac{108928}{31185} g(x) y(x) \left(\frac{d^4}{dx^4} g(x)\right) \left(\frac{d}{dx} g(x)\right)$$

$$
\begin{aligned}
&-\frac{492544}{93555}\, g(x)\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)\left(\frac{d^2}{dx^2}\, g(x)\right)\\
&-\frac{2368}{467775}\, g(x)^5 \left(\frac{d}{dx}\, y(x)\right)-\frac{18944}{13365}\, g(x)\, y(x) \left(\frac{d}{dx}\, g(x)\right)^3\\
&-\frac{393088}{467775}\, g(x)^2 \left(\frac{d}{dx}\, y(x)\right)\left(\frac{d^4}{dx^4}\, g(x)\right)-\frac{61568}{93555}\, g(x)^3\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)\\
&-\frac{87616}{467775}\, g(x)\, y(x) \left(\frac{d^7}{dx^7}\, g(x)\right)-\frac{30784}{66825}\, g(x) \left(\frac{d}{dx}\, y(x)\right)\left(\frac{d^6}{dx^6}\, g(x)\right)\\
&-\frac{139712}{51975}\, g(x) \left(\frac{d}{dx}\, y(x)\right)\left(\frac{d^2}{dx^2}\, g(x)\right)^2\\
&-\frac{4736}{13365}\, g(x)^3 \left(\frac{d}{dx}\, y(x)\right)\left(\frac{d^2}{dx^2}\, g(x)\right)\Bigg]
\end{aligned}
\tag{57}
$$

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