J Math Chem (2009) 46:692–725
DOI 10.1007/s10910-008-9509-x

ORIGINAL PAPER

High order multistep methods with improved phase-lag characteristics for the integration of the Schrödinger equation

D. S. Vlachos · Z. A. Anastassi · T. E. Simos

Received: 5 October 2008 / Accepted: 10 October 2008 / Published online: 6 January 2009

Abstract In this work we introduce a new family of 12-step linear multistep methods for the integration of the Schrödinger equation. The new methods are constructed by adopting a new methodology which improves the phase lag characteristics by vanishing both the phase lag function and its first derivatives at a specific frequency. This results in decreasing the sensitivity of the integration method on the estimated frequency of the problem. The efficiency of the new family of methods is proved via error analysis and numerical applications.

Keywords Numerical solution · Schrödinger equation · Multistep methods · Hybrid methods · P-stability · Phase-lag · Phase-fitted

T. E. Simos is a highly cited researcher, active member of the European Academy of Sciences and Arts. Corresponding member of the European Academy of Sciences, corresponding member of European Academy of Arts, Sciences and Humanities.

D. S. Vlachos · Z. A. Anastassi · 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

D. S. Vlachos
e-mail: dvlachos@uop.gr

Z. A. Anastassi
e-mail: zackanas@uop.gr

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

1 Introduction

The numerical integration of systems of ordinary differential equations with oscillatory solutions has been a subject of research during the past decades. This type of ODEs is often met in real problems, like the Schrödinger equation and the N-body problem. For problems having highly oscillatory solutions, standard methods with unspecialized use can require a huge number of steps to track the oscillations. One way to obtain a more efficient integration process is to construct numerical methods with an increased algebraic order, although the implementation of high algebraic order meets several difficulties [1].

On the other hand, there are some special techniques for optimizing numerical methods. Trigonometrical fitting and phase-fitting are some of them, producing methods with variable coefficients, which depend on $v = \omega h$, where ω is the dominant frequency of the problem and h is the step length of integration. More precisely, the coefficients of a general linear method are found from the requirement that it integrates exactly powers up to degree $p + 1$. For problems having oscillatory solutions, more efficient methods are obtained when they are exact for every linear combination of functions from the reference set

$$\{1, x, \ldots, x^K, e^{\pm\mu x}, \ldots, x^P e^{\pm\mu x}\} \tag{1}$$

This technique is known as exponential (or trigonometric if $\mu = i\omega$) fitting and has a long history [2,3]. The set (1) is characterized by two integer parameters, K and P. The set in which there is no classical component is identified by $K = -1$ while the set in which there is no exponential fitting component (the classical case) is identified by $P = -1$. Parameter P will be called the level of tuning. An important property of exponential fitted algorithms is that they tend to the corresponding classical ones when the involved frequencies tend to zero, a fact which allows us to say that exponential fitting represents a natural extension of the classical polynomial fitting. The examination of the convergence of exponential fitted multistep methods is included in Lyche's theory [2]. There is a large number of significant methods presented with high practical importance that have been presented in the bibliography. The general theory is presented in detail in [4].

Considering the accuracy of a method, when solving oscillatory problems, it is more appropriate to work with the phase-lag, rather than the principle local truncation error. We mention the pioneering paper of Brusa and Nigro [5], in which the phase-lag property was introduced. This is actually another type of a truncation error, i.e. the angle between the analytical solution and the numerical solution. On the other hand, exponential fitting is accurate only when a good estimate of the dominant frequency of the solution is known in advance. This means that in practice, if a small change in the dominant frequency is introduced, the efficiency of the method can be dramatically altered. It is well known that for equations similar to the harmonic oscillator the most efficient exponential fitted methods are those with the highest tuning level. A lot of significant work has been made during the last years in this field, mainly focusing for obvious reasons in the solution of the Schrödinger equation (see for example [6–128].

In this paper we present a new family of methods based on the 12-step linear multistep method of Quinlan and Tremaine [129]. The new methods are constructed by vanishing the phase-lag function and its first derivatives at a predefined frequency. Error analysis and numerical experiments show that the new methods exhibit improved characteristics concerning the solution of the time-independent Schrödinger equation. The paper is organized as follows: In Sect. 2 the general theory of the new methodology is presented. In Sect. 3 the new methods are described in detail. In Sect. 4 the stability properties of the new methods are investigated. Section 5 presents the results from the numerical experiments and finally, conclusions are drawn in Sect. 6.

2 Phase-lag analysis of symmetric multistep methods

Consider the differential equations

$$\frac{d^2y(t)}{dt^2} = f(t, y), \;\; y(t_0) = y_0, \;\; y'(t_0) = y'_0 \tag{2}$$

and the linear multistep methods

$$\sum_{j=0}^{J} a_j y_{n+j} = h^2 \sum_{j=0}^{J} b_j f_{n+j} \tag{3}$$

where $y_{n+j} = y(t_0 + (n+j)h)$, $f_{n+j} = f(t_0 + (n+j)h, y(t_0 + (n+j)h))$ and h is the step size of the method. With the method (3), we associate the following functional

$$L(h, a, b, y(t)) = \sum_{j=0}^{J} a_j y(t + j \cdot h) - h^2 \sum_{j=0}^{J} b_j y''(t + j \cdot h) \tag{4}$$

where a, b are the vectors of coefficients a_j and b_j respectively, and $y(t)$ is an arbitrary function. The algebraic order of the method (3) is p, if

$$L(h, a, b, y(t)) = C_{p+2} h^{p+2} y^{(p+2)}(t) + O(h^{p+3}) \tag{5}$$

The coefficients C_q are given

$$\begin{aligned} C_0 &= \sum_{j=0}^{J} a_j \\ C_1 &= \sum_{j=0}^{J} j \cdot a_j \\ c_q &= \frac{1}{q!} \sum_{j=0}^{J} j^q \cdot a_j - \frac{1}{(q-2)!} \sum_{j=0}^{J} j^{q-2} b_j \end{aligned} \tag{6}$$

The principle local truncation error (PLTE) is the leading term of (5)

$$plte = C_{p+2}h^{p+2}y^{(p+2)}(t) \tag{7}$$

The following assumptions will be considered in the rest of the paper:

(1) $a_J = 1$, since we can always divide the coefficients of (3) with a_J.
(2) $|a_0| + |b_0| \neq 0$, since otherwise we can assume that $J = J - 1$.
(3) $\sum_{j=0}^{J} |b_j| \neq 0$, since otherwise the solution of (3) would be independent of (2).
(4) The method (3) is at least of order one.
(5) The method (3) is zero stable, which means that the roots of the polynomial

$$p(z) = \sum_{j=0}^{J} a_j z^j \tag{8}$$

all lie in the unit disc, and those that lie on the unit circle have multiplicity one.

(6) The method (3) is symmetric, which means that

$$a_j = a_{J-j},\ b_j = b_{J-j},\ j = 0(1)J \tag{9}$$

It is easily proved that both the order of the method and the step number J are even numbers [130].

Consider now the test problems

$$y''(t) = -\omega^2 y(t) \tag{10}$$

where ω is a constant. The numerical solution of (10) by applying method (3) is described by the difference equation

$$\sum_{j=1}^{J/2} A_j(s^2)(y_{n+j} + y_{n-j}) + A_0(s^2)y_n = 0 \tag{11}$$

with

$$A_j(s^2) = a_{\frac{J}{2}-j} + s^2 \cdot b_{\frac{J}{2}-j} \tag{12}$$

and $s = \omega h$. The characteristic equation is then given by

$$\sum_{j=1}^{J/2} A_j(s^2)(z^j + z^{-j}) + A_0(s^2) = 0 \tag{13}$$

and the interval of periodicity $(0, s_0^2)$ is then defined such that for $s \in (0, s_0)$ the roots of (13) are of the form

$$z_1 = e^{i\lambda(s)}, \quad z_2 = e^{-i\lambda(s)}, \quad |z_j| \leq 1,\ 3 \leq j \leq J \tag{14}$$

where $\lambda(s)$ is a real function of s. The phase-lag PL of the method (3) is then defined

$$PL = s - \lambda(s) \tag{15}$$

and is of order q if

$$PL = c \cdot s^{q+1} + O(s^{q+3}) \tag{16}$$

In general, the coefficients of the method (3) depend on some parameter v, thus the coefficients A_j are functions of both s^2 and v. The following theorem was proved by Simos and Williams [131]: For the symmetric method (10) the phase-lag is given

$$PL(s, v) = \frac{2\sum_{j=1}^{J/2} A_j(s^2, v) \cdot cos(j \cdot s) + A_0(s^2, v)}{2\sum_{j=1}^{J/2} j^2 A_j(s^2, v)} \tag{17}$$

We are now in position to describe the new methodology. In order to efficiently integrate oscillatory problems, it is a good practice to calculate the coefficients of the numerical method by forcing the phase lag to be zero at a specific frequency. But, since the appropriate frequency is problem dependent and in general is not always known, we may assume that we have an error in the frequency estimation. It would be of great importance to force the phase-lag to be insensitive to this error. Thus, beyond the vanishing of the phase-lag, we also force its first derivatives to be zero.

3 Construction of the new methods

3.1 Classical method

The family of new methods is based on the 12-step linear multistep method of Quinlan and Tremaine [129] which is of the form (3) with coefficients

$$\begin{array}{llll} a_0 = 1 & a_1 = -2 & a_2 = 2 & a_3 = -1 \\ a_4 = 0 & a_5 = 0 & a_6 = 0 & \\ b_0 = 0 & b_1 = \frac{90987349}{53222400} & b_2 = -\frac{-114798419}{26611200} & b_3 = \frac{270875723}{17740800} \\ b_4 = -\frac{-67855831}{2217600} & b_5 = \frac{50277247}{985600} & b_6 = \frac{-253491379}{4435200} & \end{array} \tag{18}$$

The PLTE of the method is given:

$$plte = \left\{ \frac{16301796103 y^{(14)}\, h^{14}}{290594304000} + O\left(h^{16}\right) \right\} \tag{19}$$

3.2 New methods using phase fitting

The methods that are constructed are named as *PF-Di*, where:

- *PF-D0*: the phase lag function is zero at the frequency $v = \omega * h$.
- *PF-D1*: the phase lag function and its first derivative are zero at the frequency $v = \omega * h$.
- *PF-D2*: the phase lag function and its first and second derivatives are zero at the frequency $v = \omega * h$.
- *PF-D3*: the phase lag function and its first, second and third derivatives are zero at the frequency $v = \omega * h$.
- *PF-D4*: the phase lag function and its first, second, third and fourth derivatives are zero at the frequency $v = \omega * h$.
- *PF-D5*: the phase lag function and its first, second, third, fourth and fifth derivatives are zero at the frequency $v = \omega * h$.

The coefficients of the methods in the form:

$$
\begin{aligned}
b_1^i &= \frac{b_{1,num}^i}{b_{1,denum}^i} \\
b_2^i &= \frac{b_{2,num}^i}{b_{2,denum}^i} \\
b_3^i &= \frac{b_{3,num}^i}{b_{3,denum}^i} \\
b_4^i &= \frac{b_{4,num}^i}{b_{4,denum}^i} \\
b_5^i &= \frac{b_{5,num}^i}{b_{5,denum}^i} \\
b_6^i &= \frac{b_{6,num}^i}{b_{6,denum}^i}
\end{aligned}
$$

where the coefficients b^i correspond to the method *PF-Di*. Since for small values of v, the above formulae are subject to heavy cancelations, the Taylor expansions of the coefficients have been calculated as b_T^i. The exact formula of all coefficients are given in Appendix.

The principle local truncation errors of the methods are given by

$$plte_i = \frac{16301796103}{290594304000} coeff_i,$$

where

$$
\begin{aligned}
coeff_0 &= \left(y^{(12)}\omega^2 + y^{(14)}\right)\ h^{14}\\
coeff_1 &= \left(y^{(10)}\omega^4 + 2y^{(12)}\omega^2 + y^{(14)}\right) h^{14}\\
coeff_2 &= \left(y^{(8)}\omega^6 + 3y^{(10)}\omega^4 + 3y^{(12)}\omega^2 + y^{(14)}\right)\ h^{14}\\
coeff_3 &= \left(y^{(6)}\omega^8 + 4y^{(8)}\omega^6 + 6\ y^{(10)}\omega^4 + 4y^{(12)}\omega^2 + y^{(14)}\right) h^{14}\\
coeff_4 &= \Big(y^{(4)}\omega^{10} + 5y^{(6)}\omega^{\ 8} + 10y^{(8)}\omega^6 + 10y^{(10)}\omega^4\\
&\quad + 5y^{(12)}\omega^2 + y^{(14)}\Big) h^{14}\\
coeff_5 &= \Big(y^{(2)}\omega^{12} + 6y^{(4)}\omega^{10} + 15y^{(6)}\omega^8 + 20y^{(8)}\omega^6\\
&\quad + 15y^{(10)}\omega^4 + 6y^{(12)}\ \omega^2 + y^{(14)}\Big) h^{14}
\end{aligned}
\tag{20}
$$

4 Stability analysis

The stability of the new methods is studied by considering the test equation

$$\frac{d^2y(t)}{dt^2} = -\sigma^2 y(t) \tag{21}$$

and the linear multistep method (3) for the numerical solution. In the above equation $\sigma \neq \omega$ (ω is the frequency at which the phase-lag function and its derivatives vanish). By setting $s = \sigma h$ and $v = \omega h$, we get for the characteristic equation of the applied method

$$\sum_{j=1}^{J/2} A_j(s^2, v)(z^j + z^{-j}) + A_0(s^2, v) = 0 \tag{22}$$

where

$$A_j(s^2, v) = a_{\frac{J}{2}-j}(v) + s^2 \cdot b_{\frac{J}{2}-j}(v) \tag{23}$$

The motivation of the above analysis is straightforward: Although the coefficients of the method (3) are designed in a way that the phase-lag and its first derivatives vanish in the frequency ω, the frequency ω itself is unknown and only an estimation can be made. Thus, if the correct frequency of the problem is σ we have to check if the method is stable, that is if the roots of the characteristic equation lie in the unit disk. For this reason we draw in the s–v plane the areas in which the method is stable. Fig. 1 shows the stability region for the classical method and Fig. 2 for the six methods (the phase fitted one and those with first,second, third, fourth and fifth phase lag derivative elimination). Note here that the s-axis corresponds to the real frequency while the

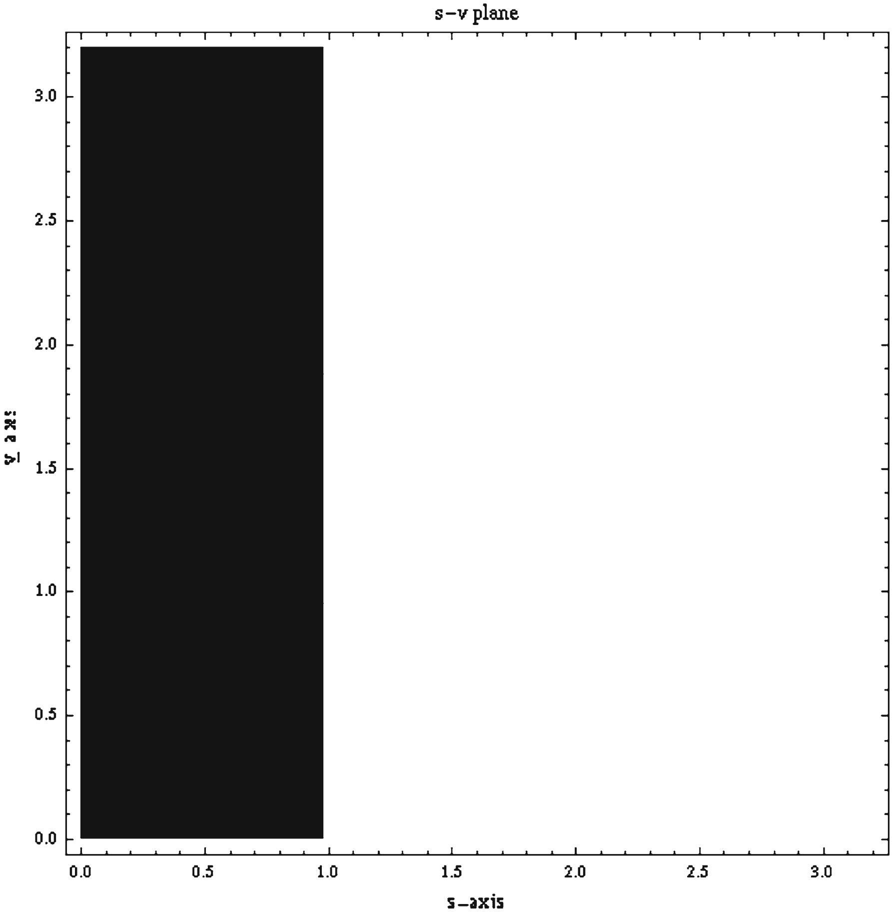

Fig. 1 The stability region (s–v plane) of the classical Quinlan-Tremaine 12-step method

v-axis corresponds to the estimated frequency used to construct the parameters of the method.

5 Numerical results

The radial Schrödinger equation is given by:

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - E \right) y(x) \tag{24}$$

where $\frac{l(l+1)}{x^2}$ is the centrifugal potential, $V(x)$ is the potential, E is the Energy and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the effective potential. It is valid that $lim_{x \to \infty} V(x) = 0$ and therefore $lim_{x \to \infty} W(x) = 0$. We consider that $E > 0$ and we divide the interval

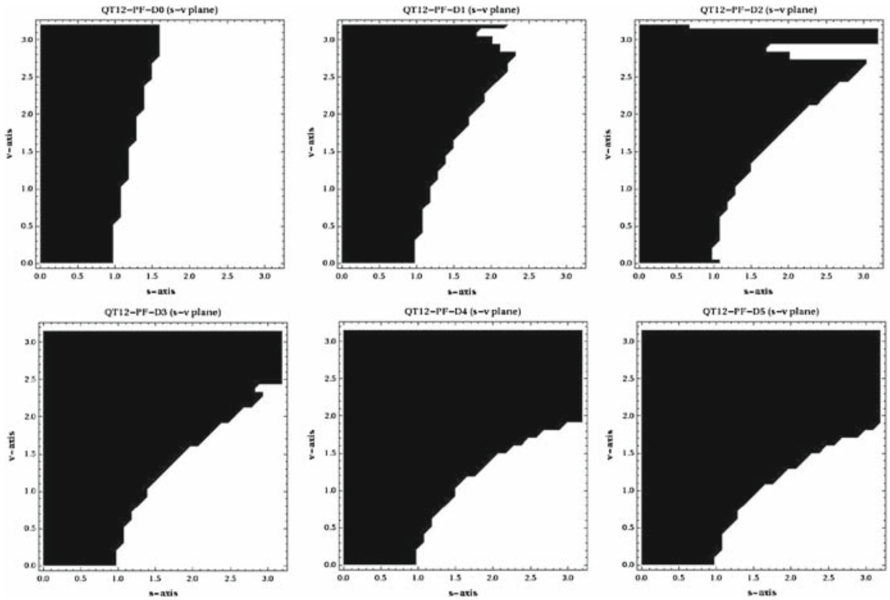

Fig. 2 The stability region of the methods PF-D0,PF-D1, PF-D2, PF-D3, PF-D4 and PF-D5 (from *left* to *right* and from *top* to *bottom*)

$[0, +\infty)$ into subintervals $[a_i, b_i]$ so that $W(x)$ can be considered constant inside each subinterval with value $\hat{W}_i$. The problem (24) can be expressed now by the equations

$$y_i'' = (\hat{W}_i - E)y_i \tag{25}$$

whose solution are

$$y_i(x) = \left(A_i e^{\sqrt{\hat{W}_i - E}x} + B_i e^{-\sqrt{\hat{W}_i - E}x}\right) \tag{26}$$

with $A_i, B_i \in R$. We will integrate problem (24) with $l = 0$ at the interval [0, 15] using the well known Woods-Saxon potential:

$$V(x) = \frac{u_0}{1+q} + \frac{U_1 q}{(1+q)^2}, \quad q = e^{\frac{x-x_0}{a}} \tag{27}$$

where $u_0 = -50, a = 0.6, x_0 = 7, u_1 = -\frac{u_0}{a}$ and with boundary condition $y(0) = 0$. The potential $V(x)$ decays more quickly than $\frac{l(l+1)}{x^2}$, so for large x (asymptotic region) the Schrödinger equation (24) becomes

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{28}$$

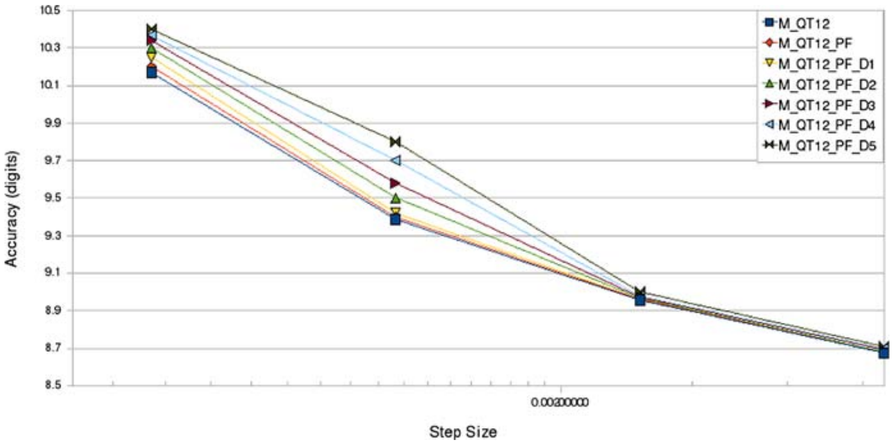

Fig. 3 The accuracy (digits) of the new methods compared to the classical one for the Schrödinger equation ($E = 989.701916$)

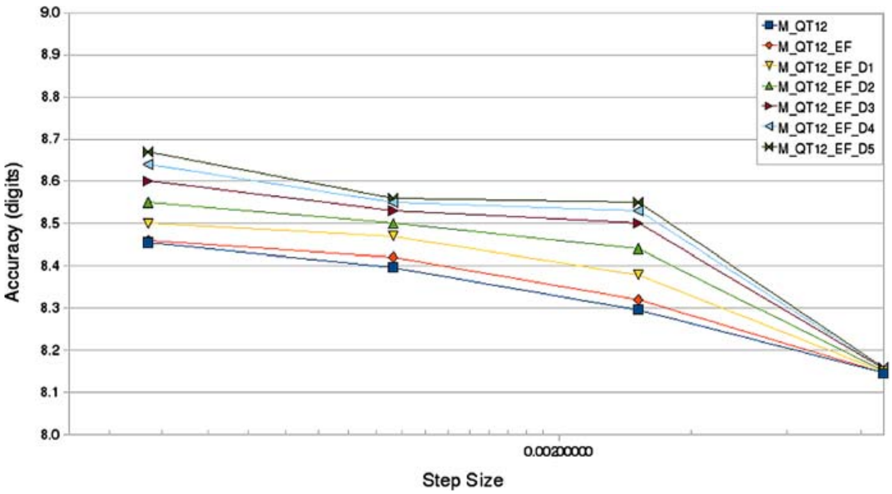

Fig. 4 The accuracy (digits) of the new methods compared to the classical one for the Schrödinger equation ($E = 341.495874$)

The last equation has two linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where j_l and n_l are the spherical *Bessel* and *Neumann* functions and $k = \sqrt{\frac{l(l+1)}{x^2} - E}$. When $x \to \infty$ the solution takes the asymptotic form

$$\begin{aligned} y(x) &\sim Akxj_l(kx) - Bkxn_l(kx) \\ &\sim D\left[sin\left(kx - \pi\frac{l}{2}\right) + tan(\delta_l)\cos\left(kx - \pi\frac{l}{2}\right)\right], \end{aligned} \tag{29}$$

where δ_l is called the *scattering phase shift* and it is given by the following expression:

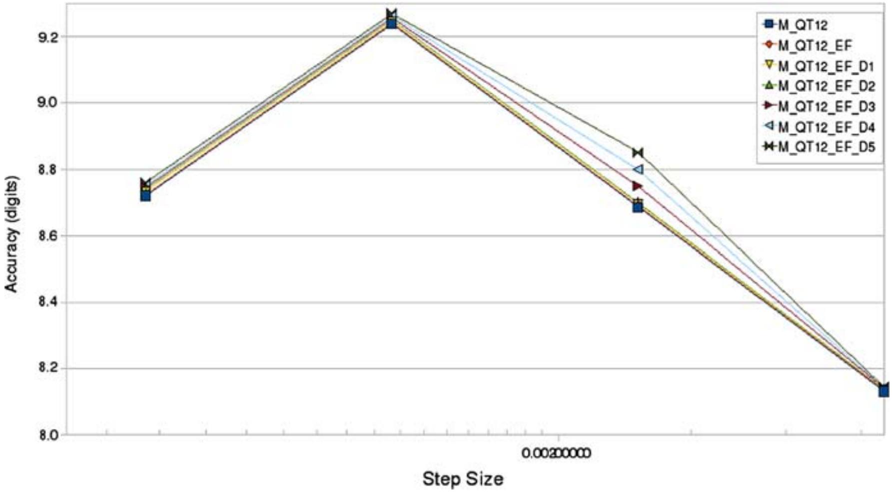

Fig. 5 The accuracy (digits) of the new methods compared to the classical one for the Schrödinger equation ($E = 163.215341$)

$$tan(\delta_l) = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})} \tag{30}$$

where $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$ and $x_i < x_{i+1}$ and both belong to the asymptotic region. Given the energy, we approximate the phase shift, the accurate value of which is $\frac{\pi}{2}$ for the above problem. We will use three different values for the energy: (i) 989.701916, (ii) 341.495874 and (iii) 163.215341. As for the frequency ω we will use the suggestion of Ixaru and Rizea [132]:

$$\omega = \begin{cases} \sqrt{E - 50}, & x \in [0, 6.5] \\ \sqrt{E}, & x \in [6.5, 15] \end{cases} \tag{31}$$

The results are shown in Figs. 3, 4 and 5. It is clear that the accuracy increases as the number of the eliminated derivatives of the phase lag function increases.

6 Conclusions

We have presented a new family of 12-step symmetric multistep numerical methods with improved characteristics concerning the integration of the Schrödinger equation. The methods were constructed by adopting a new methodology which, except for the phase fitting at a predefined frequency, it eliminates the first derivatives of the phase lag function at the same frequency. The result is that the phase lag function becomes less sensitive on the frequency near the predefined one. This behavior compensates the fact that the exact frequency can only be estimated. Experimental results demonstrate this behavior by showing that the accuracy is increased as the number of the derivatives that are eliminated is increased.

Appendix

Method *PF-D0*:

$$
\begin{aligned}
b^0_{1,num} &= ((-124184636\cos(v) + 70378348\cos(2v) - 24862148\cos(3v)\\
&\quad + 5153611\cos(4v))v^2 + 25(3013169v^2 - 16128\cos(3v)\\
&\quad + 32256\cos(4v) - 32256\cos(5v) + 16128\cos(6v)))\csc^{10}\left(\frac{v}{2}\right)\\
b^0_{2,num} &= (v^2(159588050\cos(v) - 85350160\cos(2v)\\
&\quad + 16708985\cos(3v) - 5153611\cos(5v)) - 16(6496079v^2\\
&\quad - 252000\cos(3v) + 504000\cos(4v)\\
&\quad - 504000\cos(5v) + 252000\cos(6v)))\csc^{10}\left(\frac{v}{2}\right)\\
b^0_{3,num} &= ((-367257540\cos(v) + 183567900\cos(2v)\\
&\quad - 16708985\cos(4v) + 24862148\cos(5v))v^2\\
&\quad + 81(3175117v^2 - 224000\cos(3v) + 448000\cos(4v)\\
&\quad - 448000\cos(5v) + 224000\cos(6v)))\csc^{10}\left(\frac{v}{2}\right)\\
b^0_{4,num} &= (30675810\cos(v)v^2 - 42958788v^2\\
&\quad + 75(161280 - 611893v^2)\cos(3v)\\
&\quad + 140(152411v^2 - 172800)\cos(4v)\\
&\quad + (24192000 - 17594587v^2)\cos(5v) - 12096000\cos(6v))\csc^{10}\left(\frac{v}{2}\right)\\
b^0_{5,num} &= (-61351620\cos(2v)v^2 + 85936557v^2\\
&\quad + 30(6120959v^2 - 1411200)\cos(3v)\\
&\quad + 25(3386880 - 3191761v^2)\cos(4v)\\
&\quad + (62092318v^2 - 84672000)\cos(5v) + 42336000\cos(6v))\csc^{10}\left(\frac{v}{2}\right)\\
b^0_{6,num} &= ((-171873114\cos(v) + 171835152\cos(2v)\\
&\quad - 257184477\cos(3v) + 103937264\cos(4v)\\
&\quad - 75329225\cos(5v))v^2 + 50803200(\cos(3v) - 2\cos(4v)\\
&\quad + 2\cos(5v) - \cos(6v)))\csc^{10}\left(\frac{v}{2}\right)\\
b^0_{1,denom} &= 206438400v^2\\
b^0_{2,denom} &= 206438400v^2\\
b^0_{3,denom} &= 206438400v^2\\
b^0_{4,denom} &= 51609600v^2\\
b^0_{5,denom} &= 103219200v^2\\
b^0_{6,denom} &= 103219200v^2 \qquad (32)
\end{aligned}
$$

$$\begin{aligned}
b_{T,1}^{0} &= \frac{90987349}{53222400} - \frac{16301796103v^2}{290594304000} + \frac{2012122579v^4}{581188608000} \\
&\quad - \frac{48410309v^6}{1184440320000} + \frac{991945331743v^8}{2838385676206080000} - \cdots \\
b_{T,2}^{0} &= -\frac{114798419}{26611200} + \frac{16301796103v^2}{29059430400} - \frac{2012122579v^4}{58118860800} \\
&\quad + \frac{48410309v^6}{118444032000} - \frac{991945331743v^8}{283838567620608000} + \cdots \\
b_{T,3}^{0} &= \frac{270875723}{17740800} - \frac{16301796103v^2}{6457651200} + \frac{2012122579v^4}{12915302400} \\
&\quad - \frac{48410309v^6}{26320896000} + \frac{991945331743v^8}{63075237249024000} - \cdots \\
b_{T,4}^{0} &= -\frac{67855831}{2217600} + \frac{16301796103v^2}{2421619200} - \frac{2012122579v^4}{4843238400} \\
&\quad + \frac{48410309v^6}{9870336000} - \frac{991945331743v^8}{23653213968384000} + \cdots \\
b_{T,5}^{0} &= \frac{50277247}{985600} - \frac{16301796103v^2}{1383782400} + \frac{2012122579v^4}{2767564800} \\
&\quad - \frac{48410309v^6}{5640192000} + \frac{991945331743v^8}{13516122267648000} - \cdots \\
b_{T,6}^{0} &= -\frac{253491379}{4435200} + \frac{16301796103v^2}{1153152000} - \frac{2012122579v^4}{2306304000} \\
&\quad + \frac{48410309v^6}{4700160000} - \frac{991945331743v^8}{11263435223040000} + \cdots
\end{aligned} \tag{33}$$

Method *PF-D1*:

$$\begin{aligned}
b_{1,num}^{1} &= \csc^{10}\left(\frac{v}{2}\right)\sec\left(\frac{v}{2}\right)(53760(2\cos(v)+2\cos(2v)+2\cos(3v) \\
&\quad +2\cos(5\,v)+1)\sin^3\left(\frac{v}{2}\right)+v\left(\left(304823\cos\left(\frac{v}{2}\right)-828603\cos\left(\frac{3v}{2}\right)\right.\right. \\
&\quad \left.+554639\cos\left(\frac{5v}{2}\right)-272779\cos\left(\frac{7v}{2}\right)\right)v^2+6720\left(7\cos\left(\frac{5v}{2}\right)\right. \\
&\quad \left.\left.\left.-15\cos\left(\frac{7v}{2}\right)+2\left(9\cos\left(\frac{9v}{2}\right)-6\cos\left(\frac{11v}{2}\right)+\cos\left(\frac{13v}{2}\right)\right)\right)\right)\right) \\
b_{2,num}^{1} &= \csc^7\left(\frac{v}{2}\right)\left(v((393310\cos(2v)-211395\cos(3v)\right. \\
&\quad +272779\cos(4v))v^2+(122851v^2+1088640)\cos(v) \\
&\quad -15(-1817v^2+74368\cos(2v)-65856\cos(3v)+45248\cos(4v) \\
&\quad -19040\cos(5v)+1344\cos(6v)+224\cos(7v)+36288))\csc^3\left(\frac{v}{2}\right)
\end{aligned}$$

$$
\begin{aligned}
&\quad - 26880(10\cos(v) + 10\cos(2v) + 9\cos(3v) + 2\cos(4v) \\
&\quad + 8\cos(5v) + \cos(6v) + 5)\sec\left(\frac{v}{2}\right)\Bigg) \\
b^1_{3,num} &= \csc^7\left(\frac{v}{2}\right)\Bigg(26880(90\cos(v) + 90\cos(2v) + 74\cos(3v) \\
&\quad + 32\cos(4v) + 58\cos(5v) + 16\cos(6v) + 45)\sec\left(\frac{v}{2}\right) \\
&\quad - v((2519110\cos(2v) - 654530\cos(3v) + 272779(6\cos(4v) \\
&\quad + \cos(5v)))v^2 + (1288471v^2 + 4717440)\cos(v) + 8(47587v^2 \\
&\quad - 643440\cos(2v) + 593880\cos(3v) - 416640\cos(4v) \\
&\quad + 159600\cos(5v) + 18480\cos(6v) - 6720\cos(7v) \\
&\quad -294840))\csc^3\left(\frac{v}{2}\right)\Bigg) \\
b^1_{4,num} &= \csc^7\left(\frac{v}{2}\right)\Bigg(v(1578002v^2 + 2(161489v^2 + 725760)\cos(v) \\
&\quad + 160(20521v^2 - 13776)\cos(2v) + 5(478464 - 4069v^2)\cos(3\,v) \\
&\quad + 2(738791v^2 - 900480)\cos(4v) + 3(205341v^2 + 156800)\cos(5v) \\
&\quad + 510720\cos(6v) - 94080\cos(7v) - 725760)\csc^3\left(\frac{v}{2}\right) \\
&\quad - 107520(30\cos(v) + 30\cos(2v) + 23\cos(3v) + 14\cos(4v) \\
&\quad + 16\cos(5v) + 7\cos(6v) + 15)\sec\left(\frac{v}{2}\right)\Bigg) \\
b^1_{5,num} &= -\csc^7\left(\frac{v}{2}\right)\Bigg(v(923342v^2 + 28(343339v^2 - 181440)\cos(v) \\
&\quad + 20(240593\,v^2 + 103488)\cos(2v) + 5(832859v^2 + 18816)\cos(3v) \\
&\quad + 2(1574159v^2 - 376320)\cos(4v) + 3(913431v^2 - 313600)\cos(5v) \\
&\quad + 2446080\cos(6v) - 376320\cos(7v) + 2540160)\csc^3\left(\frac{v}{2}\right) \\
&\quad - 376320(30\cos(v) + 30\cos(2v) + 22\cos(3v) + 16\cos(4v) \\
&\quad + 14\cos(5v) + 8\cos(6v) + 15)\sec\left(\frac{v}{2}\right)\Bigg) \\
b^1_{6,num} &= \csc^7\left(\frac{v}{2}\right)\Bigg(v(7(65953v^2 + 181440) + 7(379709v^2 \\
&\quad - 362880)\cos\,(v) + 2(694753v^2 + 799680)\cos(2v) + 4(360653\,v^2 \\
&\quad - 199920)\cos(3v) + 15(52889v^2 + 21952)\cos(4v) \\
&\quad + (875393v^2 - 540960)\cos(5v) + 799680\cos(6v) \\
&\quad - 117600\cos(7v))\csc^3\left(\frac{v}{2}\right) - 188160(18\cos(v) + 18\cos(2v) \\
&\quad + 13\cos(3v) + 10\cos(4v) + 8\cos(5v) + 5\cos(6v) + 9)\sec\left(\frac{v}{2}\right)\Bigg) \\
b^1_{1,denom} &= 6881280v^3 \\
b^1_{2,denom} &= 1720320v^3 \\
b^1_{3,denom} &= 3440640v^3
\end{aligned}
$$

$$b^1_{4,denom} = 1720320v^3$$
$$b^1_{5,denom} = 3440640v^3$$
$$b^1_{6,denom} = 860160v^3 \tag{34}$$

$$\begin{aligned}
b^1_{T,1} &= \frac{90987349}{53222400} - \frac{16301796103v^2}{145297152000} + \frac{1532031563v^4}{268240896000} \\
&\quad - \frac{31987133939v^6}{592812380160000} + \frac{5466168990203v^8}{2838385676206080000} + \cdots \\
b^1_{T,2} &= -\frac{114798419}{26611200} + \frac{16301796103v^2}{14529715200} - \frac{28198975459v^4}{249080832000} \\
&\quad + \frac{88492028011v^6}{11856247603200} - \frac{533071354889581v^8}{1419192838103040000} + \cdots \\
b^1_{T,3} &= \frac{270875723}{17740800} - \frac{16301796103v^2}{3228825600} + \frac{117200518583v^4}{166053888000} \\
&\quad - \frac{2285150767769v^6}{39520825344000} + \frac{308808361613933v^8}{105125395415040000} - \cdots \\
b^1_{T,4} &= -\frac{67855831}{2217600} + \frac{16301796103v^2}{1210809600} - \frac{36423021893v^4}{16144128000} \\
&\quad + \frac{989757481543v^6}{4940103168000} - \frac{1207392034807669v^8}{118266069841920000} \cdots \\
b^1_{T,5} &= \frac{50277247}{985600} - \frac{16301796103v^2}{691891200} + \frac{360410789243v^4}{83026944000} \\
&\quad - \frac{25035151487v^6}{62731468800} + \frac{125088382253381v^8}{6143691939840000} - \frac{2919882783787129v^{10}}{4460320348323840000} \cdots \\
b^1_{T,6} &= -\frac{253491379}{4435200} + \frac{16301796103v^2}{576576000} - \frac{222767191987v^4}{41513472000} \\
&\quad + \frac{3516569786117v^6}{7057290240000} - \frac{95477706318691v^8}{3754478407680000} + \cdots
\end{aligned} \tag{35}$$

Method *PF-D2*:

$$\begin{aligned}
b^2_{1,num} &= -30720(v^2-1)\cos(v) - 10(-387\csc^6\left(\frac{v}{2}\right) \\
&\quad + 72(128\cos(v)+127)\csc^2(v) + 2048(v^2-3)) - (8(-47v^4 \\
&\quad - 2040v^2 - (40((22\cos(v)+22\cos(2v)+9\cos(3v)+14\cos(4v) \\
&\quad + 8\cos(5v) - 5\cos(6v) + 11)\tan^3\left(\frac{v}{2}\right) - 27v^3)v)/(\cos(v)-1) \\
&\quad + (4817v^4+3120v^2+4410)\cos(v) \\
&\quad - 2205\cos(2v) - 2205))/((\cos(v)-1)^4)
\end{aligned}$$

$$
\begin{aligned}
b^2_{2,num} &= -1350v^4 \csc^{10}\left(\frac{v}{2}\right) + 225v^2(59v^2+12)\csc^8\left(\frac{v}{2}\right) \\
&\quad - 5(7361v^4+3696v^2-540)\csc^6\left(\frac{v}{2}\right) + 6(4817v^4+3120v^2 \\
&\quad - 7710)\csc^4\left(\frac{v}{2}\right) + 264780\csc^2\left(\frac{v}{2}\right) + 30720(3v^2-7)\cos(v) \\
&\quad + 15360(v^2-2)\cos(2v) + 30v\cot\left(\frac{v}{2}\right)\left(\frac{1}{8}(-2436\cos(v)\right. \\
&\quad \left. + 1921\cos(2v)+1595)\csc^6\left(\frac{v}{2}\right) + 8322\right) \\
&\quad + 10\left(5632v^2 - 1024(8\cos(v)+23)\sin(v)v\right. \\
&\quad \left. + \frac{6(65\cos(v)+66)\tan\left(\frac{v}{2}\right)v}{\cos(v)+1} - \frac{36}{\cos(v)+1} - 39936\right) \\
b^2_{3,num} &= 12150v^4\csc^{10}\left(\frac{v}{2}\right) - 675v^2(191v^2+36)\csc^8\left(\frac{v}{2}\right) \\
&\quad + 15(28499v^4+12432v^2-1620)\csc^6\left(\frac{v}{2}\right) - 36450v\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) \\
&\quad - 12(44896v^4+26400v^2-35955)\csc^4\left(\frac{v}{2}\right) \\
&\quad + 381960v\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right) + 12(19268v^4+12480v^2 \\
&\quad - 219885)\csc^2\left(\frac{v}{2}\right) - 817950v\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right) - 540\sec^2\left(\frac{v}{2}\right) \\
&\quad - 5120(73v^2-831) - 61440(9v^2-40)\cos(v) \\
&\quad - 61440(3v^2-8)\cos(2v) - 10240(v^2-3)\cos(3v) \\
&\quad - 1512900v\cot\left(\frac{v}{2}\right) + 1884160v\sin(v) + 532480v\sin(2v) \\
&\quad + 30720v\sin(3v) + 90v\sec^2\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right) + 7740v\tan\left(\frac{v}{2}\right) \\
b^2_{4,num} &= -4050v^4\csc^{10}\left(\frac{v}{2}\right) + 675v^2(67v^2+12)\csc^8\left(\frac{v}{2}\right) \\
&\quad - 15(11113v^4+4464v^2-540)\csc^6\left(\frac{v}{2}\right) + 12150v\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) \\
&\quad + 6(43259v^4+24000v^2-24570)\csc^4\left(\frac{v}{2}\right) - 133920v\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right) \\
&\quad + 347250v\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right) + 8(4817v^4+15840v^2-197280) \\
&\quad + 7680(19v^2-125)\cos(v) + 30720(2v^2-7)\cos(2v) \\
&\quad + 7680(v^2-3)\cos(3v) + 292500v\cot\left(\frac{v}{2}\right) - 555520v\sin(v) \\
&\quad - 194560v\sin(2v) - 23040v\sin(3v) - 30v\sec^2\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right) \\
&\quad - 3180v\tan\left(\frac{v}{2}\right) + \frac{72(4817v^4+3120v^2-26165)}{\cos(v)-1} + \frac{360}{\cos(v)+1}
\end{aligned}
$$

$$
\begin{aligned}
b^2_{5,num} &= 28350v^4 \csc^{10}\left(\frac{v}{2}\right) - 14175v^2(23v^2+4)\csc^8\left(\frac{v}{2}\right) + 45(28269v^4 \\
&\quad + 10864v^2 - 1260)\csc^6\left(\frac{v}{2}\right) - 85050v\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) \\
&\quad - 12(182576v^4 + 98160v^2 - 87255)\csc^4\left(\frac{v}{2}\right) \\
&\quad + 965160v\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right) + 180(9634v^4 + 6240v^2 \\
&\quad - 38111)\csc^2\left(\frac{v}{2}\right) - 2753430v\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right) - 256(2011v^4 \\
&\quad + 3870v^2 - 45810) - 15360(61v^2 - 479)\cos(v) - 30720(13v^2 \\
&\quad - 56)\cos(2v) - 76800(v^2-3)\cos(3v) - 1054260v\cot\left(\frac{v}{2}\right) \\
&\quad + 3537920v\sin(v) + 1372160v\sin(2v) + 230400v\sin(3v) \\
&\quad - 30v\sec^2\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right) - 2100v\tan\left(\frac{v}{2}\right) + \frac{360}{\cos(v)+1} \qquad (36) \\
b^2_{6,num} &= 93048v^4 + 156160v^2 + 1042425\csc^2\left(\frac{v}{2}\right) \\
&\quad + 15360(9v^2 - 74)\cos(v) - 268800\cos(2v) - 38400\cos(3v) \\
&\quad - \Bigg(9\left(7560\csc^2\left(\frac{v}{2}\right) + 14963\right)v^4 + 187840v^2 - 4(237663v^4 \\
&\quad + 77080v^2 + 298620)\cos(v) + 5\Big((34095v^4 - 4000v^2 \\
&\quad + 63126)\cos(2v) - 2v(v(14451v^2 - 5200)\cos(3v) \\
&\quad + 8(5v(140\cos(4v) - 16\cos(5v) - 7\cos(6v) + 2\cos(7v)) \\
&\quad - 666\sin(v) + 600\sin(2v) - 298\sin(3v) + 238\sin(4v) + 40\sin(5v) \\
&\quad + 80\sin(6v) - 30\sin(7v)) + 36\left(\sec^2\left(\frac{v}{2}\right) + 94\right)\tan\left(\frac{v}{2}\right)\Big)\Big) \\
&\quad + 878850)/((\cos(v)-1)^4) - \frac{270}{\cos(v)+1} - 1793280 \\
b^2_{1,denom} &= 5120v^4 \\
b^2_{2,denom} &= 2560v^4 \\
b^2_{3,denom} &= 5120v^4 \\
b^2_{4,denom} &= 640v^4 \\
b^2_{5,denom} &= 2560v^4 \\
b^2_{6,denom} &= 320v^4 \qquad (37) \\
b^2_{T,1} &= \frac{90987349}{53222400} - \frac{16301796103v^2}{96864768000} + \frac{1568734969v^4}{232475443200} \\
&\quad - \frac{112423833619v^6}{889218570240000} - \frac{128168340031v^8}{189225711747072000} - \cdots
\end{aligned}
$$

$$
\begin{aligned}
b^2_{T,2} &= -\frac{114798419}{26611200} + \frac{16301796103v^2}{9686476800} - \frac{10540703911v^4}{44706816000} \\
&\quad + \frac{871935134531v^6}{44460928512000} - \frac{463103326062011v^8}{473064279367680000} + \cdots \\
b^2_{T,3} &= \frac{270875723}{17740800} - \frac{16301796103v^2}{2152550400} + \frac{639312597971v^4}{387459072000} \\
&\quad - \frac{2472777112313v^6}{11856247603200} + \frac{58110459403753v^8}{3185618042880000} - \cdots \\
b^2_{T,4} &= -\frac{67855831}{2217600} + \frac{16301796103v^2}{807206400} - \frac{89147839889v^4}{16144128000} \\
&\quad + \frac{1282661397349v^6}{1482030950400} - \frac{3541527647083319v^8}{39422023280640000} + \cdots \\
b^2_{T,5} &= \frac{50277247}{985600} - \frac{16301796103v^2}{461260800} + \frac{300047111873v^4}{27675648000} \\
&\quad - \frac{18727460555953v^6}{9880206336000} + \frac{4749826752625121v^8}{22526870446080000} - \cdots \\
b^2_{T,6} &= -\frac{253491379}{4435200} + \frac{16301796103v^2}{384384000} - \frac{37309797113v^4}{2767564800} \\
&\quad + \frac{90333884682737v^6}{37050773760000} - \frac{69221174089601v^8}{250298560512000} + \cdots
\end{aligned} \tag{38}
$$

Method *PF-D3*:

$$
\begin{aligned}
b^3_{1,num} &= -108v^5\csc^{10}\left(\frac{v}{2}\right) + 9v^3(53v^2+12)\csc^8\left(\frac{v}{2}\right) \\
&\quad + 486v\csc^6\left(\frac{v}{2}\right) - 2484v\csc^4\left(\frac{v}{2}\right) - 6144v(4v^2-9)\cos(v) \\
&\quad + 3\cot\left(\frac{v}{2}\right)\left(99v^2\csc^6\left(\frac{v}{2}\right) + 9(16-9v^2)\csc^4\left(\frac{v}{2}\right) - 8(113v^2\right. \\
&\quad \left. + 276)\csc^2\left(\frac{v}{2}\right) - 11266v^2 + 10032\right) - 6144(v^3 - 6v + 4\sin(v)) \\
&\quad + 2v^2\left(26624\sin(v) - 5635\tan\left(\frac{v}{2}\right)\right) + 5520\tan\left(\frac{v}{2}\right) \\
&\quad - 9v\sec^4\left(\frac{v}{2}\right)\left(v\tan\left(\frac{v}{2}\right) - 6\right) - 6\sec^2\left(\frac{v}{2}\right)\left((61v^2+24)\tan\left(\frac{v}{2}\right)\right. \\
&\quad \left. - 363v\right) + \frac{32508v}{\cos(v)-1} \\
b^3_{2,num} &= 540v^5\csc^{10}\left(\frac{v}{2}\right) - 45v^3(71v^2+12)\csc^8\left(\frac{v}{2}\right) \\
&\quad + 18v(212v^4+48v^2-135)\csc^6\left(\frac{v}{2}\right) - 1485v^2\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) \\
&\quad + 15984v\csc^4\left(\frac{v}{2}\right) + 27(131v^2-80)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right) \\
&\quad + 55782v\csc^2\left(\frac{v}{2}\right) + 6(1777v^2+5952)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)
\end{aligned}
$$

$$
\begin{aligned}
&+54v\sec^4\left(\frac{v}{2}\right)+6144v(5v^2-39)+6144v(8v^2-33)\cos(v)\\
&+18432v(v^2-4)\cos(2v)+6(20035v^2-31704)\cot\left(\frac{v}{2}\right)\\
&-20480(7v^2-6)\sin(v)+3072(12-19v^2)\sin(2v)\\
&-9v^2\sec^4\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right)-12(23v^2+12)\sec^2\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right)\\
&+14(456-337v^2)\tan\left(\frac{v}{2}\right)+\frac{3276v}{\cos(v)+1}\\
b^3_{3,num}&=-1620v^5\csc^{10}\left(\frac{v}{2}\right)+135v^3(85v^2+12)\csc^8\left(\frac{v}{2}\right)\\
&-6v(3872v^4+768v^2-1215)\csc^6\left(\frac{v}{2}\right)+4455v^2\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)\\
&+36v(424v^4+96v^2-1563)\csc^4\left(\frac{v}{2}\right)+9(720\\
&-1781v^2)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)-96642v\csc^2\left(\frac{v}{2}\right)-24(685v^2\\
&+4716)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)-54v\sec^4\left(\frac{v}{2}\right)+1024v(606-67v^2)\\
&-49152v(2v^2-13)\cos(v)-49152v(v^2-5)\cos(2v)\\
&+2048v(21-4v^2)\cos(3v)+6(111720-46199v^2)\cot\left(\frac{v}{2}\right)\\
&+32768(11v^2-15)\sin(v)+4096(41v^2-36)\sin(2v)\\
&+4096(7v^2-6)\sin(3v)+9v^2\sec^4\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right)+6(61v^2\\
&+24)\sec^2\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right)+10(1055v^2-552)\tan\left(\frac{v}{2}\right)-\frac{4356v}{\cos(v)+1}\\
b^3_{4,num}&=1620v^5\csc^{10}\left(\frac{v}{2}\right)-135v^3(95v^2+12)\csc^8\left(\frac{v}{2}\right)\\
&+18v(1844v^4+336v^2-405)\csc^6\left(\frac{v}{2}\right)-4455v^2\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)\\
&-216v(169v^4+36v^2-288)\csc^4\left(\frac{v}{2}\right)+27(737v^2\\
&-240)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)+18v(848v^4+192v^2+2229)\csc^2\left(\frac{v}{2}\right)\\
&+18(35v^2+6528)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)-54v\sec^4\left(\frac{v}{2}\right)+384v(133v^2\\
&-1350)+768v(112v^2-843)\cos(v)+3072v(13v^2-81)\cos(2v)\\
&+1536v(8v^2-45)\cos(3v)+768v(v^2-6)\cos(4v)+54(4447v^2\\
&-13800)\cot\left(\frac{v}{2}\right)+512(1146-659v^2)\sin(v)-512(289v^2\\
&-348)\sin(2v)+1024(42-43v^2)\sin(3v)+256(12\\
&-11v^2)\sin(4v)+\left(9v^2\sec^4\left(\frac{v}{2}\right)+5258v^2+\frac{552v^2+288}{\cos(v)+1}\right.\\
&\left.-6384\right)\tan\left(\frac{v}{2}\right)-\frac{3276v}{\cos(v)+1}
\end{aligned}
\tag{39}
$$

$$
\begin{aligned}
b^3_{5,num} &= -11340v^5\csc^{10}\left(\frac{v}{2}\right)+945v^3(101v^2+12)\csc^8\left(\frac{v}{2}\right)\\
&\quad -18v(15472v^4+2688v^2-2835)\csc^6\left(\frac{v}{2}\right)\\
&\quad +31185v^2\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)+108v(3500v^4+720v^2-4263)\csc^4\left(\frac{v}{2}\right)\\
&\quad +189(240-823v^2)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)+864(87v^2\\
&\quad -973)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)+54v\sec^4\left(\frac{v}{2}\right)+384v(159v^4-796v^2\\
&\quad +8568)+3072v(1395-172v^2)\cos(v)-24576v(11v^2\\
&\quad -75)\cos(2v)+3072v(171-28v^2)\cos(3v)\\
&\quad -12288v(v^2-6)\cos(4v)+18(307848-88943v^2)\cot\left(\frac{v}{2}\right)\\
&\quad +2048(1055v^2-2154)\sin(v)+2048(505v^2-708)\sin(2v)\\
&\quad +2048(155v^2-174)\sin(3v)+4096(11v^2-12)\sin(4v)\\
&\quad -9v^2\sec^4\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right)-6\,(61v^2+24)\sec^2\left(\frac{v}{2}\right)\tan\left(\frac{v}{2}\right)+10(552\\
&\quad -1019v^2)\tan\left(\frac{v}{2}\right)+\frac{36v(256(53v^2+12)v^2+1479)}{\cos(v)-1}+\frac{4356v}{\cos(v)+1}\\
b^3_{6,num} &= 2268v^5\csc^{10}\left(\frac{v}{2}\right)-189v^3(103v^2+12)\csc^8\left(\frac{v}{2}\right)\\
&\quad +6v(9820v^4+1680v^2-1701)\csc^6\left(\frac{v}{2}\right)-6237v^2\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)\\
&\quad -144v(590v^4+120v^2-651)\csc^4\left(\frac{v}{2}\right)+63(511v^2\\
&\quad -144)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)+18v(3392v^4+768v^2-677)\csc^2\left(\frac{v}{2}\right)\\
&\quad +6(28224-3463v^2)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)+54v\sec^4\left(\frac{v}{2}\right)\\
&\quad -128v(141v^4-460v^2+5016)+3072v(32v^2-269)\cos(v)\\
&\quad +6144v(9v^2-62)\cos(2v)+2048v(8v^2-51)\cos(3v)\\
&\quad +3072v(v^2-6)\cos(4v)+1002(317v^2-1128)\cot\left(\frac{v}{2}\right)\\
&\quad -6144(67v^2-146)\sin(v)-3072(69v^2-100)\sin(2v)\\
&\quad -12288(5v^2-6)\sin(3v)+1024(12-11v^2)\sin(4v)\\
&\quad -\left(9v^2\sec^4\left(\frac{v}{2}\right)+5438v^2+\frac{552v^2+288}{\cos(v)+1}-6384\right)\tan\left(\frac{v}{2}\right)\\
&\quad +\frac{3276v}{\cos(v)+1}\\
b^3_{1,denom} &= 3072v^5\\
b^3_{2,denom} &= 1536v^5\\
b^3_{3,denom} &= 1024v^5
\end{aligned}
$$

$$
\begin{aligned}
b^3_{4,denom} &= 384v^5\\
b^3_{5,denom} &= 1536v^5\\
b^3_{6,denom} &= 256v^5
\end{aligned} \tag{40}
$$

$$
\begin{aligned}
b^3_{T,1} &= \frac{90987349}{53222400} - \frac{16301796103v^2}{72648576000} + \frac{1273143229v^4}{193729536000}\\
&\quad - \frac{421960559v^6}{1221454080000} - \frac{124506164597657v^8}{5676771352412160000} - \cdots\\
b^3_{T,2} &= -\frac{114798419}{26611200} + \frac{16301796103v^2}{7264857600} - \frac{38969308351v^4}{96864768000}\\
&\quad + \frac{5604849953v^6}{158789030400} - \frac{5242236508523657v^8}{2838385676206080000} + \cdots\\
b^3_{T,3} &= \frac{270875723}{17740800} - \frac{16301796103v^2}{1614412800} + \frac{578948920601v^4}{193729536000}\\
&\quad - \frac{733132845253v^6}{1482030950400} + \frac{3064860132866873v^8}{57341124771840000} - \cdots\\
b^3_{T,4} &= -\frac{67855831}{2217600} + \frac{16301796103v^2}{605404800} - \frac{247322293877v^4}{24216192000}\\
&\quad + \frac{844539338551v^6}{370507737600} - \frac{80127849554001773v^8}{236532139683840000} + \cdots\\
b^3_{T,5} &= \frac{50277247}{985600} - \frac{16301796103v^2}{345945600} + \frac{279925886083v^4}{13837824000}\\
&\quad - \frac{644885438797v^6}{123502579200} + \frac{122198747647321067v^8}{135161222676480000} - \cdots\\
b^3_{T,6} &= -\frac{253491379}{4435200} + \frac{16301796103v^2}{288288000} - \frac{1220113637v^4}{48384000}\\
&\quad + \frac{55089606671v^6}{8096760000} - \frac{1634963205351829v^8}{1325110026240000} + \cdots
\end{aligned} \tag{41}
$$

Method *PF-D4*:

$$
\begin{aligned}
b^4_{1,num} &= 216v^6\csc^{10}\left(\frac{v}{2}\right) - 810v^2\csc^6\left(\frac{v}{2}\right) - 54(157v^2\\
&\quad + 80)\csc^4\left(\frac{v}{2}\right) + 36(1840 - 2257v^2)\csc^2\left(\frac{v}{2}\right) - 12288(20v^4\\
&\quad - 71v^2 + 20)\cos(v) - 3v\cot\left(\frac{v}{2}\right)\left((4682v^2 + 9\csc^2\left(\frac{v}{2}\right)\left(5\csc^2\left(\frac{v}{2}\right)v^2\right.\right.\\
&\quad \left.\left. + 54v^2 + 96\right) + 5856)\csc^2\left(\frac{v}{2}\right) + 2520(31v^2 - 48)\right)\\
&\quad - 45v^2\sec^6\left(\frac{v}{2}\right)\left(v\tan\left(\frac{v}{2}\right) - 6\right) + 56v\left(1024(11v^2 - 12)\sin(v)\right.\\
&\quad \left. + 135(48 - 31v^2)\tan\left(\frac{v}{2}\right)\right) - 18\sec^4\left(\frac{v}{2}\right)(-373v^2 + 3(21v^2
\end{aligned}
$$

$$+ 16) \tan\left(\frac{v}{2}\right) v - 80) - 2\sec^2\left(\frac{v}{2}\right)\left(-39246v^2\right.$$
$$\left. + (6733v^2 + 6384)\tan\left(\frac{v}{2}\right) v + 28320\right)$$

$$\begin{aligned}
b^4_{2,num} = & -1080v^6\csc^{10}\left(\frac{v}{2}\right) + 2160v^6\csc^8\left(\frac{v}{2}\right) + 4050v^2\csc^6\left(\frac{v}{2}\right) \\
& + 54(617v^2 + 400)\csc^4\left(\frac{v}{2}\right) + 293508v^2\csc^2\left(\frac{v}{2}\right) + 12288(20v^4 \\
& - 71v^2 + 20)\cos(v) + 24576(10v^4 - 59v^2 + 20)\cos(2v) \\
& + 3v\cot\left(\frac{v}{2}\right)\left(\left(16978v^2 + 9\csc^2\left(\frac{v}{2}\right)\left(25\csc^2\left(\frac{v}{2}\right)v^2 + 214v^2 + 480\right)\right.\right. \\
& \left.\left. + 20064\right)\csc^2\left(\frac{v}{2}\right) + 120(2341v^2 - 5136)\right) + (72(4096v^4 \\
& - 31783v^2 - 80(257\cos(v) + 251)\csc^2(v) + 1024(4v^4 - 35v^2 \\
& + 20)\cos(v) + 25600))/(\cos(v) + 1) - v\left(135v(v\tan\left(\frac{v}{2}\right)\right. \\
& - 6)\sec^6\left(\frac{v}{2}\right) + 18((161v^2 + 144)\tan\left(\frac{v}{2}\right) - 951v)\sec^4\left(\frac{v}{2}\right) \\
& + 18(1407v^2 + 1616)\tan\left(\frac{v}{2}\right)\sec^2\left(\frac{v}{2}\right) + 8\left(7168(11v^2 - 12)\sin(v)\right. \\
& \left.\left. + 1024(107v^2 - 156)\sin(2v) + 15(3217v^2 - 9168)\tan\left(\frac{v}{2}\right)\right)\right)
\end{aligned}$$

$$\begin{aligned}
b^4_{3,num} = & \,9720v^6\csc^{10}\left(\frac{v}{2}\right) - 34560v^6\csc^8\left(\frac{v}{2}\right) + 270v^2(128v^4 \\
& - 135)\csc^6\left(\frac{v}{2}\right) - 6075v^3\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) - 162(1459v^2 \\
& + 1200)\csc^4\left(\frac{v}{2}\right) - 54v(767v^2 + 2160)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right) \\
& + 108(32720 - 18831v^2)\csc^2\left(\frac{v}{2}\right) - 234v(1511v^2 \\
& + 1488)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right) + 3510v^2\sec^6\left(\frac{v}{2}\right) + 90(701v^2 \\
& + 208)\sec^4\left(\frac{v}{2}\right) - 12288(98v^4 - 825v^2 + 540) - 12288(220v^4 \\
& - 1717v^2 + 940)\cos(v) - 98304(10v^4 - 59v^2 + 20)\cos(2v) \\
& - 24576(20v^4 - 147v^2 + 60)\cos(3v) + 360v(45744 \\
& - 16567v^2)\cot\left(\frac{v}{2}\right) + 8192v(1279v^2 - 2868)\sin(v) + 32768v(107v^2 \\
& - 156)\sin(2v) + 147456v(13v^2 - 24)\sin(3v) - v(585v^2\sec^6\left(\frac{v}{2}\right) \\
& + (42991v^2 + (32281v^2 + 46128)\cos(v) + 57360)\sec^4\left(\frac{v}{2}\right) \\
& + 120(8741v^2 - 38928))\tan\left(\frac{v}{2}\right) + \frac{24(30457v^2 - 69040)}{\cos(v) + 1}
\end{aligned}$$

$$\begin{aligned}
b^4_{4,num} &= -3240v^6\csc^{10}\left(\frac{v}{2}\right)+15120v^6\csc^8\left(\frac{v}{2}\right)-810v^2(32v^4\\
&\quad-15)\csc^6\left(\frac{v}{2}\right)+2025v^3\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)+54(320v^6+1179v^2\\
&\quad+1200)\csc^4\left(\frac{v}{2}\right)+54v(209v^2+720)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)\\
&\quad+108(5237v^2-11440)\csc^2\left(\frac{v}{2}\right)+18v(5461v^2\\
&\quad+3888)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)+270v^2\sec^6\left(\frac{v}{2}\right)+90(41v^2+16)\sec^4\left(\frac{v}{2}\right)\\
&\quad+76800(5v^4-54v^2+48)+6144(100v^4-819v^2+480)\cos(v)\\
&\quad+73728(5v^4-39v^2+20)\cos(2v)+6144(20v^4-147v^2\\
&\quad+60)\cos(3v)+6144(5v^4-41v^2+20)\cos(4v)+360v(4705v^2\\
&\quad-14928)\cot\left(\frac{v}{2}\right)-36864v(67v^2-154)\sin(v)-86016v(17v^2\\
&\quad-36)\sin(2v)-36864v(13v^2-24)\sin(3v)-2048v(61v^2\\
&\quad-132)\sin(4v)-v(((1087+\frac{90}{\cos(v)+1})v^2+(457v^2\\
&\quad+1776)\cos(v)+2640)\sec^4\left(\frac{v}{2}\right)+120(349v^2\\
&\quad-2832))\tan\left(\frac{v}{2}\right)+\frac{24(349v^2-5680)}{\cos(v)+1}
\end{aligned}\tag{42}$$

$$\begin{aligned}
b^4_{5,num} &= 22680v^6\csc^{10}\left(\frac{v}{2}\right)-120960v^6\csc^8\left(\frac{v}{2}\right)+4050v^2(64v^4\\
&\quad-21)\csc^6\left(\frac{v}{2}\right)-14175v^3\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)-54(5120v^6+7077v^2\\
&\quad+8400)\csc^4\left(\frac{v}{2}\right)-378v(181v^2+720)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)+108(1280v^6\\
&\quad-33131v^2+82320)\csc^2\left(\frac{v}{2}\right)-378v(1643v^2+784)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)\\
&\quad-1890v^2\sec^6\left(\frac{v}{2}\right)-126(277v^2+80)\sec^4\left(\frac{v}{2}\right)-15360(160v^4\\
&\quad-1833v^2+1740)-30720(120v^4-1079v^2+740)\cos(v)\\
&\quad-6144(400v^4-3271v^2+1780)\cos(2v)-6144(140v^4-1113v^2\\
&\quad+540)\cos(3v)-49152(5v^4-41v^2+20)\cos(4v)-6144(4v^4\\
&\quad-35v^2+20)\cos(5v)+360v(102576-30047v^2)\cot\left(\frac{v}{2}\right)\\
&\quad+20480v(755v^2-1956)\sin(v)+4096v(2429v^2-5412)\sin(2v)\\
&\quad+12288v(281v^2-588)\sin(3v)+16384v(61v^2-132)\sin(4v)\\
&\quad+20480v(5v^2-12)\sin(5v)+v(((25429+\frac{630}{\cos(v)+1})v^2+(19507v^2
\end{aligned}$$

$$
\begin{aligned}
&+ 26256)\cos(v) + 32304)\sec^4\left(\frac{v}{2}\right) + 120(5347v^2 - 20976))\tan\left(\frac{v}{2}\right)\\
&+ \frac{885120 - 443976v^2}{\cos(v)+1}\\
b^4_{6,num} &= -13608v^6\csc^{10}\left(\frac{v}{2}\right) + 75600v^6\csc^8\left(\frac{v}{2}\right) + 270v^2(189\\
&- 640v^4)\csc^6\left(\frac{v}{2}\right) + 8505v^3\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) + 162(1280v^6\\
&+ 1337v^2 + 1680)\csc^4\left(\frac{v}{2}\right) + 378v(103v^2 + 432)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)\\
&+ 126v(2863v^2 + 1104)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right) - 1890v^2\sec^6\left(\frac{v}{2}\right)\\
&- 126(253v^2 + 80)\sec^4\left(\frac{v}{2}\right) + 3072(18v^6 + 400v^4 - 4575v^2 + 4500)\\
&+ 30720(80v^4 - 753v^2 + 540)\cos(v) + 30720(40v^4 - 327v^2\\
&+ 180)\cos(2v) + 6144(100v^4 - 819v^2 + 420)\cos(3v) + 24576(5v^4\\
&- 41v^2 + 20)\cos(4v) + 6144(4v^4 - 35v^2 + 20)\cos(5v)\\
&+ 360v(17495v^2 - 61104)\cot\left(\frac{v}{2}\right) - 552960v(19v^2 - 52)\sin(v)\\
&- 552960v(9v^2 - 20)\sin(2v) - 12288v(203v^2 - 444)\sin(3v)\\
&- 8192v(61v^2 - 132)\sin(4v) - 20480v(5v^2 - 12)\sin(5v)\\
&+ v(63(48(v^2+1) + (43v^2 + 48)\cos(v))\sec^6\left(\frac{v}{2}\right) + 840(659v^2\\
&- 2928) + \frac{57964v^2 + 86592}{\cos(v)+1})\tan\left(\frac{v}{2}\right)\\
&+ \frac{216(1280v^6 - 19257v^2 + 49840)}{\cos(v)-1} + \frac{908160 - 325608v^2}{\cos(v)+1}\\
b^4_{1,denom} &= 24576v^6\\
b^4_{2,denom} &= 12288v^6\\
b^4_{3,denom} &= 24576v^6\\
b^4_{4,denom} &= 3072v^6\\
b^4_{5,denom} &= 12288v^6\\
b^4_{6,denom} &= 6144v^6
\end{aligned} \tag{43}
$$

$$
\begin{aligned}
b^4_{T,1} &= \frac{90987349}{53222400} - \frac{16301796103v^2}{58118860800} + \frac{451826777v^4}{87178291200}\\
&\quad - \frac{567827928197v^6}{711374856192000} - \frac{7456559915267v^8}{87334943883264000} - \cdots\\
b^4_{T,2} &= -\frac{114798419}{26611200} + \frac{16301796103v^2}{5811886080} - \frac{53423656079v^4}{87178291200}\\
&\quad + \frac{3768047264957v^6}{71137485619200} - \frac{18073625620419v^8}{567677135241216000} + \cdots
\end{aligned}
$$

$$
\begin{aligned}
b_{T,3}^4 &= \frac{270875723}{17740800} - \frac{16301796103v^2}{1291530240} + \frac{137191770479v^4}{29059430400} \\
&\quad - \frac{6482264498201v^6}{6774998630400} + \frac{177746918811101v^8}{1557413265408000} - \cdots \\
b_{T,4}^4 &= -\frac{67855831}{2217600} + \frac{16301796103v^2}{484323840} - \frac{4393734833v^4}{269068800} \\
&\quad + \frac{3998343544387v^6}{846874828800} - \frac{42449166474915191v^8}{47306427936768000} + \cdots \\
b_{T,5}^4 &= \frac{50277247}{985600} - \frac{16301796103v^2}{276756480} + \frac{9638045471v^4}{296524800} \\
&\quad - \frac{87748735805873v^6}{7904165068800} + \frac{70694795981650949v^8}{27032244535296000} - \cdots \\
b_{T,6}^4 &= -\frac{253491379}{4435200} + \frac{16301796103v^2}{230630400} - \frac{84219941177v^4}{2075673600} \\
&\quad + \frac{863717128805537v^6}{59281238016000} - \frac{183092352668191v^8}{500597121024000} + \cdots \qquad (44)
\end{aligned}
$$

Method *PF-D5*:

$$
\begin{aligned}
b_{1,num}^5 &= -\cos^5\left(\frac{v}{2}\right)\csc^{13}(v)\sin^7\left(\frac{v}{2}\right)\Bigg(60(-5v^5 + 3v^3 + 3\sin(v) \\
&\quad - 6\sin(3v) + 3\sin(4v) + 3\sin(5v) - 6\sin(6v) + 3\sin(8v)) \\
&\quad + \frac{1}{2}v\Bigg(15(200v^4 + 283v^2 - 100)\cos(v) + 300(2\cos(2v) + 6\cos(3v) \\
&\quad - 10\cos(4v) + \cos(5v) + 12\cos(6v) - 2\cos(7v) - 4\cos(8v)) \\
&\quad + v\Bigg(v\Bigg(15(366\cos(3v) + 686\cos(4v) - 503\cos(5v) - 480\cos(6v) \\
&\quad + 142\cos(7v) + 116\cos(8v)) + 2\Bigg(15(72v^2 - 155)\cos(2v) \\
&\quad + v\Bigg(-60v(45\cos(3v) + 24\cos(4v) - 25\cos(5v) - 14\cos(6v) \\
&\quad + 5\cos(7v) + 3\cos(8v)) + 405\cot\left(\frac{v}{2}\right) + 357\sin(v) - 2530\sin(2v) \\
&\quad + 4516\sin(3v) + 3752\sin(4v) - 3373\sin(5v) - 2324\sin(6v) \\
&\quad + 770\sin(7v) + 522\sin(8v) + 315\tan\left(\frac{v}{2}\right)\Bigg)\Bigg)\Bigg) - 60(49\sin(v) \\
&\quad - 44\sin(2v) - 6\sin(3v) + 131\sin(4v) - 67\sin(5v) - 114\sin(6v) \\
&\quad + 28\sin(7v) + 31\sin(8v))\Bigg)\Bigg)\Bigg) \\
b_{2,num}^5 &= \csc^7\left(\frac{v}{2}\right)\sec^9\left(\frac{v}{2}\right)\Bigg(4(3875v^4 - 519v^2 - 90)\cos(v) \\
&\quad - 36(147v^4 - 76v^2 - 10\cos(2v) + 20\cos(4v) - 20\cos(5v) \\
&\quad + 10\cos(7v) - 20\cos(8v) + 10\cos(10v)) + v\Bigg(v(2(5117v^2 \\
&\quad - 4254)\cos(2v) + 12(516\cos(3v) + 482\cos(4v) - 158\cos(5v)
\end{aligned}
$$

$$+ 348\cos(6v) - 317\cos(7v) - 486\cos(8v) + 132\cos(9v)$$
$$+ 137\cos(10v)) + v(3(-12\sin(v) - 3789\sin(2v) + 3900\sin(3v)$$
$$+ 2058\sin(4v) + 708\sin(5v) + 1632\sin(6v) - 2142\sin(7v)$$
$$- 1792\sin(8v) + 614\sin(9v) + 461\sin(10v))$$
$$- 2v(-393216v(15\cos(2v) + 17)\sin^7\left(\frac{v}{2}\right)\cos^9\left(\frac{v}{2}\right) + 4476\cos(3v)$$
$$+ 1918\cos(4v) + 2288\cos(5v) + 1242\cos(6v) - 2476\cos(7v)$$
$$- 1400\cos(8v) + 582\cos(9v) + 351\cos(10v))))$$
$$- 15360\cos^3\left(\frac{v}{2}\right)(186\cos(v) + 156\cos(2v) + 132\cos(3v)$$
$$+78\cos(4v) + 48\cos(5v) + 19\cos(6v) + 98)\sin^5\left(\frac{v}{2}\right)))$$

$$\begin{aligned} b^5_{3,num} = & -\cos^6\left(\frac{v}{2}\right)\csc^{14}(v)\sin^8\left(\frac{v}{2}\right)(7290\cot\left(\frac{v}{2}\right)v^4 \\ & + 5670\tan\left(\frac{v}{2}\right)v^4 + 32(56v^2 - 93)\sin(9v)v^2 + 12(250v^4 - 751v^2 \\ & + 100)v + 3(2140v^4 + 13737v^2 - 2220)\cos(v)v - 6(260v^4 \\ & - 591v^2 + 540)\cos(2v)v + 6(-1702v^4 + 2971v^2 + 1100)\cos(3v)v \\ & - 6(584v^4 - 3933v^2 + 1020)\cos(4v)v + 15(236v^4 - 1395v^2 \\ & + 228)\cos(5v)v + 12(182v^4 - 1121v^2 + 800)\cos(6v)v + 12(61v^4 \\ & - 201v^2 - 180)\cos(7v)v + 12(10v^4 - 171v^2 + 60)\cos(8v)v \\ & - 60(8v^4 - 53v^2 + 20)\cos(9v)v - 24(10v^4 - 93v^2 + 90)\cos(10v)v \\ & + 6(1327v^4 - 974v^2 - 60)\sin(v) - 4(1295v^4 + 1098v^2 \\ & - 180)\sin(2v) + 8(3403v^4 + 579v^2 - 270)\sin(3v) + 4(3256v^4 \\ & - 4557v^2 + 90)\sin(4v) + 2(-6097v^4 + 8058v^2 + 180)\sin(5v) \\ & - 8(935v^4 - 1929v^2 + 270)\sin(6v) - 4(593v^4 + 126v^2 \\ & - 180)\sin(7v) - 4(v^2 - 3)(199v^2 + 30)\sin(8v) + 8(127v^4 - 363v^2 \\ & + 90)\sin(10v)) \end{aligned} \quad (45)$$

$$\begin{aligned} b^5_{4,num} = & 5670v^3\sec^8\left(\frac{v}{2}\right) - 945v^4\tan\left(\frac{v}{2}\right)\sec^8\left(\frac{v}{2}\right) + 270v(257v^2 \\ & + 160)\sec^6\left(\frac{v}{2}\right) - 1080v^2(11v^2 + 18)\tan\left(\frac{v}{2}\right)\sec^6\left(\frac{v}{2}\right) + 4320v(51v^2 \\ & - 46)\sec^4\left(\frac{v}{2}\right) - 18(2267v^4 + 9816v^2 + 2880)\tan\left(\frac{v}{2}\right)\sec^4\left(\frac{v}{2}\right) \\ & + 4(-61651v^4 + 89664v^2 + 570240)\tan\left(\frac{v}{2}\right)\sec^2\left(\frac{v}{2}\right) \\ & + 7290v^3\csc^6\left(\frac{v}{2}\right) + 1215v^4\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right) + 78732v^3\csc^4\left(\frac{v}{2}\right) \\ & + 81v^2(167v^2 + 240)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right) + 756v(1127v^2 \\ & - 2640)\csc^2\left(\frac{v}{2}\right) + 9(16297v^4 + 2592v^2 - 17280)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right) \end{aligned}$$

$$
\begin{aligned}
&+46080v(30v^4-443v^2+980)+73728v(101v^2-370)\cos(v)\\
&+36864v(40v^4-431v^2+580)\cos(2v)+73728v(13v^2\\
&-40)\cos(3v)+6144v(30v^4-307v^2+340)\cos(4v)+9(342973v^4\\
&-1171680v^2+328320)\cot\left(\frac{v}{2}\right)+73728(17v^4-271v^2\\
&+210)\sin(v)-98304(67v^4-243v^2+90)\sin(2v)\\
&+16384(10v^4-147v^2+90)\sin(3v)-24576(33v^4-107v^2\\
&+30)\sin(4v)+(-3937883v^4+28223520v^2-21006720)\tan\left(\frac{v}{2}\right)\\
&+\frac{24v(115673v^2-893360)}{\cos(v)+1}
\end{aligned}
$$

$$
\begin{aligned}
b^5_{5,num} &= 39690v^3\sec^8\left(\frac{v}{2}\right)-6615v^4\tan\left(\frac{v}{2}\right)\sec^8\left(\frac{v}{2}\right)+1890v(239v^2\\
&+160)\sec^6\left(\frac{v}{2}\right)-1890v^2(41v^2+72)\tan\left(\frac{v}{2}\right)\sec^6\left(\frac{v}{2}\right)+756v(1471v^2\\
&-2160)\sec^4\left(\frac{v}{2}\right)-378(561v^4+2968v^2+960)\tan\left(\frac{v}{2}\right)\sec^4\left(\frac{v}{2}\right)\\
&+84v(99661v^2-859120)\sec^2\left(\frac{v}{2}\right)-56(26371v^4-61404v^2\\
&-289440)\tan\left(\frac{v}{2}\right)\sec^2\left(\frac{v}{2}\right)-51030v^3\csc^6\left(\frac{v}{2}\right)\\
&-8505v^4\cot\left(\frac{v}{2}\right)\csc^6\left(\frac{v}{2}\right)-503496v^3\csc^4\left(\frac{v}{2}\right)-1701v^2(51v^2\\
&+80)\cot\left(\frac{v}{2}\right)\csc^4\left(\frac{v}{2}\right)-756v(7131v^2-18320)\csc^2\left(\frac{v}{2}\right)\\
&-189(4913v^4+256v^2-5760)\cot\left(\frac{v}{2}\right)\csc^2\left(\frac{v}{2}\right)-92160v(373v^2\\
&-2140)-245760v(60v^4-767v^2+1400)\cos(v)-12288v(1829v^2\\
&-6620)\cos(2v)-884736v(5v^4-54v^2+70)\cos(3v)-24576v(61v^2\\
&-220)\cos(4v)-49152v(6v^4-65v^2+80)\cos(5v)-9(2193517v^4\\
&-8002080v^2+2378880)\cot\left(\frac{v}{2}\right)+245760(287v^4-1321v^2\\
&+690)\sin(v)-24576(151v^4-2446v^2+1860)\sin(2v)\\
&+16384(1211v^4-4317v^2+1530)\sin(3v)-49152(5v^4-82v^2\\
&+60)\sin(4v)+49152(27v^4-95v^2+30)\sin(5v)+(-24636373v^4\\
&+185682720v^2-157806720)\tan\left(\frac{v}{2}\right)
\end{aligned}
$$

$$
\begin{aligned}
b^5_{6,num} &= 119070v^3\sec^8\left(\frac{v}{2}\right)-19845v^4\tan\left(\frac{v}{2}\right)\sec^8\left(\frac{v}{2}\right)\\
&+5670v(233v^2+160)\sec^6\left(\frac{v}{2}\right)-45360v^2(5v^2+9)\tan\left(\frac{v}{2}\right)\sec^6\left(\frac{v}{2}\right)\\
&+30240v(97v^2-170)\sec^4\left(\frac{v}{2}\right)-126(4501v^4+25800v^2\\
&+8640)\tan\left(\frac{v}{2}\right)\sec^4\left(\frac{v}{2}\right)+28(-151573v^4+398400v^2
\end{aligned}
$$

$$
\begin{aligned}
&+ 1745280) \tan\left(\frac{v}{2}\right) \sec^2\left(\frac{v}{2}\right) + 153090v^3 \csc^6\left(\frac{v}{2}\right) \\
&+ 25515v^4 \cot\left(\frac{v}{2}\right) \csc^6\left(\frac{v}{2}\right) + 1462860v^3 \csc^4\left(\frac{v}{2}\right) + 2835v^2(89v^2 \\
&+ 144) \cot\left(\frac{v}{2}\right) \csc^4\left(\frac{v}{2}\right) + 3780v(4139v^2 - 10960) \csc^2\left(\frac{v}{2}\right) \\
&+ 63(42779v^4 + 480v^2 - 51840) \cot\left(\frac{v}{2}\right) \csc^2\left(\frac{v}{2}\right) + 61440v(400v^4 \\
&- 6273v^2 + 15540) + 184320v(737v^2 - 3260) \cos(v) \\
&+ 184320v(150v^4 - 1739v^2 + 2660) \cos(2v) + 368640v(61v^2 \\
&- 220) \cos(3v) + 61440v(72v^4 - 779v^2 + 980) \cos(4v) \\
&+ 614400v(v^2 - 4) \cos(5v) + 30720v(4v^4 - 45v^2 + 60) \cos(6v) \\
&+ 27(2129819v^4 - 7933600v^2 + 2405760) \cot\left(\frac{v}{2}\right) + 122880(173v^4 \\
&- 3222v^2 + 3060) \sin(v) - 491520(259v^4 - 1035v^2 + 450) \sin(2v) \\
&+ 8192(451v^4 - 7365v^2 + 5490) \sin(3v) - 24576(809v^4 \qquad (46) \\
&- 2860v^2 + 960) \sin(4v) + 49152(2v^4 - 35v^2 + 30) \sin(5v) \\
&- 4096(137v^4 - 510v^2 + 180) \sin(6v) + (-71232167v^4 \\
&+ 545068320v^2 - 484318080) \tan\left(\frac{v}{2}\right) + \frac{4200v(11495v^2 - 101648)}{\cos(v) + 1}
\end{aligned}
$$

$$
\begin{aligned}
b^5_{1,denom} &= 30v^7 \\
b^5_{2,denom} &= 393216v^7 \\
b^5_{3,denom} &= 6v^7 \\
b^5_{4,denom} &= 6144v^7 \\
b^5_{5,denom} &= 24576v^7 \\
b^5_{6,denom} &= 61440v^7 \qquad (47)
\end{aligned}
$$

$$
\begin{aligned}
b^5_{T,1} &= \frac{90987349}{53222400} - \frac{16301796103v^2}{48432384000} + \frac{3000167803v^4}{1162377216000} \\
&\quad - \frac{2795461105681v^6}{1778437140480000} - \frac{423149542577683v^8}{1892257117470720000} - \cdots \\
b^5_{T,2} &= -\frac{114798419}{26611200} + \frac{16301796103v^2}{4843238400} - \frac{9164631311v^4}{10567065600} \\
&\quad + \frac{1149042063431v^6}{16167610368000} - \frac{1015140295561079v^8}{189225711747072000} - \cdots \\
b^5_{T,3} &= \frac{270875723}{17740800} - \frac{16301796103v^2}{1076275200} + \frac{106131595741v^4}{15498362880} \\
&\quad - \frac{193910381341843v^6}{118562476032000} + \frac{12701953007551v^8}{62296530616320} - \cdots
\end{aligned}
$$

$$
\begin{aligned}
b^5_{T,4} &= -\frac{67855831}{2217600} + \frac{16301796103v^2}{403603200} - \frac{15415020883v^4}{645765120} \\
&\quad + \frac{125531790304181v^6}{14820309504000} - \frac{361081038637727v^8}{185515403673600} + \cdots \\
b^5_{T,5} &= \frac{50277247}{985600} - \frac{16301796103v^2}{230630400} + \frac{263828905451v^4}{5535129600} \\
&\quad - \frac{400330948542829v^6}{19760412672000} + \frac{54441481708734389v^8}{9010748178432000} - \cdots \\
b^5_{T,6} &= -\frac{253491379}{4435200} + \frac{16301796103v^2}{192192000} - \frac{117727186937v^4}{1976832000} \\
&\quad + \frac{3958504514434801v^6}{148203095040000} - \frac{7164842887862063v^8}{834328535040000} + \cdots
\end{aligned}
\tag{48}
$$

References

1. G. Quinlan, Resonances and instabilities in symmetric multistep methods. preprint arXiv astro-ph/9901136 (1999)
2. T. Lyche, Chebyshevian multistep methods for ordinary differential equations. Num. Math. **19**, 65–75 (1972)
3. W. Gautschi, Numerical integration of ordinary differential equations based on trigonometric polynomials. Numer. Math. **3**, 381–397 (1961)
4. L.Gr. Ixaru, G.V. Berghe, *Exponential Fitting, Mathematics and its Applications* (Kluwer Academic Publishers, Dordrecht/Boston/London 2004)
5. L. Brusa, L. Nigro, A one-step method for direct integration of structural dynamic equations. Int. J. Numer. Methods Eng. **15**, 685–699 (1980)
6. L.Gr. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
7. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
8. I. Prigogine, S. Rice (eds.), *Advances in Chemical Physics Vol. 93: New Methods in Computational Quantum Mechanics* (Wiley, 1997)
9. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
10. T.E. Simos, in *Atomic Structure Computations in Chemical Modelling: Applications and Theory*, ed by A. Hinchliffe (UMIST, The Royal Society of Chemistry, 2000), pp. 38–142
11. T.E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems. Chem. Model.: Appl. Theory, Roy. Soc. Chem. **2**, 170–270 (2002)
12. T.E. Simos, *Numerical Solution of Ordinary Differential Equations with Periodical Solution*. Doctoral Dissertation, National Technical University of Athens, Greece, 1990 (in Greek)
13. A. Konguetsof, T.E. Simos, On the Construction of exponentially-fitted methods for the numerical solution of the Schrödinger Equation. J. Comput. Methods Sci. Eng. **1**, 143–165 (2001)
14. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
15. A.D. Raptis, Exponential multistep methods for ordinary differential equations. Bull. Greek Math. Soc. **25**, 113–126 (1984)
16. L.Gr. Ixaru, *Numerical Methods for Differential Equations and Applications* (Reidel, Dordrecht-Boston-Lancaster, 1984)
17. L.Gr. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. Comput. Phys. Commun. **19**, 23–27 (1980)
18. T.E. Simos, P.S. Williams, A New Runge-Kutta-Nystrom method with phase-lag of order infinity for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 123–137 (2002)
19. T.E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 7–26 (2004)

20. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Shrödinger equation with automatic error control. Comput. Phys. Commun. **28**, 427–431 (1983)
21. A.D. Raptis, On the numerical solution of the Schrodinger equation. Comput. Phys. Commun. **24**, 1–4 (1981)
22. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation. Appl. Math. Comput. **112**, 99–112 (2000)
23. A.D. Raptis, T.E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problem. BIT **31**, 160–168 (1991)
24. P. Henrici, *Discrete Variable Methods in Ordinary Differential Equations* (Wiley, 1962)
25. M.M. Chawla, Uncoditionally stable Noumerov-type methods for second order differential equations. BIT **23**, 541–542 (1983)
26. M.M. Chawla, P.S. Rao, A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems. J. Comput. Appl. Math. **11**(3), 277–281 (1984)
27. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. J. Math. Chem. **41**(1), 79–100 (2007)
28. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **40**(3), 257–267 (2006)
29. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor-Corrector methods. J. Math. Chem. **40**(3), 269–293 (2006)
30. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
31. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
32. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods. J. Math. Chem. **37**(3), 271–279 (2005)
33. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
34. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. J. Math. Chem. **37**(3), 295–316 (2005)
35. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 317–331 (2005)
36. T.E. Simos, Exponentially - fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
37. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation. J. Math. Chem. **35**(1), 55–63 (2004)
38. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. J. Math. Chem. **34**(1–2), 39–58 (2003)
39. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34**(1–2), 83–94 (2003)
40. J. Vigo-Aguiar, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **32**(3), 257–270 (2002)
41. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
42. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. J. Math. Chem. **31**(2), 135–144 (2002)
43. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nystrom methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem. **31**(2), 211–232
44. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
45. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)

46. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
47. J. Vigo-Aguiar, T.E. Simos, A family of P-stable eighth algebraic order methods with exponential fitting facilities. J. Math. Chem. **29**(3), 177–189 (2001)
48. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)
49. G. Avdelas, T.E. Simos, Embedded eighth order methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **26**(4), 327–341 (1999)
50. T.E. Simos, A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **25**(1), 65–84 (1999)
51. T.E. Simos, Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. J. Math. Chem. **24**(1–3), 23–37 (1998)
52. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. J. Math. Chem. **21**(4), 359–372 (1997)
53. P. Amodio, I. Gladwell, G. Romanazzi, Numerical solution of general bordered ABD linear systems by cyclic reduction. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 5–12 (2006)
54. S.D. Capper, J.R. Cash, D.R. Moore, Lobatto-Obrechkoff formulae for 2nd order two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 13–25 (2006)
55. S.D. Capper, D.R. Moore, On high order MIRK schemes and Hermite-Birkhoff interpolants. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 27–47 (2006)
56. J.R. Cash, N. Sumarti, T.J. Abdulla, I. Vieira, The derivation of interpolants for nonlinear two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 49–58 (2006)
57. J.R. Cash, S. Girdlestone, Variable step Runge-Kutta-Nystrm methods for the numerical solution of reversible systems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 59–80 (2006)
58. J.R. Cash, F. Mazzia, Hybrid mesh selection algorithms based on conditioning for two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 81–90 (2006)
59. F. Iavernaro, F. Mazzia, D. Trigiante, Stability and conditioning in numerical analysis. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 91–112 (2006)
60. F. Iavernaro, D. Trigiante, Discrete conservative vector fields induced by the trapezoidal method. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 113–130 (2006)
61. F. Mazzia, A. Sestini, D. Trigiante, BS linear multistep methods on non-uniform meshes. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 131–144 (2006)
62. L.F. Shampine, P.H. Muir, H. Xu, A user-friendly fortran BVP solver. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(2), 201–217 (2006)
63. G.V. Berghe, M. Van Daele, Exponentially-fitted Strmer/Verlet methods. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(3), 241–255 (2006)
64. L. Aceto, R. Pandolfi, D. Trigiante, Stability analysis of linear multistep methods via polynomial type variation. JNAIAM J. Numer. Anal. Indust. Appl. Math. **2**(1–2), 1–9 (2007)
65. G. Psihoyios, A block implicit advanced step-point (BIAS) algorithm for stiff differential systems. Comput. Lett. **2**(1–2), 51–58 (2006)
66. W.H. Enright, On the use of 'arc length' and 'defect' for mesh selection for differential equations. Comput. Lett. **1**(2), 47–52 (2005)
67. T.E. Simos, P-stable four-step exponentially-fitted method for the numerical integration of the Schrödinger equation. Comput. Lett. **1**(1), 37–45(2005)
68. T.E. Simos, Stabilization of a four-step exponentially-fitted method and its application to the Schrödinger equation. Int. J. Modern Phys. C **18**(3), 315–328 (2007)
69. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**, 162–174 (2005)
70. T.E. Simos, A Runge-Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution. Comput. Math. Appl. **25**, 95–101 (1993)
71. T.E. Simos, Runge-Kutta interpolants with minimal phase-lag. Comput. Math. Appl. **26**, 43–49 (1993)
72. T.E. Simos, Runge-Kutta-Nyström interpolants for the numerical integration of special second-order periodic initial-value problems. Comput. Math. Appl. **26**, 7–15 (1993)
73. T.E. Simos, G.V. Mitsou, A family of four-step exponential fitted methods for the numerical integration of the radial Schrödinger equation. Comput. Math. Appl. **28**, 41–50 (1994)

74. T.E. Simos, G. Mousadis, A two-step method for the numerical solution of the radial Schrödinger equation. Comput. Math. Appl. **29**, 31–37 (1995)
75. G. Avdelas, T.E. Simos, Block Runge-Kutta methods for periodic initial-value problems. Comput. Math. Appl. **31**, 69–83 (1996)
76. G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation. Computers and Mathematics with Applications **31**, 85–102 (1996)
77. G. Papakaliatakis, T.E. Simos, A new method for the numerical solution of fourth order BVPs with oscillating solutions. Comput. Math. Appl. **32**, 1–6 (1996)
78. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **33**, 67–78 (1997)
79. T.E. Simos, A new hybrid imbedded variable-step procedure for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **36**, 51–63 (1998)
80. T.E. Simos, Bessel and Neumann fitted methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **42**, 833–847 (2001)
81. A. Konguetsof, T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems. Comput. Math. Appl. **45**, 547–554 (2003)
82. Z.A. Anastassi, T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
83. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
84. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. J. Comput. Appl. Math. **175**(1), 161–172 (2005)
85. K. Tselios, T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
86. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
87. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
88. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 93–106 (2003)
89. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
90. Ch. Tsitouras, T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
91. T.E. Simos, An exponentially fitted eighth-order method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **108**(1–2), 177–194 (1999)
92. T.E. Simos, An accurate finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **91**(1), 47–61 (1998)
93. R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **87**(2) 215–226 (1997)
94. Z.A. Anastassi, T.E. Simos, Special optimized Runge-Kutta methods for IVPs with oscillating solutions. Int. J. Modern Phys. C, **15**, 1–15 (2004)
95. Z.A. Anastassi, T.E. Simos, A dispersive-fitted and dissipative-fitted explicit Runge-Kutta method for the numerical solution of orbital problems. New Astron. **10**, 31–37 (2004)
96. Z.A. Anastassi, T.E. Simos, A trigonometrically-fitted Runge-Kutta method for the numerical solution of orbital problems. New Astron. **10**, 301–309 (2005)
97. T.V. Triantafyllidis, Z.A. Anastassi, T.E. Simos, Two optimized Runge-Kutta methods for the solution of the Schr̈dinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
98. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted fifth order Runge-Kutta methods for the numerical solution of the Schrödinger equation. Math. Comput. Model. **42**(7–8), 877–886 (2005)
99. Z.A. Anastassi, T.E. Simos, New trigonometrically fitted six-step symmetric methods for the efficient solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
100. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two new optimized eight-step symmetric methods for the efficient solution of the Schrödinger equation and related problems. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)

101. Z.A. Anastassi, T.E. Simos, A six-step P-stable trigonometrically-fitted method for the numerical integration of the radial Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
102. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. (in press, corrected proof)
103. T.E. Simos, P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**(2), 189–205 (1997)
104. G. Avdelas, T.E. Simos, A generator of high-order embedded P-stable methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **72**(2), 345–358 (1996)
105. R.M. Thomas, T.E. Simos, G.V. Mitsou, A family of Numerov-type exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **67**(2), 255–270 (1996)
106. T.E. Simos, A family of 4-step exponentially fitted predictor-corrector methods for the numerical-integration of the Schrödinger-equation. J. Comput. Appl. Math. **58**(3), 337–344 (1995)
107. T.E. Simos, An explicit 4-step phase-fitted method for the numerical-integration of 2nd-order initial-value problems. J. Comput. Appl. Math. **55**(2), 125–133 (1994)
108. T.E. Simos, E. Dimas, A.B. Sideridis, A Runge-Kutta-Nyström method for the numerical-integration of special 2nd-order periodic initial-value problems. J. Comput. Appl. Math. **51**(3), 317–326 (1994)
109. A.B. Sideridis, T.E. Simos, A low-order embedded Runge-Kutta method for periodic initial-value problems. J. Comput. Appl. Math. **44**(2), 235–244 (1992)
110. T.E. Simos, A.D. Raptis, A 4th-order Bessel fitting method for the numerical-solution of the SchrÖdinger-equation. J. Comput. Appl. Math. **43**(3), 313–322 (1992)
111. T.E. Simos, Explicit 2-step methods with minimal phase-lag for the numerical-integration of special 2nd-order initial-value problems and their application to the one-dimensional Schrödinger-equation. J. Comput. Appl. Math. **39**(1), 89–94 (1992)
112. T.E. Simos, A 4-step method for the numerical-solution of the Schrödinger-equation. J. Comput. Appl. Math. **30**(3), 251–255 (1990)
113. C.D. Papageorgiou, A.D. Raptis, T.E. Simos, A method for computing phase-shifts for scattering. J. Comput. Appl. Math. **29**(1), 61–67 (1990)
114. A.D. Raptis, Two-step methods for the numerical solution of the Schrödinger equation. Computing **28**, 373–378 (1982)
115. T.E. Simos, A new Numerov-type method for computing eigenvalues and resonances of the radial Schrödinger equation. Int. J. Modern Phys. C-Phys. Comput. **7**(1), 33–41 (1996)
116. T.E. Simos, Predictor corrector phase-fitted methods for $Y''=F(X,Y)$ and an application to the Schrödinger-equation. Int. J. Quantum Chem. **53**(5), 473–483 (1995)
117. T.E. Simos, Two-step almost P-stable complete in phase methods for the numerical integration of second order periodic initial-value problems. Int. J. Comput. Math. **46**, 77–85 (1992)
118. R.M. Corless, A. Shakoori, D.A. Aruliah, L. Gonzalez-Vega, Barycentric Hermite interpolants for event location in initial-value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 1–16 (2008)
119. M. Dewar, Embedding a general-purpose numerical library in an interactive environment. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 17–26 (2008)
120. J. Kierzenka, L.F. Shampine, A BVP solver that controls residual and error. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 27–41 (2008)
121. R. Knapp, A method of lines framework in mathematica. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 43–59 (2008)
122. N.S. Nedialkov, J.D. Pryce, Solving differential algebraic equations by Taylor series (III): the DAETS code. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 61–80 (2008)
123. R.L. Lipsman, J.E. Osborn, J.M. Rosenberg, The SCHOL Project at the University of Maryland: using mathematical software in the teaching of Sophomore differential equations. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 81–103 (2008)
124. M. Sofroniou, G. Spaletta, Extrapolation methods in mathematica. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 105–121 (2008)
125. R.J. Spiteri, Thian-Peng Ter, pythNon: A PSE for the numerical solution of nonlinear algebraic equations. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 123–137 (2008)
126. S.P. Corwin, S. Thompson, S.M. White, Solving ODEs and DDEs with impulses. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 139–149 (2008)

127. W. Weckesser, VFGEN: a code generation tool. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 151–165 (2008)
128. A. Wittkopf, Automatic code generation and optimization in maple. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 167–180 (2008)
129. D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits. Astron. J. **100**(5), 1694–1700 (1990)
130. J. Lambert, I. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
131. T. Simos, P. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
132. L.G. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schröodinger equation. Compu. Phys. Commun. **38**(3), 329–337 (1985)