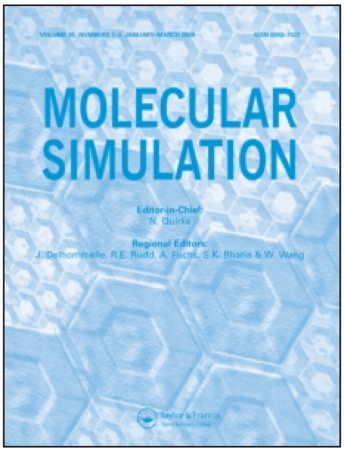

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

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To cite this Article Simos, T. E.(1999) 'High Algebraic Order Methods for the Numerical Solution of the Schrödinger Equation', Molecular Simulation, 22: 4, 303 — 349
To link to this Article: DOI: 10.1080/08927029908022103
URL: http://dx.doi.org/10.1080/08927029908022103

Molecular Simulation, 1999, Vol. 22, pp. 303–349
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HIGH ALGEBRAIC ORDER METHODS FOR THE NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

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(Received October 1998; accepted November 1998)

A family of new hybrid four-step tenth algebraic order methods with phase-lag of order 16(2)22 is developed for the numerical solution of the Schrödinger equation. Based on the new methods a variable-step procedure is introduced. Numerical illustrations obtained for the approximation of the phase shift problem for the well known case of the Lenard-Jones potential and for the numerical solution of the coupled equations arising from the Schrödinger equation show that these new methods are better than other finite difference methods.

Keywords: Schrödinger equation; eigenvalue problems; resonance problems; scattering problems; phase shift problems; finite differences; multistep methods; exponential fitting; Bessel and Neumann fitting; phase-lag; coupled differential equations

1. INTRODUCTION

There is much activity concerning the numerical solution of the radial Schrödinger equation (1) (see [1–3, 8, 13–17, 19, 21–29, 31]). The construction of a great number of schemes is the result of this activity. The radial Schrödinger equation has the form:

$$y''(r) + W(r)y(r) = 0 \tag{1}$$

where $0 \leq r < \infty$ and $W(r) = E - l(l+1)/r^2 - V(r)$. We call the term $l(l+1)/r^2$ the *centrifugal potential*, and the function $V(r)$ *the potential*,

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where $V(r) \to 0$ as $r \to \infty$. Based on the sign of the energy E there are two main categories of problems arising from (1) (see for details [1]).

In many scientific areas, such as nuclear physics, quantum mechanics, quantum chemistry, physical and theoretical chemistry and theoretical physics (see [2–4]), there is the need for the accurate solution of the Schrödinger equation. The most important characteristics of an efficient method for the solution of the problem (1) are the accuracy and the computational efficiency. The development of methods with the above mentioned characteristics is an open problem.

One of the most important properties for the numerical solution of the general second order differential equations with periodic or oscillating solution is the algebraic order of the method. Another important property is the interval of periodicity. The interval of periodicity defines the stepsize which can be used in order the approximation of the solution of problems with high oscillatory or periodic solution to be of the same order with the algebraic order of the method. It is obvious that when we have a large interval of periodicity then we can have a large stepsize for the same accuracy. It is obvious, also, that when we have small interval of periodicity or zero interval of periodicity then we can have only very small stepsizes or we may have divergence of the method. Another important new insight is the **phase-lag** first introduced by Brusa and Nigro [5]. This property defines the approximation of a method to the accurate solution of the test equation $y'' = -w^2 y$. When we have a method with minimal phase-lag then this approximation is accurate and it has been proved that the method is accurate for the numerical approximation of problems with oscillatory solution. The most widely used scheme for the numerical integration of (1) is **Numerov's method**, with interval of periodicity (0, 6) and phase-lag of order four. In the literature many methods with minimal phase-lag for the approximate solution of general second order differential equations with periodic solutions have been developed (see [1, 6–14]). All these methods have algebraic order **four** and **six**.

The purpose of this paper is to introduce a four-parameter family of tenth algebraic order methods. This family contains a free parameter which is defined in order to have minimal phase-lag *i.e.*, phase-lag of orders 16(2)22 for the numerical solution of the phase shift problem of the radial Schrödinger equation and for the numerical solution of the coupled equations arising from the Schrödinger equation. The phase shifts calculated by these methods are more accurate than those computed by Cash and Raptis [16] and by Simos [31]. We introduce a new error control procedure, which is based on the phase-lag order. Based on the new methods an embedded scheme is introduced for the numerical solution of (1) and for the numerical solution of the coupled Schrödinger equations. The numerical results given by this new embedded scheme are better than those of the most well known variable-step method of Raptis and Cash [17] and the variable-step method of Simos [25].

2. PHASE-LAG ANALYSIS OF GENERAL SYMMETRIC 2*K*-STEP, $K \in N$ METHODS

In recent years there has been considerable interest in the numerical solution of second order periodic initial-value problems (see [5–7, 9–12, 18–19]).

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \tag{2}$$

To investigate the absolute stability properties we introduce the scalar test equation:

$$y'' = -w^2 y \tag{3}$$

When we apply a symmetric $2k$ method to the scalar test equation (3) we obtain a difference equation of the form

$$\begin{aligned} &A_k(H)y_{n+k} + \cdots + A_1(H)y_{n+1} + A_0(H)y_n + A_1(H)y_{n-1} \\ &\quad + \cdots + A_k(H)y_{n-k} = 0 \end{aligned} \tag{4}$$

where $H = wh$, h is the step length and $A_0(H), A_1(H), \ldots, A_k(H)$ are polynomials of H and y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2, \ldots$.

The characteristic equation associated with (4) is

$$A_k(H)s^k + \cdots + A_1(H)s + A_0(H) + A_1(H)s^{-1} + \cdots + A_k(H)s^{-k} = 0 \tag{5}$$

DEFINITION 1 [12] and [19] The method (4) with the characteristic equation (5) is unconditionally stable if $|s_i| \leq 1$, $i = 1, \ldots, 2k$ for all values of H.

From Lambert and Watson [18] we have the following definitions

DEFINTION 2 A symmetric $2k$-step method with the characteristic equation given by (5) is said to have an **interval of periodicity** (H_0^2, H_1^2) if, for all

$H \in (H_0^2, H_1^2)$, the roots s_i, $i = 1, \ldots, 2k$ of (5) satisfy:

$$s_1 = e^{i\theta(H)}, \quad s_2 = e^{-i\theta(H)}, \quad \text{and} \quad |s_i| \leq 1, \quad i = 3, \ldots, 2k \tag{6}$$

where $\theta(H)$ is a real function of H.

We note here that the quantities s_i, $i = 1, 2$ express the accuracy of the approximation of the numerical method to the true solution of the test equation $y'' = -w^2 y$ which is e^{iH}, $H = wh$.

DEFINITION 3 The method (5) is **P-stable** if its **interval of periodicity** is $(0, \infty)$.

DEFINITION 4 For any method corresponding to the characteristic equation (5) **the phase-lag** is defined as the leading term in the expansion of

$$t = H - \theta(H) \tag{7}$$

Then if the quantity $t = O(H^{q+1})$ as $H \to 0$, the order of phase-lag is q.

The phase-lag theory is also valid for the case where w is imaginary. In that case we now have an **exponential error** which corresponds to the **phase-lag**.

THEOREM 1 *For all H in the interval of periodicity, the symmetric $2k$-step method with characteristic equation given by* (5) *has phase-lag order q and phase-lag constant c given by*

$$\begin{aligned} &-cH^{q+2} + O(H^{q+3}) \\ &= \frac{2A_k(H)\,cos(kH) + \cdots + 2A_j(H)\,cos(jH) + \cdots + A_0(H)}{2k^2 A_k(H) + \cdots + 2j^2 A_j(H) + \cdots + 2A_1(H)} \end{aligned} \tag{8}$$

Proof If we put $s = e^{i\theta(H)}$ then (5) becomes

$$2A_k(H)\cos(k\theta(H)) + \cdots + 2A_j(H)\cos(j\theta(H)) + \cdots + A_0(H) = 0 \tag{9}$$

By definition the phase-lag order q and phase-lag constant c are given by

$$t = H - \cos(\theta(H)) = cH^{q+1} + O(H^{q+2}) \tag{10}$$

then since

$$\theta(H) = H - t \tag{11}$$

we may show from trigonometric expansions that

$$\cos(\theta(H)) = \cos(H - t) = \cos H + cH^{q+2} + O(H^{q+3}) \tag{12}$$

$$\sin(\theta(H)) = \sin(H - t) = \sin H - cH^{q+1} + O(H^{q+2}) \tag{13}$$

By an inductive argument using the familiar identities

$$\cos(j\theta(H)) = \cos((j-1)\theta(H))\cos(\theta(H)) - \sin((j-1)\theta(H))\sin(\theta(H)) \tag{14}$$

$$\sin(j\theta(H)) = \sin((j-1)\theta(H))\cos(\theta(H)) + \cos((j-1)\theta(H))\sin(\theta(H)) \tag{15}$$

it is now straightforward to show that

$$\cos(j\theta(H)) = \cos(jH) + cj^2H^{q+2} + O(H^{q+3}) \tag{16}$$

$$\sin(j\theta(H)) = \sin(jH) - cjH^{q+1} + O(H^{q+2}) \tag{17}$$

Then substituting (16) and (17) into (9) for $j = 1, 2, \ldots, k$ will give the result.

The converse of the theorem may also be easily shown. The converse states that if (8) is true then the method will have phase-lag order q and phase-lag constant c. To prove this we suppose that the method has phase-lag order p and phase-lag constant d. This means

$$t = H - \theta(H) = dH^{q+1} + O(H^{p+1}) \tag{18}$$

Then we may show by trigonometric expansions that

$$\cos(j\theta(H)) = \cos(jH) + dj^2H^{p+2} + O(H^{p+3}) \tag{19}$$

Substituting for $\cos(jH)$ in (8) and using (9) we have

$$-2dH^{p+1}\sum_{j=0}^{k} A_j j^2 = -2cH^{q+1}\sum_{j=0}^{k} A_j j^2 + O(H^{q+2}) \tag{20}$$

Equating highest powers gives

$$p = q \quad \text{and} \quad d = c \tag{21}$$

i.e., the theorem is proved. ∎

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric $2k$-step method. For the symmetric four-step methods the phase-lag order and the phase-lag constant are given by (8) with $k = 2$.

The calculation of the exponential error follows the same principle. Now w is imaginary and cos is replaced by cosh in formula (8).

For the symmetric four-step methods (*i.e.*, for the case $k = 2$) we have the following lemma (for the proof see [29]).

LEMMA 1 (for the proof see [ ]) *All symmetric four-step methods with characteristic equation given by (5) for $k = 2$ have an interval of periodicity $[H_0^2, H_1^2]$ if for all $H \in [H_0^2, H_1^2]$ the following relations*

$$\begin{aligned} P_1(H) &= 2A_2(H) - 2A_1(H) + A_0(H) \geq 0, \\ P_2(H) &= 12A_2(H) - 2A_0(H) \geq 0, \\ P_3(H) &= 2A_2(H) + 2A_1(H) + A_0(H) \geq 0, \\ S(H) &= P_2(H)^2 - 4P_1(H)P_3(H) \geq 0. \end{aligned} \tag{22}$$

are satisfied.

3. THE NEW TENTH ORDER METHODS

Consider approximations at the point x_{n+s} of algebraic order eight

$$\begin{aligned} \hat{y}_{n+s} &= z_0 y_{n+2} + z_1 y_{n+1} + z_2 y_n + z_3 y_{n-1} + z_4 y_{n-2} \\ &\quad + h^2 (z_5 f_{n+2} + z_6 f_{n+1} + z_7 f_n + z_8 f_{n-1} + z_9 f_{n-2}) \end{aligned} \tag{23}$$

where $f_i = f(x_i, y_i)$, $i = n + 2(-1)n - 2$. After straightforward calculations, using algebraic manipulation packages, it can be seen that for

$$\begin{aligned} z_0 &= -\frac{2}{3}s^3 - \frac{1}{42}s^7 + \frac{1}{4}s^5 + \frac{37}{84}s + \frac{11}{632}s^8 \\ &\quad + \frac{139}{7584}s^4 - \frac{31}{15168}s^{10} - \frac{511}{15168}s^6, \\ z_1 &= -\frac{8}{21}s + \frac{4}{3}s^3 + \frac{1}{21}s^7 - \frac{1}{2}s^5 + \frac{232}{237}s^4 \\ &\quad + \frac{19}{158}s^8 - \frac{2}{237}s^{10} - \frac{140}{237}s^6, \\ z_2 &= 1 - \frac{2521}{1264}s^4 - \frac{87}{316}s^8 + \frac{53}{2528}s^{10} + \frac{3157}{2528}s^6, \end{aligned}$$

$$
\begin{aligned}
z_3 &= \frac{8}{21}s - \frac{4}{3}s^3 - \frac{1}{21}s^7 + \frac{1}{2}s^5 + \frac{232}{237}s^4 \\
&\quad + \frac{19}{158}s^8 - \frac{2}{237}s^{10} - \frac{140}{237}s^6, \\
z^4 &= \frac{2}{3}s^3 + \frac{1}{42}s^7 - \frac{1}{4}s^5 - \frac{37}{84}s + \frac{11}{632}s^8 \\
&\quad + \frac{139}{7584}s^4 - \frac{31}{15168}s^{10} - \frac{511}{15168}s^6, \\
z_5 &= \frac{1}{1592640}s \\
&\quad (161s^9 - 1050s^7 - 42976 + 3160s^6 \\
&\quad + 1869s^5 + 66360s^2 - 980s^3 - 26544s^4), \\
z_6 &= \frac{1}{99540}s \\
&\quad (1975s^6 - 3045s^7 + 8904s^5 - 21567s^4 \\
&\quad - 6160s^3 - 46768 + 301s^9 + 66360s^2), \\
z_7 &= \frac{1}{12640}s^2(-1610s^6 - 11720s^2 + 6879s^4 + 6320 + 131s^8), \\
z_8 &= \frac{1}{99540}s \\
&\quad (46768 - 66360s^2 - 6160s^3 + 301s^9 \\
&\quad + 21567s^4 + 8904s^5 - 1975s^6 - 3045s^7), \\
z_9 &= \frac{1}{1592640}s \\
&\quad (-66360s^2 + 42976 + 1869s^5 - 980s^3 \\
&\quad - 3160s^6 + 161s^9 - 1050s^7 + 26544s^4), \qquad (24)
\end{aligned}
$$

the approximation is of order $O(h^9)$.

Consider, now, approximations at the points x_{n-s} of algebraic order eight

$$
\begin{aligned}
\hat{y}_{n-s} &= x_0 y_{n+2} + x_1 y_{n+1} + x_2 y_n + x_3 y_{n-1} + x_4 y_{n-2} \\
&\quad + h^2(x_5 f_{n+2} + x_6 f_{n+1} + x_7 f_n + x_8 f_{n-1} + x_9 f_{n-2}) \qquad (25)
\end{aligned}
$$

where $f_i = f(x_i, y_i)$, $i = n + 2(-1)n - 2$. After straightforward calculations, using algebraic manipulation packages, it can be seen that for

$$
\begin{aligned}
x_0 &= \frac{2}{3}s^3 + \frac{1}{42}s^7 - \frac{1}{4}s^5 - \frac{37}{84}s \\
&\quad + \frac{11}{632}s^8 + \frac{139}{7584}s^4 - \frac{31}{15168}s^{10} - \frac{511}{15168}s^6, \\
x_1 &= \frac{8}{21}s - \frac{4}{3}s^3 - \frac{1}{21}s^7 + \frac{1}{2}s^5 \\
&\quad + \frac{232}{237}s^4 + \frac{19}{158}s^8 - \frac{2}{237}s^{10} - \frac{140}{237}s^6, \\
x_2 &= 1 - \frac{2521}{1264}s^4 - \frac{87}{316}s^8 + \frac{53}{2528}s^{10} + \frac{3157}{2528}s^6, \\
x_3 &= -\frac{8}{21}s + \frac{4}{3}s^3 + \frac{1}{21}s^7 - \frac{1}{2}s^5 \\
&\quad + \frac{232}{237}s^4 + \frac{19}{158}s^8 - \frac{2}{237}s^{10} - \frac{140}{237}s^6, \\
x_4 &= -\frac{2}{3}s^3 - \frac{1}{42}s^7 + \frac{1}{4}s^5 + \frac{37}{84}s \\
&\quad + \frac{11}{632}s^8 + \frac{139}{7584}s^4 - \frac{31}{15168}s^{10} - \frac{511}{15168}s^6, \\
x_5 &= \frac{1}{1592640}s(-66360s^2 + 42976 + 1869s^5 - 980s^3 \\
&\quad - 3160s^6 + 161s^9 - 1050s^7 + 26544s^4), \\
x_6 &= \frac{1}{99540}s(46768 - 66360s^2 - 6160s^3 + 301s^9 \\
&\quad + 21567s^4 + 8904s^5 - 1975s^6 - 3045s^7), \\
x_7 &= \frac{1}{12640}s^2(-1610s^6 - 11720s^2 + 6879s^4 + 6320 + 131s^8), \\
x_8 &= \frac{1}{99540}s(1975s^6 - 3045s^7 + 8904s^5 - 21567s^4 \\
&\quad - 6160s^3 - 46768 + 301s^9 + 66360s^2), \\
x_9 &= \frac{1}{1592640}s(161s^9 - 1050s^7 - 42976 + 3160s^6 \\
&\quad + 1869s^5 + 66360s^2 - 980s^3 - 26544s^4),
\end{aligned} \tag{26}
$$

the approximation is of order $O(h^9)$.

Finally, we consider the following general formula

$$
\begin{aligned}
&y_{n+2} + q_0(y_{n+1} + y_{n-1}) + q_1 y_n + y_{n-2} \\
&\quad = h^2[w_0(f_{n+2} + f_{n-2}) + w_1(f_{n+1} + f_{n-1}) + w_2(f_{n+s} + f_{n-s}) + w_3 f_n]
\end{aligned} \tag{27}
$$

where $f_i = f(x_i, y_i)$, $i = n+2(-1)n-2$. In order the above formula has algebraic order ten the following system of equations must satisfied

$$\begin{aligned}
2+q_1+2q_0=0,\ 4-2w_1-2w_2-w_3+q_0-2w_0&=0,\\
\frac{4}{3}-w_1-w_2s^2+\frac{1}{12}q_0-4w_0&=0,\\
\frac{8}{45}-\frac{1}{12}w_2s^4-\frac{1}{12}w_1+\frac{1}{360}q_0-\frac{4}{3}w_0&=0,\\
\frac{4}{315}-\frac{1}{360}w_2s^6-\frac{1}{360}w_1+\frac{1}{20160}q_0-\frac{8}{45}w_0&=0,\\
\frac{8}{14175}-\frac{1}{20160}w_2s^8-\frac{1}{20160}w_1+\frac{1}{1814400}q_0-\frac{4}{315}w_0&=0.
\end{aligned} \tag{28}$$

The solution of the above equation is given by

$$\begin{aligned}
w_2&=-\frac{1264}{s^2(465\,s^6+2555\,s^2-556-2464\,s^4)},\\
w_0&=\frac{1}{3}\frac{69\,s^4-211\,s^2+56}{465\,s^4-1999\,s^2+556}\\
w_1&=\frac{16}{3}\frac{129\,s^4-296\,s^2+88}{(465\,s^2-139)(s^2-1)},\quad q_0=128\frac{15\,s^2-58}{465\,s^2-139}\\
w_3&=2\frac{1179\,s^4-3121\,s^2+316}{(465\,s^2-139)s^2},\quad q_1=-6\frac{795\,s^2-2521}{465\,s^2-139}
\end{aligned} \tag{29}$$

Consider now the following four parameter family of methods of algebraic order ten

$$\begin{aligned}
\hat{y}_{n+(1/2)}&=\frac{1}{64}(19y_{n+1}+29y_n-13y_{n-1})+\frac{h^2}{768}(-25f_{n+1}+62f_n+23f_{n-1})\\
\hat{y}_{n-(1/2)}&=\frac{1}{64}(-13y_{n+1}+29y_n+19y_{n-1})+\frac{h^2}{768}(23f_{n+1}+62f_n-25f_{n-1})\\
\hat{y}_n&=y_n-t_ih^2[f_{n+1}-2f_n+f_{n-1}-4(\hat{f}_{n+(1/2)}-2f_n+\hat{f}_{n-(1/2)})],\ i=1(1)4\\
\hat{\hat{y}}_n&=y_n-\frac{h^2}{20}(-f_{n+2}-f_{n-2}+20f_{n+1}+20f_{n-1}\\
&\qquad-102\hat{f}_n-64\hat{f}_{n+(1/2)}-64\hat{f}_{n-(1/2)})\\
\hat{y}_{n+s}&=z_0y_{n+2}+z_1y_{n+1}+z_2y_n+z_3y_{n-1}+z_4y_{n-2}\\
&\quad+h^2(z_5f_{n+2}+z_6f_{n+1}+z_7\hat{\hat{f}}_n+z_8f_{n-1}+z_9f_{n-2})
\end{aligned} \tag{30}$$

$$\hat{y}_{n-s} = x_0 y_{n+2} + x_1 y_{n+1} + x_2 y_n + x_3 y_{n-1} + x_4 y_{n-2} + h^2(x_5 f_{n+2} + x_6 f_{n+1} + x_7 \hat{\hat{f}}_n + x_8 f_{n-1} + x_9 f_{n-2}) \tag{31}$$

$$y_{n+2} + q_0(y_{n+1} + y_{n-1}) + q_1 y_n + y_{n-2} = h^2[w_0(f_{n+2} + f_{n-2}) + w_1(f_{n+1} + f_{n-1}) + w_2(\hat{f}_{n+s} + \hat{f}_{n-s}) + w_3 f_n] \tag{32}$$

with the coefficients given by (24), (26) and (29). The local truncation error of the above family of methods is given by

$$\begin{aligned} L.T.E(h) = h^{12}\Bigg[\frac{1}{2452488192000}&(-217964888064000\, t_i(D^{(6)})(y)(x_n) \\ &- 2927657779200\, s^2(D^{(8)})(y)(x_n) \\ &+ 131744600064000\, s^2 t_i(D^{(6)})(y)(x_n) \\ &- 18071772364800\, s^4 t_i(D^{(6)})(y)(x_n) \\ &+ 401594941440\, s^4(D^{(8)})(y)(x_n) + 1187512320(D^{(12)})(y)(x_n) \\ &- 4698931200\, s^2(D^{(12)})(y)(x_n) + 1708523520\, s^4(D^{(12)})(y)(x_n) \\ &+ 4843664179200(D^{(8)})(y)(x_n))/(465 s^2 - 139)\Bigg], \quad i = 1(1)4 \end{aligned} \tag{33}$$

where $(D^{(j)})(y)(x_n)) = y^{(j)}(x_n)$.

We apply this method to the scalar test equation (3). Setting $H = wh$ we obtain the *difference equation* (4) and the corresponding characteristic equation (5) with $k = 2$ and

$$\begin{aligned} A_2(H) = -\frac{1}{14400}&(-6696000 s^2 + 2001600 + 5600 H^4 s^2 \\ &- 3680 H^4 s^4 - 137520 h^6 s^2 + 18864 H^6 s^4 \\ &+ 227520 H^6 - 69600 s^2 H^2 \\ &- 74400 s^4 H^2 + 67200 H^2)/(465 s^2 - 139), \\ A_1(H) = -\frac{1}{14400}&(106905600 - 6366600 H^{10} s^4 t_4 t_3 \\ &- 110080 H^4 s^4 - 307200 s^4 H^2 + 563200 H^4 s^2 \\ &+ 1670868000 H^{14} s^2 t_4 t_3 t_2 t_1 + 278478000 H^{12} s^2 t_4 t_3 t_2 \\ &+ 46413000 H^{10} s^2 t_4 t_3 \end{aligned}$$

$$
\begin{aligned}
& - 1061100\, H^8 s^4 t_4 - 229197600\, H^{14} s^4 t_4 t_3 t_2 t_1 \\
& - 38199600\, H^{12} s^4 t_4 t_3 t_2 \\
& - 2764368000\, H^{14} t_4 t_3 t_2 t_1 - 460728000\, H^{12} t_4 t_3 t_2 \\
& - 76788000\, H^{10} t_4 t_3 \\
& - 773550\, H^{12} s^2 t_4 t_3 + 3144\, H^8 s^4 \\
& + 7735500\, H^8 s^2 t_4 + 37920\, H^8 - 7065600\, s^2 H^2 \\
& - 3185280\, H^6 - 12798000\, H^8 t_4 \\
& + 213300\, H^{10} t_4 - 22920\, H^8 s^2 + 1925280\, H^6 s^2 \\
& - 27648000\, s^2 - 264096\, H^6 s^4 \\
& + 6758400\, H^2 - 27847800\, H^{16} s^2 t_4 t_3 t_2 t_1 \\
& - 4641300\, H^{14} s^2 t_4 t_3 t_2 - 128925\, H^{10} s^2 t_4 \\
& + 46072800\, H^{16} t_4 t_3 t_2 t_1 \\
& + 7678800\, H^{14} t_4 t_3 t_2 + 1279800\, H^{12} t_4 t_3 \\
& + 3819960\, H^{16} s^4 t_4 t_3 t_2 t_1 \\
& + 636660\, H^{14} s^4 t_4 t_3 t_2 \\
& + 106110\, H^{12} s^4 t_4 t_3 + 17685\, H^{10} s^4 t_4)/(465\, s^2 - 139),
\end{aligned}
$$

$$
\begin{aligned}
A_0(H) = -\frac{1}{14400} & (-217814400 + 12733200\, H^{10} s^4 t_4 t_3 \\
& - 377280\, H^4 s^4 + 763200\, s^4 H^2 \\
& + 2750400\, H^4 s^2 \\
& - 3341736000\, H^{14} s^2 t_4 t_3 t_2 t_1 - 556956000\, H^{12} s^2 t_4 t_3 t_2 \\
& - 92826000\, H^{10} s^2 t_4 t_3 + 2122200\, H^8 s^4 t_4 \\
& + 458395200\, H^{14} s^4 t_4 t_3 t_2 t_1 \\
& + 76399200\, H^{12} s^4 t_4 t_3 t_2 + 5528736000\, H^{14} t_4 t_3 t_2 t_1 \\
& + 921456000\, H^{12} t_4 t_3 t_2 \\
& + 153576000\, H^{10} t_4 t_3 + 47960100\, H^{12} s^2 t_4 t_3 \\
& - 194928\, H^8 s^4 - 15471000\, H^8 s^2 t_4 \\
& - 2351040\, H^8 - 40161600\, s^2 H^2 - 4550400\, H^4 \\
& + 5915520\, H^6 + 25596000\, H^8 t_4 \\
& - 13224600\, H^{10} t_4 + 1421040\, H^8 s^2 \\
& - 3575520\, H^6 s^2 + 68688000\, s^2 + 490464\, H^6 s^4 \\
& + 101260800\, H^2 + 1726563600\, H^{16} s^2 t_4 t_3 t_2 t_1
\end{aligned}
$$

$$
\begin{aligned}
&+ 287760600\, H^{14} s^2 t_4 t_3 t_2 \\
&+ 7993350\, H^{10} s^2 t_4 - 2856513600\, H^{16} t_4 t_3 t_2 t_1 \\
&- 476085600\, H^{14} t_4 t_3 t_2 \\
&- 79347600\, H^{12} t_4 t_3 - 236837520\, H^{16} s^4 t_4 t_3 t_2 t_1 \\
&- 39472920\, H^{14} s^4 t_4 t_3 t_2 \\
&- 6578820\, H^{12} s^4 t_4 t_3 - 1096470\, H^{10} s^4 t_4)/(465 s^2 - 139)
\end{aligned} \tag{34}
$$

THEOREM 2 *The above family of methods produces methods with phase-lag of order* 16(2)22 *for the value of parameters presented in the Table* I. *The interval of periodicity of the methods produced by the above family are, also, shown in Table* I. *equal to* (0, 9.1672).

Proof Considering (8) with $k = 2$ and (34) we have that the phase-lag of the above family of methods is given by the formula (65) given in the Appendix A.

To have maximal phase-lag order it follows from (65) that we must have the following systems of equations:

Case I $t_1 = t_2 = t_3 = 0$ and $t_4 \neq 0$

$$
\begin{aligned}
&\frac{1}{4191264000}(820523\, s^4 - 5965895\, s^2 + 9856876 + 36767115\, s^4 t_4 \\
&\qquad - 268035075\, s^2 t_4 + 443450700\, t_4)/(9 s^2 - 19) = 0 \\
&-\frac{1}{45768602880000}(896011116\, s^8 - 148590285660\, s^4 + 11808680598\, s^6 \\
&\qquad + 410088330450\, s^2 - 4951853426520\, s^4 t_4 \\
&\qquad + 13414079153475\, s^2 t_4 - 9460133783100\, t_4 \\
&\qquad + 345398978925\, s^6 t_4 + 40149689580\, s^8 t_4 \\
&\qquad - 313868656168)/(9 s^2 - 19)^2 = 0
\end{aligned} \tag{35}
$$

Case II $t_1 = t_2 = 0$ and $t_3, t_4 \neq 0$

$$
\begin{aligned}
&\frac{1}{4191264000}(- 5965895\, s^2 + 9856876 \\
&\qquad + 36767115\, s^4 t_2 - 268035075\, s^2 t_2 \\
&\qquad + 443450700\, t_2 + 820523\, s^4)/(9 s^2 - 19) = 0
\end{aligned}
$$

$$\frac{1}{45768602880000}(-345398978925s^6 t_2 - 40149689580s^8 t_2 + 21680832373200 t_2 s^6 t_1 + 313868656168 - 410088330450 s^2 - 203825569147200 s^4 t_2 t_1 + 595165512942000 s^2 t_2 t_1 + 4951853426520 s^4 t_2 - 13414079153475 s^2 t_2 - 552042907416000 t_2 t_1 + 9460133783100 t_2 - 11808680598 s^6 + 148590285660 s^4 - 896011116 s^8)/(9s^2-19)^2 = 0$$

$$-\frac{1}{19222813209600000}(4522574269988775 s^6 t_2 - 403043997901545 s^8 t_2 - 128845738824402600 t_2 s^6 t_1 + 5911281704928600 t_2 t_1 s^8 + 910594959674400 t_2 s^{10} t_1 - 37632466872 s^{12} - 3666340928250 s^{10} t_2 - 1686286962360 s^{12} t_2 - 224755333605704 + 554495862713990 s^2 + 541326057262590600 s^4 t_2 t_1 - 856821944069091000 s^2 t_2 t_1 - 14311205248375035 s^4 t_2 + 16205000498361675 s^2 t_2 + 452951205534828000 t_2 t_1 - 5320655568528300 t_2 + 129570499668974 s^6 - 438981953860614 s^4 - 254041583796 s^{10} - 10516916005882 s^8)/(9s^2-19)^3 = 0 \tag{36}$$

Case III $t_1 = 0$ and $t_2, t_3, t_4 \neq 0$

$$\frac{1}{4191264000}(9856876 + 36767115 s^4 t_3 - 5965895 s^2 - 268035075 s^2 t_3 + 820523 s^4 + 443450700 t_3)/(9s^2-19) = 0$$

$$
\begin{aligned}
\frac{1}{45768602880000}(&21680832373200\, t_3 s^6 t_2 \\
&+ 595165512942000\, s^2 t_3 t_2 - 203825569147200\, s^4 t_3 t_2 \\
&+ 313868656168 - 345398978925\, s^6 t_3 \\
&- 40149689580\, s^8 t_3 + 4951853426520\, s^4 t_3 \\
&- 410088330450\, s^2 - 13414079153475\, s^2 t_3 \\
&- 552042907416000\, t_3 t_2 + 148590285660\, s^4 \\
&- 896011116\, s^8 - 11808680598\, s^6 \\
&+ 9460133783100\, t_3)/(9 s^2 - 19)^2 = 0
\end{aligned}
$$

$$
\begin{aligned}
\frac{1}{19222813209600000}(&1288457388244402600 t_3 s^6 t_2 \\
&+2643181440707808000 t_3 t_2 t_1 \\
&+856821944069091000 s^2 t_3 t_2 \\
&-541326057262590600 s^4 t_3 t_2 \\
&+224755333605704+1686286962360 s^{12} t_3 \\
&-4522574269988775 s^6 t_3 \\
&+403043997901545 s^8 t_3+14311205248375035 s^4 t_3 \\
&-554495862713990 s^2-4101685789985784000 s^2 t_3 t_2 t_1 \\
&+2325752208429249600 s^4 t_3 t_2 t_1 \\
&-16205000498361675 s^2 t_3 \\
&-452951205534828000 t_3 t_2+37632466872 s^{12} \\
&+491721278224176000 t_3 t_2 t_1 s^8+438981953860614 s^4 \\
&+254041583796 s^{10}+10516916005882 s^8 \\
&+3666340928250 s^{10} t_3-129570499668974 s^6 \\
&-910594959674400 t_3 s^{10} t_2+5320655568528300 t_3 \\
&-5911281704928600 t_3 t_2 s^8 \\
&-5660842162287312000 t_3 t_2 t_1 s^6)/(9 s^2-19)^3=0
\end{aligned}
$$

$$
\begin{aligned}
-\frac{1}{1372508863165440000000}(&-9199022848363541793600\, t_3\, s^6\, t_2 \\
&- 3686841632571285988800000\, t_3\, t_2\, t_1 \\
&- 1524165416664824033100\, s^2\, t_3\, t_2 \\
&+ 1789674861611567090160\, s^4\, t_3\, t_2 \\
&+ 330717958499035107\, s^{12}\, t_3 \\
&+ 3510889926520616640\, t_3\, t_2\, t_1\, s^{12} + 4167058118958512361 \\
&- 512228973446190\, s^{14}\, t_3 + 120400889112504\, s^{16}\, t_3 \\
&+ 1537965900775696392000\, t_3\, t_2\, s^{10}\, t_1 \\
&+ 8652667887864\, s^{14} + 26869581346608\, s^{16} \\
&- 6501648012075216\, t_3\, s^{14}\, t_2 - 41024272413524400\, s^{12}\, t_3\, t_2 \\
&- 14906406781735582113\, s^6\, t_3 + 375210358534015174170\, s^8\, t_3 \\
&+ 3381038102409852224340\, s^4\, t_3 - 856666003619323103\, s^2 \\
&+ 87205865640048559404000\, s^2\, t_3\, t_2\, t_1 \\
&- 770974026324736970736000\, s^4\, t_3\, t_2\, t_1 \\
&- 40167781486658473898\, s^2\, t_3 + 4330800806559295068000\, t_3\, t_2 \\
&+ 7410195751037679\, s^{12} - 5448930991768034971200\, t_3\, t_2\, t_1\, s^8 \\
&+ 711659624925322648\, s^4 - 115331039260111615\, s^{10} \\
&+ 791862894073252714\, s^8 - 531019213338181317\, s^{10} t_3 \\
&- 311728911733490655\, s^6 - 15241338896896132020\, t_3\, s^{10}\, t_2 \\
&+ 19265944749392498157\, t_3 + 20717854280688136572\, t_3\, t_2\, s^8 \\
&+ 3135889522116751720320\, t_3\, t_2\, t_1\, s^6)/(9s^2 - 19)^4 = 0 \qquad (37)
\end{aligned}
$$

'ase IV t_1, t_2, t_3 and $t_4 \neq 0$

$$
\begin{aligned}
\frac{1}{4191264000}(&820523\, s^4 + 36767115\, s^4\, t_4 - 268035075\, s^2\, t_4 \\
&+ 9856876 - 5965895\, s^2 + 443450700\, t_4)/(9\, s^2 - 19) = 0
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{45768602880000}(148590285660\,s^4 - 896011116\,s^8 \\
&\quad - 11808680598\,s^6 + 595165512942000\,s^2\,t_4\,t_3 \\
&\quad - 203825569147200\,s^4\,t_4\,t_3 + 313868656168 \\
&\quad - 345398978925\,t_4\,s^6 - 40149689580\,s^8\,t_4 \\
&\quad + 21680832373200\,t_4\,s^6\,t_3 - 552042907416000\,t_4\,t_3 \\
&\quad + 4951853426520\,s^4\,t_4 - 13414079153475\,s^2\,t_4 \\
&\quad - 410088330450\,s^2 + 9460133783100\,t_4)/(9\,s^2 - 19)^2 = 0
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{19222813209600000}(438981953860614\,s^4 + 10516916005882\,s^8 \\
&\quad + 254041583796\,s^{10} - 129570499668974\,s^6 \\
&\quad + 26431814407078080000\,t_4\,t_3\,t_2 \\
&\quad + 856821944069091000\,s^2\,t_4\,t_3 - 541326057262590600\,s^4\,t_4\,t_3 \\
&\quad - 4522574269988775\,t_4\,s^6 + 403043997901545\,s^8\,t_4 \\
&\quad - 5660842162287312000\,t_4\,t_3\,t_2\,s^6 + 491721278224176000\,t_4\,t_3\,t_2\,s^8 \\
&\quad + 37632466872\,s^{12} + 224755333605704 + 3666340928250\,s^{10}\,t_4 \\
&\quad + 1686286962360\,s^{12}\,t_4 - 5911281704928600\,t_4\,s^8\,t_3 \\
&\quad + 128845738824402600\,t_4\,s^6\,t_3 - 452951205534828000\,t_4\,t_3 \\
&\quad + 14311205248375035\,s^4\,t_4 - 41016857899857840000\,s^2\,t_4\,t_3\,t_2 \\
&\quad + 23257522084292496000\,s^4\,t_4\,t_3\,t_2 - 16205000498361675\,s^2\,t_4 \\
&\quad - 910594959674400\,t_4\,s^{10}\,t_3 - 554495862713990\,s^2 \\
&\quad + 5320655568528300\;t_4)/(9\,s^2 - 19)^3 = 0
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{1372508863165440000000}(-711659624925322648l2\,s^4 \\
&\quad - 7918628940732527144\,s^8 + 1153310392601116152\,s^{10} \\
&\quad + 31172891173349065576\,s^6 + 368684163257128598880000\,t_4\,t_3\,t_2 \\
&\quad + 152416541666482403310000\,s^2\,t_4\,t_3 \\
&\quad - 178967486161156709016000\,s^4\,t_4\,t_3 \\
&\quad + 149064067817355821130\,t_4\,s^6 - 37521035853401517417\,s^8\,t_4
\end{aligned}
$$

$$- 3135889522116751720320000\, t_4\, t_3\, t_2\, s^6$$
$$+ 135748693012351952332800000\, t_4\, t_3\, t_2\, s^6\, t_1$$
$$- 258283575571484631168000\, t_4\, t_3\, t_2\, t_1\, s^8$$
$$+ 5448930991768034971200\, t_4\, t_3\, t_2\, s^8 - 74101957510376796\, s^{12}$$
$$+ 53101921333818131775\, s^{10}\, t_4$$
$$- 3307179584990351070\, s^{12}\, t_4$$
$$- 2071785428068813657200\, t_4\, s^8\, t_3$$
$$- 153796590077569639200\, t_4\, t_3\, s^{10}\, t_2$$
$$+ 18958805603211329856000\, t_4\, t_3\, t_2\, t_1\, s^{10}$$
$$+ 5122289734461900\, s^{14}\, t_4$$
$$- 1204008891125040\, s^{16}\, t_4 - 8652667887864\, s^{14}$$
$$- 26869581346608\, s^{16}$$
$$- 351088992652061664000\, t_4\, t_3\, t_2\, s^{12}$$
$$+ 41024272413524400\, s^{12}\, t_4\, t_3$$
$$+ 650164801207521600\, t_4\, s^{14}\, t_3$$
$$+ 9199022848363541793600\, t_4\, s^6\, t_3$$
$$- 215144396547852739968000000\, t_4\, t_3\, t_2\, t_1$$
$$- 4330800806559295068000\, t_4\, t_3$$
$$- 338103810240985222434 0\, s^4\, t_4$$
$$- 8720586564004855940400000\, s^2\, t_4\, t_3\, t_2$$
$$+ 770974026324736970736000\, s^4\, t_4\, t_3\, t_2$$
$$+ 4357713201896131197120000\, s^2\, t_4\, t_3\, t_2\, t_1$$
$$- 3474515240759990883456000\, s^4\, t_4\, t_3\, t_2\, t_1$$
$$+ 401677814866584738982 5\, s^2\, t_4$$
$$+ 15241338896896132020 0\, t_4\, s^{10}\, t_3$$
$$+ 856666003619323103 60\, s^2$$
$$- 192659447493924981570 0\, t_4$$
$$- 41670581189585123616)/(9\, s^2 - 19)^4 = 0$$

$$
\begin{aligned}
&-\frac{1}{547631036403010560000000}(756456343568132061254400000\,s^{14}\,t_4\,t_3\,t_2\,t_1\\
&\quad+1716737937834147761332800000\,t_4\,t_3\,t_2\,t_1\,s^{12}\\
&\quad+257614364688018528489897 8\,s^4\\
&\quad+561833293085997561270576\,s^8\\
&\quad-1098572170828047579755558\,s^{10}\\
&\quad-1598137795263778528921256\,s^6\\
&\quad-19699080548715609546304800000\,t_4\,t_3\,t_2\\
&\quad+22421757542725581090265215000\,s^2\,t_4\,t_3\\
&\quad-24033540111736888613749869000\,s^4\,t_4\,t_3\\
&\quad-16513040304042966684000\,s^{16}\,t_4\,t_3\\
&\quad+614433165968658854317500\,t_4^2\,s^{14}\\
&\quad-480399547558890960\,s^{20}\,t_4\\
&\quad-8409680708810597986770000000\,t_4^2\\
&\quad+259415755681801118400\,t_4\,s^{18}\,t_3-10720962957296592\,s^{20}\\
&\quad-140084508068172603936000\,t_4\,t_3\,t_2\,s^{16}\\
&\quad-534288303645818329262655000\,t_4^2\,s^8\\
&\quad-270505502860619109519686 25\,t_4\,s^6\\
&\quad+930163539365620897152816 0\,s^8\,t_4\\
&\quad+804030098963492307269563200 0\,t_4\,t_3\,t_2\,s^6\\
&\quad-30875313451493039646525408000 0\,t_4\,t_3\,t_2\,s^6\,t_1\\
&\quad+9235088315268361643601504000 0\,t_4\,t_3\,t_2\,t_1\,s^8\\
&\quad-292439378271978929496304800 0\,t_4\,t_3\,t_2\,s^8\\
&\quad+988800903797516033909 0\,s^{12}\\
&\quad+149274980267470782838863750 0\,t_4^2\,s^6\\
&\quad-2457429656329378666548112500\,t_4^2\,s^4\\
&\quad+22116731910746059662075000 00\,t_4^2\,s^2\\
&\quad-128499394175481097293525 00\,t_4^2\,s^{12}\\
&\quad+112428174375396261046665000\,t_4^2\,s^{10}\\
&\quad+758083009617977450539176\\
&\quad-1559342785863702968978850\,s^{10}\,t_4
\end{aligned}
$$

$$
\begin{aligned}
&+ 4871000520028831654966\,5 s^{12} t_4 \\
&- 491841624202056994329664200\, t_4 s^8 t_3 \\
&+ 5157136424381283366864840\,00 t_4 t_3 s^{10} t_2 \\
&- 12439825884490241409812640000\, t_4 t_3 t_2 t_1 s^{10} \\
&+ 2265232780530634031617\,5 s^{14} t_4 \\
&- 2544160963044421710990\, s^{16} t_4 \\
&+ 638802921047759624\,52 s^{14} - 565830016387644495\,6 s^{16} \\
&- 3282032848670239034170\,8000 t_4 t_3 t_2 s^{12} \\
&- 1294564367661316575994\,1700 s^{12} t_4 t_3 \\
&+ 71489483809063838137620\,0 t_4 s^{14} t_3 \\
&+ 1406511288419251448248214400\, t_4 s^6 t_3 \\
&+ 16769967849913751448655680\,0000 t_4 t_3 t_2 t_1 \\
&- 876330762870867171169302000\, t_4 t_3 \\
&+ 4134160888286102922104356\,5 s^4 t_4 \\
&+ 78659331560228843123099400\,00 s^2 t_4 t_3 t_2 \\
&- 11424481882272403928019036000\, s^4 t_4 t_3 t_2 \\
&- 4761012902657058052197192\,00000 s^2 t_4 t_3 t_2 t_1 \\
&+ 5385790037221184846008353\,60000 s^4 t_4 t_3 t_2 t_1 \\
&- 3070351366296189634779120\,0 s^2 t_4 \\
&+ 10499676378763942484584470\,0 t_4 s^{10} t_3 \\
&+ 2868948717430353077520\,00 s^{14} t_4 t_3 t_2 + 6546806166679178\,4 s^{18} \\
&- 2189520197359245512726510\, s^2 \\
&+ 513207640978602570\,0 s^{18} t_4 \\
&+ 810176060096256720386520\,0 t_4)/(9 s^2 - 19)^5 = 0
\end{aligned}
\tag{38}
$$

From the systems of Eqs. (35)–(38) it is easy for one to see that for

Case I $t_1 = t_2 = t_3 = 0$ and $t_4 \neq 0$

$$
\begin{aligned}
s &= \frac{1}{43209114}\sqrt{6788049187754250 - 43209114\sqrt{2242996609537505}} \\
t_4 &= -\frac{12564854753320544}{1362804686459892225} \\
&\quad - \frac{575603638}{3179877601739748525}\sqrt{2242996609537505}
\end{aligned}
\tag{39}
$$

Case II $t_1 = t_2 = 0$ and $t_3, t_4 \neq 0$

$$s = \frac{1}{1696313222} \sqrt{10470365214812644010 - 1696313222\sqrt{3473276111843421473}}$$

$$t_4 = -\frac{2643322959713995502559869}{4625675092246750461274111840} + \frac{61343015880179}{308378339483116697418274556}\sqrt{3473276111843421473}$$

$$t_3 = -\frac{56001078927638919}{10163442033626782285} - \frac{3485543753}{493943282834261619051}\sqrt{3473276111843421473} \tag{40}$$

Case III $t_1 = 0$ and $t_2, t_3, t_4 \neq 0$

$$s = \frac{1}{48200052638} \sqrt{8460331716383036275610 - 48200052638\sqrt{2822060490600354539065}}$$

$$t_4 = -\frac{259010010234729918217705934069}{35924416714821461921084043642960} - \frac{368521289492125627}{3991601857202384657898227071440}\sqrt{2822060490600354539065}$$

$$t_3 = -\frac{1140345057937919624168950733}{321713080252666803046600428096} + \frac{3582446979327609}{35745897805851867005177825344}\sqrt{2822060490600354539065}$$

$$t_2 = \frac{3193561969013358932323}{465026045079370275980325} - \frac{41939694353}{93005209015874055196065}\sqrt{2822060490600354539065} \tag{41}$$

Case IV t_1, t_2, t_3 and $t_4 \neq 0$

$$s = \frac{1}{38319300742294}(5348231235666415523466100490 - 38319300742294\sqrt{1788796154098194863439291665})^{1/2}$$

$$
\begin{aligned}
t_4 &= -\frac{2375925617513508020710381147997 19419}{23673407598076420902692904230455 2677304} \\
&\quad - \frac{241822666143533541785}{26303786220084912114103226922728075256} \\
&\quad \sqrt{17887961540981948634392916 65} \\
t_3 &= -\frac{28201142611083647674914315754909037}{66532454999134452792672852351820 41360} \\
&\quad - \frac{281056998771022929 51}{739249499990382808807476137242449040} \\
&\quad \sqrt{1788796154098194863439291665} \\
t_2 &= \frac{99939414677289793971732988430 09}{30551552153722251933535488339705 6} \\
&\quad + \frac{299832534935839007}{305515521537222519335354883397056} \\
&\quad \sqrt{1788796154098194863439291665} \\
t_1 &= \frac{1551905708180384730024068 9}{6926270548701011543324241 75} \\
&\quad - \frac{94805037119}{1385254109740202308664848 35} \\
&\quad \sqrt{1788796154098194863439291665}
\end{aligned} \tag{42}
$$

the phase-lag is given by

Case I $t_1 = t_2 = t_3 = 0$ and $t_4 \neq 0$

$$
\begin{aligned}
\text{phase-lag} = H^{16}\Bigg(&-\frac{1}{1516925029701463200 00} \\
&(837426275306822656398444 1551\sqrt{2242996609537505} \\
&- 3951273539893193816939932048067950 13) \\
&(-197635153 + 3\sqrt{2242996609537505})^3\Bigg)
\end{aligned} \tag{43}
$$

Case II $t_1 = t_2 = 0$ and $t_3, t_4 \neq 0$

phase-lag

$$
\begin{aligned}
= H^{18}\Bigg(&-\frac{19}{1113618430436730538320 0000} \\
&(-16034801621299552489749785200771887438133246377000115 13 \\
&+85967157142268749211332221449999994281365282 5 \\
&\sqrt{347327611184342147 3})(-23321868877+9\sqrt{347327611184342147 3})^4\Bigg)
\end{aligned} \tag{44}
$$

Case III $t_1 = 0$ and $t_2,\ t_3,\ t_4 \neq 0$

phase-lag

$$
\begin{aligned}
&= -\frac{1}{8332871917416877277402155200000} \\
&\quad H^{20}\Bigl(-466071004615080411075044294 13 \\
&\qquad 6429055114565093021937895941360124332625760 1899 \\
&\qquad + 8768578298844167643865349780920779195722323473341 83973 \\
&\qquad 92194561663\sqrt{2822060490600354539065})(-663927263233 \\
&\qquad + 9\sqrt{2822060490600354539065})^5\Bigr)
\end{aligned}
\tag{45}
$$

Case IV t_1, t_2, t_3 and $t_4 \neq 0$

hboxphase-lag

$$
\begin{aligned}
&= H^{22}\Bigl(\frac{1}{39748067594280045797198107305600000} \\
&\qquad (230813976047169433850654096 25 \\
&\qquad 9194802972759337971833867514780336315398734457 5204 \\
&\qquad 7277987670508169\sqrt{178879615409819486343929166 5} \\
&\qquad - 976267423159888804135576412554812\backslash \\
&\qquad 2590092022117199834894666 24 \\
&\qquad 1439574762899862938133088207436327742636500561 45) \\
&\qquad (-528064796351429 \\
&\qquad + 9\sqrt{178879615409819486343929166 5})^6\Bigr)
\end{aligned}
\tag{46}
$$

i.e., the methods are of phase-lag order 16(2)22.

To examine the interval of periodicity of the above method we calculate the polynomials $P_i(H)$, $i = 1(1)3$ and $S(H)$ and we substitute the above value of s and t_i, $i = 1(1)4$. We note here that for the first case we have that $t_1 = t_2 = t_3 = 0$ and $t_4 \neq 0$, for the second case we have that $t_1 = t_2 = 0$ and $t_3,\ t_4 \neq 0$, for the third case we have that $t_1 = 0$ and $t_2, t_3, t_4 \neq 0$ and for the final case we have that t_1, t_2, t_3 and $t_4 \neq 0$. The resulting polynomials are given in Appendix B.

It is easy for one to see that $P_i(H) \geq 0$, $i = 1(1)3$ and $S(H) \geq 0$ for $H^2 \in (0, 23.6551)$ for the Case I, for $H^2 \in (0, 17.9845)$ for the Case II, for $H^2 \in (0,\ 9.8214)$ for the Case III and for $H^2 \in (0,\ 9.8547)$ for the last case. ∎

In the following section we present some numerical illustrations of the method obtained in this paper.

4. NUMERICAL ILLUSTRATION

4.1. One-dimensional Schrödinger Equation

The methods developed in previous section can be applied in both the open channel problem and the bound state problem. We investigate in this paper the first case, *i.e.*, the case $E = k^2 > 0$.

In this case, in general, the potential function $V(r)$ dies away much faster than $l(l+1)/r^2$ so the latter is the predominant term. We note that we not consider Coulombic potentials. Then, Eq. (1) effectively reduces to: $y''(r) + (k^2 - l(l+1)/r^2)\, y(r) = 0$, for large r. It is well known that the Eq. (1) has two linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus the asymptotic solution of (1) (*i.e.*, for $r \to \infty$) has the form of

$$\begin{aligned} y(r) &\cong Akrj_l(kr) - Bkrn_l(kr) \\ &\cong G\left[\sin(kr - l\pi/2) + \tan\delta_l \cos(kr - l\pi/2)\right] \end{aligned} \tag{47}$$

where δ_l is the real scattering phase shift of the lth partial were induced by the potential $V(r)$. The value of δ_l can be computed using the formula

$$\tan\delta_l = \frac{y(r_b)S(r_a) - y(r_a)S(r_b)}{y(r_a)C(r_b) - y(r_b)C(r_a)} \tag{48}$$

where r_a and r_b are two distinct points in the asymptotic region, $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$.

The term $l\pi/2$ in (47) is conventional. The reason for inserting it is that, with this definition, all phase shifts vanish when the potential function vanishes itself.

4.2. The Woods-Saxon Potential

As a test for the accuracy of our methods we consider the numerical solution of the radial Schrödinger equation (1) with $l = 0$ in the well-known case where the potential $V(r)$ is the Woods-Saxon one

$$V(r) = V_w(r) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \tag{49}$$

with $z = \exp[(r - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$.

The problem considered here consists either of finding the **phase shift** $\delta(E) = \delta_l$ or finding those E, for $E \in [1, 1000]$, at which δ equals $\pi/2$. In our case we find the phase shifts for given energies. The obtained phase shift is then compared to the accurate value of the phase shift which is equal to $\pi/2$.

The boundary conditions for this problem are (considering that the phase shift is equal to $\pi/2$):

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

The domain of numerical integration is $[0, 15]$.

The new methods are four-step methods. So, to start integration we want to know the values y_0, y_1 and y_2. The value y_0 is known by the boundary conditions given above. To determine the value y_1 we use high order Runge-Kutta-Nyström method (see [30]) and to determine y_2 and y_3 we use the eighth order method developed by Simos [31] with steplength equal to the half of step size used.

In our numerical illustration we use the present methods, the method of Cash and Raptis [16] and the method of Simos [31]. From the results presented it is obvious that our new methods are much more accurate than the other methods.

Table I shows the absolute errors of the phase shifts in 10^{-7} units for energies given in the first column and for different choices of constant stepsize, which are shown in column 2. The empty areas indicate that the corresponding absolute errors are larger than 1.

TABLE I Absolute errors for phase shifts computed using the method of Cash and Rapits [16] (which is indicated as Method [a]), the method of Simos [31] (which is indicated as Method [b]), the present tenth order method with phase-lag of order 16 (which is indicated as Method [c]) and the present tenth order method with phase-lag of order 22 (which is indicated as Method [d])

The resonance	*h*	[*a*]	[*b*]	[*c*]	[*d*]
53.5888719	1/2	912345	3	0	0
	1/4	5981	1	0	0
	1/8	54	0	0	0
	1/16	5	0	0	0
341.4958743	1/2	934561	9	1	0
	1/4	9978	2	0	0
	1/8	79	0	0	0
	1/16	8	0	0	0
989.7019159	1/2	–	44	6	0
	1/4	555457	9	0	0
	1/8	657	1	0	0
	1/16	89	0	0	0

4.3. Error Estimation – The Phase Shift Problem

Several methods have been proposed for the estimation of the local truncation error (LTE) for the numerical integration of systems of initial-value problems, (see for example [20] and references therein).

In this paper we base our local error estimation technique on an embedded pair of integration methods and on the fact that when the local phase-lag error is of higher order then the approximation of the solution for the problems which have a periodic or oscillating solution is better.

We denote the solution obtained using the tenth order method with phase-lag of order 22 developed in this paper as y_{n+1}^H and the solution obtained with the tenth order method with phase-lag of order 20 developed in this paper as y_{n+1}^L and then, we have the following definition.

Definition 5 We define the **local phase-lag error** estimate in the lower order solution y_{n+1}^L by the quantity

$$L.PL.E = |y_{n+1}^H - y_{n+1}^L|. \tag{50}$$

Under the assumption that h is sufficiently small, the **local phase-lag error** in y_{n+1}^H can be neglected compared with that in y_{n+1}^L.

If the local phase-lag error of acc is requested and the step size of the integration used for the nth step length is h_n, the estimated step size for the $(n+1)st$ step must be

$$h_{n+1} = h_n \left(\frac{\text{acc}}{L.PL.E} \right)^{1/q}, \tag{51}$$

where q is the phase-lag order of the method.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in [17] for the Local Error, the step control procedure which we have actually used is

$$\begin{gathered} \text{If } L.PL.E < \text{acc}, h_{n+1} = 2h_n \\ \text{If } 100 \text{ acc} > L.PL.E \geq \text{acc}, h_{n+1} = h_n \end{gathered} \tag{52}$$

$$\text{If } L.PL.E \geq 100 \text{ acc}, h_{n+1} = \frac{h_n}{2} \text{ and repeat the step.} \tag{53}$$

We note that the local phase-lag error estimate is in the lower order solution y_{n+1}^L. However, if this error estimate is acceptable, *i.e.*, less than acc, we adopt the widely used procedure of performing local extrapolation. Thus, although we are actually controlling an estimate of the local phase-lag error in lower order solution y^L_{n+1}, it is the higher order solution y^H_{n+1} which we actually accept at each point.

4.4. Close Coupled Differential Equations

Many problems in theoretical physics and chemistry, in quantum mechanics, in quantum chemistry, in nuclear physics, in chemical physics and in physical chemistry can be transformed to the solution of coupled differential equations of the Schrödinger type.

The close-coupling differential equations of the Schrödinger type may be written in the form

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii}\right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{54}$$

for $1 \le i \le N$ and $m \neq i$.

We have investigated the case in which all channels are open. So we have the following boundary conditions (see for details [21]):

$$y_{ij} = 0 \quad \text{at } x = 0 \tag{55}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{li}(k_i x) \tag{56}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. We note here that since the methods presented in this paper have much larger intervals of periodicity (the property which must have a method to avoid instabilities) than the Numerov's method and other finite difference methods and have high algebraic order and minimal phase-lag, we can use the present methods to problems involve close channels.

Based on the detailed analysis developed in [21] and defining a matrix K' and diagonal matrices M, N by:

$$K'_{ij} = \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}$$
$$M_{ij} = k_i x j_{l_i}(k_i x)\delta_{ij}$$
$$N_{ij} = k_i x n_{l_i}(k_i x)\delta_{ij}$$

we find that the asymptotic condition (56) may be written as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}' \tag{57}$$

One of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation is the Iterative Numerov method of Allison [21].

A real problem in theoretical physics and chemistry, in quantum mechanics, in quantum chemistry, in nuclear physics, in chemical physics and in physical chemistry that can be transformed to close-coupling differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [21], the entrance channel by the quantum numbers (j, l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we find that

$$\begin{aligned}\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right] y_{j'l'}^{Jjl}(x) \\ = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J|V|j''l''; J\rangle y_{j''l''}^{Jjl}(x)\end{aligned} \tag{58}$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}\right] \tag{59}$$

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

Following the detailed analysis given in [21], the potential V can be expanded as $V(x, \hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2$ where $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i, $i = 0, 2$ are Legendre polynomials (see for details [22] and [24]).

The coupling matrix element may then be written

$$\langle j'l'; J|V|j''l''; J\rangle = \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x) \tag{60}$$

where the f_2 coefficients can be obtained from formulas given by Bernstein *et al.* [22]. The boundary conditions are given by

$$y_{j'l'}^{Jjl}(x) = 0 \quad \text{at}\, x = 0 \tag{61}$$

$$y_{j'l'}^{Jjl}(x) \sim \delta_{jj'}\delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[i(k_{j'j}x - 1/2l'\pi)] \tag{62}$$

where the scattering S matrix is related to the K matrix of (56) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \tag{63}$$

To calculate the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles a computer program has been obtained. In this program the numerical method for step-by-step integration from the initial value to matching points is included. We note here that the program developed for the applications of this paper is also based on an analogous program which has been written for the numerical applications of [21].

For numerical purposes we choose the **S** matrix which is calculated using the following parameters

$$\frac{2\mu}{\hbar^2} = 1000.0, \quad \frac{\mu}{I} = 2.351, \quad E = 1.1,$$
$$V_0(x) = \frac{1}{x^{12}} - 2\frac{1}{x^6}, \quad V_2(x) = 0.2283 V_0(x).$$

As is described in [21], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2$, 4 and 6 giving rise to sets of **four, nine and sixteen coupled differential equations**, respectively. Following the procedure obtained by Bernstein [23] and Allison [21] we assumed the potential infinite for values of x less than some x_0. The wavefunctions will then be zero in this region and effectively the boundary condition (61) may be written as

$$y_{j'l'}^{Jjl}(x_0) = 0 \tag{64}$$

For the numerical solution of this problem we have used (1) the well known Iterative Numerov method of Allison [21], (2) the variable-step method of Raptis and Cash [17], (3) the variable-step method developed by Simos [25], (4) the variable-step method developed by Simos [31] and (5) the new variable-step method. In Table II we present the real time of computation required by the methods mentioned above to calculate the square of the modulus of the **S** matrix for sets of 4, 9 and 16 coupled differential equations. In Table II N indicates the number of equations of the set of coupled differential equations.

TABLE II Real time of computation (in seconds) to calculate $|S|^2$ for the Variable-step Methods (1)–(3). acc = 10^{-6}. $h$max is the maximum stepsize

Method	*N*	*h max*	*Real time of computation (in seconds)*
Iterative Numerov [21]	4	0.014	3.25
	9	0.014	23.51
	16	0.014	99.15
Variable-step Method of Raptis and Cash[17]	4	0.056	1.65
	9	0.056	8.68
	16	0.056	45.21
Variable-step Method of Simos [25]	4	0.056	1.05
	9	0.056	5.25
	16	0.056	27.15
Variable-step Method of Simos [31]	4	0.448	0.37
	9	0.448	3.22
	16	0.448	14.22
New Variable-step Method	4	0.448	0.24
	9	0.448	2.70
	16	0.448	10.76

In all cases the variable step method developed in this paper is more accurate than other well known finite difference ones for a given value of hmax so that the new embedded method can use a larger value of $h$max and still gets converged results.

All computations were carried out on an PC-AT 80486 using double precision arithmetic of 16 digits accuracy.

5. CONCLUSIONS

In this paper a tenth algebraic order method with phase-lag of order 16(2)22, for the numerical solution of the phase shift problem of the radial Schrödinger equation and for the numerical solution of the coupled equations arising from the Schrödinger equation, is introduced. Based on the new methods, a new variable step method for the solution of (1) and for the numerical solution of the coupled Schrödinger equations is obtained. The numerical results given by this new variable-step method are better than those of the most well known variable-step method of Raptis and Cash [17], the variable-step methods of Raptis and Cash [17], the variable-step methods of Simos (see [25] and [31]).

APPENDIX A

$$\text{phase-lag} = H^{12}\Bigg(\frac{1}{4191264000}(820523s^4+36767115s^4t_4 -268035075s^2t_4+9856876-5965895s^2 +443450700t_4)/(9s^2-19)\Bigg)$$

$$+H^{14}\Bigg(\frac{1}{45768602880000}(148590285660s^4 -896011116s^8-11808680598s^6 +595165512942000s^2t_4t_3-203825569147200s^4t_4t_3 +313868656168 -345398978925t_4s^6-40149689580s^8t_4 +21680832373200t_4s^6t_3 -552042907416000t_4t_3+4951853426520s^4t_4 -13414079153475s^2t_4 -410088330450s^2+9460133783100t_4)/(9s^2-19)^2\Bigg)$$

$$+H^{16}\Bigg(\frac{1}{19222813209600000}(438981953860614s^4 +10516916005882s^8 +254041583796s^{10}-129570499668974s^6 +2643181440707808000t_4t_3t_2 +856821944069091000s^2t_4t_3 -541326057262590600s^4t_4t_3 -4522574269988775t_4s^6+403043997901545s^8t_4 -5660842162287312000t_4t_3t_2s^6 +491721278224176000t_4t_3t_2s^8 +37632466872s^{12}+224755333605704 +3666340928250s^{10}t_4 +1686286962360s^{12}t_4-5911281704928600t_4s^8t_3 +128845738824402600t_4s^6t_3-452951205534828000t_4t_3 +143112052483750035s^4t_4-4101685789985784000s^2t_4t_3t_2$$

$$
\begin{aligned}
&+ 23257522084292496000\, s^4\, t_4\, t_3\, t_2 \\
&- 16205000498361675\, s^2\, t_4 \\
&- 910594959674400\, t_4\, s^{10}\, t_3 - 554495862713990\, s^2 \\
&+ 5320655568528300\, t_4)/(9\, s^2 - 19)^3 \Big) \\
+ H^{18} \Bigg(&\frac{1}{137250886316544000000} (-711659624925322648 12\, s^4 \\
&- 7918628940732527144\, s^8 + 1153310392601116152\, s^{10} \\
&+ 3117289117334906557 6\, s^6 \\
&+ 3686841632571285988 80000\, t_4\, t_3\, t_2 \\
&+ 1524165416664824033 1000\, s^2\, t_4\, t_3 \\
&- 1789674861611567090 1600\, s^4\, t_4\, t_3 \\
&+ 1490640678173558211300\, t_4\, s^6 \\
&- 375210358534015174170\, s^8\, t_4 \\
&- 313588952211675172032000\, t_4\, t_3\, t_2\, s^6 \\
&+ 1357486930123519523328 0000\, t_4\, t_3\, t_2\, s^6\, t_1 \\
&- 2582835755714846311680000\, t_4\, t_3\, t_2\, t_1\, s^8 \\
&+ 544893099176803497120 00\, t_4\, t_3\, t_2\, s^8 \\
&- 74101957510376796\, s^{12} \\
&+ 5310192133381813177 5\, s^{10}\, t_4 \\
&- 3307179584990351070\, s^{12}\, t_4 \\
&- 2071785428068813657200\, t_4\, s^8\, t_3 \\
&- 1537965900775696392000\, t_4\, t_3\, s^{10}\, t_2 \\
&+ 18958805603211329856 0000\, t_4\, t_3\, t_2\, t_1\, s^{10} \\
&+ 5122289734461900\, s^{14}\, t_4 \\
&- 1204008891125040\, s^{16}\, t_4 - 8652667887864\, s^{14} \\
&- 26869581346608\, s^{16} - 3510889926520616640 00\, t_4\, t_3\, t_2\, s^{12} \\
&+ 41024272413524400\, s^{12}\, t_4\, t_3 \\
&+ 650164801207521600\, t_4\, s^{14}\, t_3 \\
&+ 9199022848363541793600\, t_4\, s^6\, t_3 \\
&- 21514439654785273996800000\, t_4\, t_3\, t_2\, t_1 \\
&- 433080080655929506800 0\, t_4\, t_3
\end{aligned}
$$

$$
\begin{aligned}
&- 338103810240985224340\, s^4\, t_4 \\
&- 87205865640048559404000\, s^2\, t_4\, t_3\, t_2 \\
&+ 77097402632473697073600\, s^4\, t_4\, t_3\, t_2 \\
&+ 43577132018961311971200000\, s^2\, t_4\, t_3\, t_2\, t_1 \\
&- 34745152407599908834560000\, s^4\, t_4\, t_3\, t_2\, t_1 \\
&+ 40167781486658473898 25\, s^2\, t_4 \\
&+ 1524133889689613202 00\, t_4\, s^{10}\, t_3 \\
&+ 856666003619323103 60\, s^2 \\
&- 1926594474939249815700\, t_4 \\
&- 416705811895851236 16)/(9\, s^2 - 19)^4\Bigg) \\
+ H^{20}\Bigg(&- \frac{1}{547631036403010560000000} \\
&(75645634356813206125440000\, s^{14}\, t_4\, t_3\, t_2\, t_1 \\
&+ 17167379378341477613328 0000\, t_4\, t_3\, t_2\, t_1\, s^{12} \\
&+ 2576143646880185284898978\, s^4 \\
&+ 5618332930859975612705 76\, s^8 \\
&- 1098572170828047579755 58\, s^{10} \\
&- 1598137795263778528921256\, s^6 \\
&- 19699080548715609546304 80000\, t_4\, t_3\, t_2 \\
&+ 22421757542725581090265 21500\, s^2\, t_4\, t_3 \\
&- 24033540111736888613749 86900\, s^4\, t_4\, t_3 \\
&- 165130403040429666 8400\, s^{16}\, t_4\, t_3 \\
&+ 614433165968658854317500\, t_4^2\, s^{14} \\
&- 480399547558890960\, s^{20}\, t_4 \\
&- 84096807088105979867 7000000\, t_4^2 \\
&+ 25941575568180111 8400\, t_4\, s^{18}\, t_3 \\
&- 10720962957296592\, s^{20} \\
&- 14008450806817260 3936000\, t_4\, t_3\, t_2\, s^{16} \\
&- 53428830364581832926 2655000\, t_4^2\, s^8 \\
&- 27050550286061910951968625\, t_4\, s^6 \\
&+ 9301635393656208971528160\, s^8\, t_4
\end{aligned}
$$

$$
\begin{aligned}
&+ 80403009896349230726956320000\, t_4\, t_3\, t_2\, s^6 \\
&- 308753134514930396465254080000\, t_4\, t_3\, t_2\, s^6\, t_1 \\
&+ 923508831526836164360150400000\, t_4\, t_3\, t_2\, t_1\, s^8 \\
&- 29243937827197892949630480000\, t_4\, t_3\, t_2\, s^8 \\
&+ 98880090379751603390 90\, s^{12} \\
&+ 149274980267470782838863750 0\, t_4^2\, s^6 \\
&- 24574296563293786665481125 00\, t_4^2\, s^4 \\
&+ 22116731910746059662075000 00\, t_4^2\, s^2 \\
&- 128499394175481097293525 00\, t_4^2\, s^{12} \\
&+ 112428174375396261046665000\, t_4^2\, s^{10} \\
&+ 7580830096179774505391 76 \\
&- 1559342785863702968978850\, s^{10}\, t_4 \\
&+ 48710005200288316549665\, s^{12}\, t_4 \\
&- 4918416242020569943296642 00\, t_4\, s^8\, t_3 \\
&+ 51571364243812833668648400 0\, t_4\, t_3\, s^{10}\, t_2 \\
&- 124398258844902414098126400 00\, t_4\, t_3\, t_2\, t_1\, s^{10} \\
&+ 2265232780530634031617 5\, s^{14}\, t_4 \\
&- 254416096304442171099 0\, s^{16}\, t_4 \\
&+ 638802921047759624 52\, s^{14} \\
&- 565803001638764449 56\, s^{16} \\
&- 328203284867023903417080 00\, t_4\, t_3\, t_2\, s^{12} \\
&- 1294564367661316575994170 0\, s^{12}\, t_4\, t_3 \\
&+ 714894838090638381376200\, t_4\, s^{14}\, t_3 \\
&+ 1406511288419251448248214400\, t_4\, s^6\, t_3 \\
&+ 16769967849913751448655680 0000\, t_4\, t_3\, t_2\, t_1 \\
&- 8763307628708671711693020 00\, t_4\, t_3 \\
&+ 4134160888286102922104356 5\, s^4\, t_4 \\
&+ 78659331560228843123099400 00\, s^2\, t_4\, t_3\, t_2 \\
&- 114244818822724039280190360 00\, s^4\, t_4\, t_3\, t_2 \\
&- 4761012902657058052197192000 00\, s^2\, t_4\, t_3\, t_2\, t_1 \\
&+ 5385790037221184846008353600 00\, s^4\, t_4\, t_3\, t_2\, t_1
\end{aligned}
$$

$$
\begin{aligned}
&- 307035136629618963477912 00\, s^2\, t_4 \\
&+ 1049967637876394248458447 00\, t_4\, s^{10}\, t_3 \\
&+ 286894871743035307752000\, s^{14}\, t_4\, t_3\, t_2 \\
&+ 65468061666791784\, s^{18} \\
&- 218952019735924551272651 0\, s^2 \\
&+ 5132076409786025700\, s^{18}\, t_4 \\
&+ 8101760600962567203865200\, t_4)/(9\, s^2 - 19)^5\Big) \\
+ H^{22}\Bigg(&\frac{1}{253005538818190878720000000} \\
&\quad (833911734191213417833613520 0000\, s^{14}\, t_4\, t_3\, t_2\, t_1 \\
&- 1459460501228406723817147977600 00\, t_4\, t_3\, t_2\, t_1\, s^{12} \\
&- 59929077046304588782331632132\, s^4 \\
&- 28011817737425079191324465552\, s^8 \\
&+ 88186538303003564029493807 67\, s^{10} \\
&+ 53431019044464065665804592993\, s^6 \\
&- 4615458861888283217114479773600 00\, t_4\, t_3\, t_2 \\
&- 647190427274957430184320 00\, t_4\, t_3\, t_2\, s^{20} \\
&- 18192153810736912834474959312000\, s^2\, t_4\, t_3 \\
&+ 29433711155060980770986173390200\, s^4\, t_4\, t_3 \\
&- 6991261436884061808823552200\, s^{16}\, t_4\, t_3 \\
&- 8120297469546862522824651 7500\, t_4^2\, s^{14} \\
&- 17503380594481294363851 00\, s^{20}\, t_4 \\
&+ 13334810215925524697721850500000\, t_4^2 \\
&+ 6374202390638284324734612 00\, t_4\, s^{18}\, t_3 \\
&- 388250845220515243926 96\, s^{20} \\
&- 1792216730135857983550472880 00\, t_4\, t_3\, t_2\, s^{16} \\
&+ 265705949167092981223399860637 50\, t_4^2\, s^8 \\
&+ 393448816919610226746240243975\, t_4\, s^6 \\
&- 3013016220210350542713281757 00\, s^8\, t_4 \\
&+ 1340370124092263249899201292004000\, t_4\, t_3\, t_2\, s^6 \\
&+ 7084845465210240615889524563040000\, t_4\, t_3\, t_2\, s^6\, t_1
\end{aligned}
$$

$$
\begin{aligned}
&- 354611400837697923404724439200000\,t_4\,t_3\,t_2\,t_1\,s^8 \\
&\quad - 6099395828695742290825120693680000\,t_4\,t_3\,t_2\,s^8 \\
&\quad - 16063287047105648755780715008\,s^{12} \\
&\quad - 551590575930011053624509696375000\,t_4^2\,s^6 \\
&\quad + 683685653769012292840270391062500\,t_4^2\,s^4 \\
&\quad - 4654482576548199098601622725000\,t_4^2\,s^2 \\
&\quad + 124421132524508514579705195375\,t_4^2\,s^{12} \\
&\quad - 769404757671105479180890132500\,t_4^2\,s^{10} \\
&\quad + 1193809644392230514867599631255\,s^{10}\,t_4 \\
&\quad - 2656831214121849532370322720\,s^{12}\,t_4 \\
&\quad + 116475566144975776854215838738000\,t_4\,s^8\,t_3 \\
&\quad + 178004343957603111223174111212000\,t_4\,t_3\,s^{10}\,t_2 \\
&\quad + 10011938221122464656734186081600000\,t_4\,t_3\,t_2\,t_1\,s^{10} \\
&\quad + 328963849239532065224258092 5\,s^{14}\,t_4 \\
&\quad - 231346791301104881467065000\,s^{16}\,t_4 \\
&\quad + 146388789273990458204105283\,s^{14} \\
&\quad - 35516687618698437032786 52\,s^{16} \\
&\quad - 33012804241338905852987430312000\,t_4\,t_3\,t_2\,s^{12} \\
&\quad + 4146794237561644672612210602 00\,s^{12}\,t_4\,t_3 \\
&\quad - 221644088869185895087375200\,t_4\,s^{14}\,t_3 \\
&\quad - 245608884087592568302487840112000\,t_4\,s^6\,t_3 \\
&\quad - 1037511174339753723584781206400000\,t_4\,t_3\,t_2\,t_1 \\
&\quad + 426703527331496489493172353600 0\,t_4\,t_3 \\
&\quad - 16676691647930058052215309402 0\,s^4\,t_4 \\
&\quad + 1399536124981294846725405806580000\,s^2\,t_4\,t_3\,t_2 \\
&\quad - 1825176497780876246548914684312000\,s^4\,t_4\,t_3\,t_2 \\
&\quad + 4634282336143489736568611349600000\,s^2\,t_4\,t_3\,t_2\,t_1 \\
&\quad - 7979439121519818879044149711680000\,s^4\,t_4\,t_3\,t_2\,t_1 \\
&\quad - 1337205711407575822465380477 75\,s^2\,t_4 \\
&\quad - 883213998562662394244061766 8 \\
&\quad - 314184665646804609391862607480 0\,t_4\,s^{10}\,t_3
\end{aligned}
$$

$$
\begin{aligned}
&+36061999977670300164934723320000s^{14}t_4t_3t_2\\
&-8858421271432731495344047200000000t_4^2t_3\\
&+695327276649403633435 2s^{18}\\
&+3604865654979097558608227 1005s^2\\
&+548596419707754945871344000t_4t_3t_2s^{18}\\
&-145354241311797595618981440000t_4t_3t_2t_1s^{16}\\
&+349482830728477012299532800000t_4t_3t_2t_1s^{18}\\
&+11985007912499211670 0800s^{22}t_4t_3\\
&+3797805957571050024600s^{22}t_4\\
&-495308488627102 5504s^{24}\\
&-34890962555891189933322637 50t_4^2s^{16}\\
&+567736245355040781389370000t_4^2s^{18}\\
&-2219445909722076235 20s^{24}t_4\\
&+18377129131239707706027150s^{18}t_4\\
&+620875044732286824 48s^{22}\\
&+11809224403322728965560367 3900t_4\\
&-1307620369070931413364904837800000t_4^2t_3s^8\\
&-15333672564217343824488 00t_4s^{20}t_3\\
&+2798562033467537017572301410000000t_4^2t_3s^6\\
&-3692094558209699705094013983000000t_4^2t_3s^4\\
&+2749297501197160537712208120000000t_4^2t_3s^2\\
&-6963277407121619527635471780000 0t_4^2t_3s^{12}\\
&+3850158337471849191050093832000 00t_4^2t_3s^{10}\\
&-3065775724917220219502598000 00t_4^2t_3s^{16}\\
&+7058825091484551321341605200000t_4^2t_3s^{14})/(9s^2-19)^6\Big)
\end{aligned}
\tag{65}
$$

APPENDIX B

$$
\begin{aligned}
P_1(H)=\frac{1}{900}(&-5492400\,h^2-111391200\,h^{16}\,s^2\,t_4\,t_3\,t_2\,t_1\\
&+15279840\,h^{16}\,s^4\,t_4\,t_3\,t_2\,t_1
\end{aligned}
$$

$$
\begin{aligned}
&+ 417717000\,h^{14}\,s^2\,t_4\,t_3\,t_2\,t_1 + 184291200\,h^{16}\,t_4\,t_3\,t_2\,t_1\\
&- 796320\,h^6 - 6912000\,s^2\\
&+ 30715200\,h^{14}\,t_4\,t_3\,t_2 - 515700\,h^{10}\,s^2\,t_4\\
&+ 70740\,h^{10}\,s^4\,t_4 + 5119200\,h^{12}\,t_4\,t_3\\
&+ 151680\,h^8 - 19197000\,h^{10}\,t_4\,t_3\\
&- 115182000\,h^{12}\,t_4\,t_3\,t_2 + 1933875\,h^8\,s^2\,t_4\\
&+ 11603250\,h^{10}\,s^2\,t_4\,t_3 + 481320\,h^6\,s^2\\
&+ 853200\,h^{10}\,t_4 - 3199500\,h^8\,t_4\\
&- 3094200\,h^{12}\,s^2\,t_4\,t_3 - 91680\,h^8\,s^2\\
&- 1591650\,h^{10}\,s^4\,t_4\,t_3 + 12576\,h^8\,s^4\\
&- 57299400\,h^{14}\,s^4\,t_4\,t_3\,t_2\,t_1 - 18565200\,h^{14}\,s^2\,t_4\,t_3\,t_2\\
&+ 2546640\,h^{14}\,s^4\,t_4\,t_3\,t_2\\
&+ 424440\,h^{12}\,s^4\,t_4\,t_3 - 691092000\,h^{14}\,t_4\,t_3\,t_2\,t_1\\
&+ 69619500\,h^{12}s^2\,t_4\,t_3\,t_2\\
&+ 284400\,h^4 - 9549900\,h^{12}\,s^4\,t_4\,t_3\,t_2\\
&- 265275\,h^8\,s^4\,t_4 + 26726400 - 76800\,s^4\,h^2\\
&+ 10280\,s^4\,h^4 - 66024\,h^6\,s^4 + 1635600\,s^2\,h^2\\
&- 102200\,s^2\,h^4)/(465\,s^2 - 139)
\end{aligned}
$$

$$
\begin{aligned}
P_2(H) = -\frac{1}{1200}(&-16809600\,h^2 - 287760600\,h^{16}\,s^2\,t_4\,t_3\,t_2\,t_1\\
&+ 39472920\,h^{16}\,s^4\,t_4\,t_3\,t_2\,t_1 + 556956000\,h^{14}\,s^2\,t_4\,t_3\,t_2\,t_1\\
&+ 476085600\,h^{16}\,t_4\,t_3\,t_2\,t_1 - 758400\,h^6\\
&- 18144000\,s^2 + 79347600\,h^{14}\,t_4\,t_3\,t_2\\
&- 1332225\,h^{10}\,s^2\,t_4 + 182745\,h^{10}\,s^4\,t_4\\
&+ 13224600\,h^{12}\,t_4\,t_3 + 391840\,h^8\\
&- 25596000\,h^{10}\,t_4\,t_3 - 153576000\,h^{12}\,t_4\,t_3\,t_2\\
&+ 2578500\,h^8\,s^2\,t_4\\
&+ 15471000\,h^{10}\,s^2\,t_4\,t_3 + 458400\,h^6\,s^2\\
&+ 2204100\,h^{10}\,t_4 - 4266000\,h^8\,t_4\\
&- 7993350\,h^{12}\,s^2\,t_4\,t_3 - 236840\,h^8\,s^2\\
&- 2122200\,h^{10}\,s^4\,t_4\,t_3 + 32488\,h^8\,s^4\\
&- 76399200\,h^{14}\,s^4\,t_4\,t_3\,t_2\,t_1 - 47960100\,h^{14}\,s^2\,t_4\,t_3\,t_2
\end{aligned}
$$

$$
\begin{aligned}
&+6578820\,h^{14}\,s^4\,t_4\,t_3\,t_2\\
&+1096470\,h^{12}\,s^4\,t_4\,t_3-921456000\,h^{14}\,t_4\,t_3\,t_2\,t_1\\
&+92826000\,h^{12}\,s^2\,t_4\,t_3\,t_2\\
&+758400\,h^4-12733200\,h^{12}\,s^4\,t_4\,t_3\,t_2-353700\,h^8\,s^4\,t_4\\
&-201600\,s^4\,h^2+59200\,s^4\,h^4\\
&-62880\,h^6\,s^4+6624000\,s^2\,h^2-452800\,s^2\,h^4\\
&+38304000)/(465\,s^2-139)
\end{aligned}
$$

$$
\begin{aligned}
P_3(H)=\frac{1}{80}\,h^2(&-638400-9282600\,h^{14}\,s^2\,t_4\,t_3\,t_2\,t_1\\
&+1273320\,h^{14}\,s^4\,t_4\,t_3\,t_2\,t_1\\
&+15357600\,h^{14}\,t_4\,t_3\,t_2\,t_1+2559600\,h^{12}\,t_4\,t_3\,t_2\\
&-42975\,h^8\,s^2\,t_4+5895\,h^8\,s^4\,t_4\\
&+426600\,h^{10}\,t_4\,t_3+12640\,h^6+71100\,h^8\,t_4\\
&-257850\,h^{10}\,s^2\,t_4\,t_3-7640\,h^6\,s^2\\
&+1048\,h^6\,s^4-1547100\,h^{12}\,s^2\,t_4\,t_3\,t_2\\
&+212220\,h^{12}\,s^4\,t_4\,t_3\,t_2+35370\,h^{10}\,s^4\,t_4\,t_3\\
&+25280\,h^2+3360\,s^4\,h^2+302400\,s^2\\
&-21600\,s^2\,h^2)/(465\,s^2-139)
\end{aligned}
$$

$$
\begin{aligned}
S(H)=\frac{1}{1440000}(&77220864000000\,h^2-656651124000\,h^{28}\,s^6\,t_4^2\,t_3^2\,t_2^2\\
&-322214355000\,h^{18}\,s^4\,t_4^2\\
&+25751623680000\,h^{16}\,t_4\,t_3\,t_2\\
&+266887872000\,h^{20}\,s^8\,t_4\,t_3\,t_2+74135520\,h^{20}\,s^8\,t_4\,t_3\\
&+329204736000000\,s^4\\
&-3860905305600000\,h^{16}\,s^2\,t_4\,t_3\,t_2\,t_1\\
&-2841799680000\,h^{12}\,s^2\,t_4\\
&+572825520000\,h^{16}\,s^4\,t_4+253532160000\,h^{16}\,s^8\,t_4\,t_3\\
&+444813120\,h^{22}\,s^8\,t_4\,t_3\,t_2\\
&-48216384000\,h^{14}\,s^8\,t_4\,t_3+855671040000\,h^{12}\,s^8\,t_4\,t_3\\
&-16013440\,h^{16}\,s^6+324268764480000\,h^{24}\,s^8\,t_4^2\,t_3^2\,t_2\,t_1\\
&+1501244280000\,h^{18}\,s^8\,t_4^2\,t_3\\
&+54044794080000\,h^{22}\,s^8\,t_4^2\,t_3^2\,t_2-150124428000\,h^{22}\,s^8\,t_4^2\,t_3^2
\end{aligned}
$$

$$+ 4503732840000\, h^{20} s^8 t_4^2 t_3^2 - 7762527360000\, h^{14} s^2 t_4$$
$$- 2679687360000\, s^6 h^{10} t_4$$
$$- 1801493136000\, h^{24} s^8 t_4^2 t_3^2 t_2 - 6111045000\, h^{20} s^2 t_4^2$$
$$+ 2685119625\, h^{20} s^4 t_4^2$$
$$+ 44481312000\, h^{18} s^8 t_4 t_3 - 180151200\, h^{18} s^6 t_4$$
$$+ 2897550351360000\, h^{16} s^4 t_4 t_3 t_2 t_1$$
$$+ 4291937280000\, h^{14} t_4 t_3$$
$$+ 8512330176000\, h^{14} s^4 t_4 t_3$$
$$- 17050798080000\, h^{14} s^2 t_4 t_3$$
$$+ 76105080576000000\, h^{14} s^2 t_4 t_3 t_2 t_1$$
$$- 681140275200000\, h^{16} t_4 t_3 t_2 t_1$$
$$+ 181987560000\, h^{24} t_4^2 t_3^2 + 6470668800000\, h^{18} t_4 t_3$$
$$- 57963601920000\, h^6 - 1303689600000\, h^{16} s^2 t_4$$
$$+ 34751025\, h^{20} s^8 t_4^2$$
$$+ 849081159936000000\, h^{28} t_4^2 t_3^2 t_2^2 t_1^2 - 108090720000\, h^{16} s^6 t_4$$
$$+ 5836837760640000\, h^{28} s^8 t_4^2 t_3^2 t_2^2 t_1^2 + 954709200\, h^{18} s^4 t_4$$
$$+ 1521192960000\, h^{18} s^8 t_4 t_3 t_2 - 289298304000\, h^{16} s^8 t_4 t_3 t_2$$
$$- 5404479408000\, h^{26} s^8 t_4^2 t_3^2 t_2^2 - 141186240000\, h^{12} s^6 t_4$$
$$+ 733325400000\, h^{18} s^2 t_4^2 + 15012442800\, h^{26} s^8 t_4^2 t_3^2 t_2$$
$$+ 45037328400\, h^{28} s^8 t_4^2 t_3^2 t_2^2 + 38824012800000\, h^{16} t_4 t_3$$
$$+ 6081030000\, h^{18} s^6 t_4^2 - 2172816000\, h^{18} s^2 t_4$$
$$- 506675250\, h^{20} s^6 t_4^2$$
$$- 684703744000\, h^{12} s^2 + 1078444800000\, h^{16} t_4$$
$$+ 1251036900\, h^{24} s^8 t_4^2 t_3^2$$
$$- 1389975552000000\, s^2 - 5082704640000\, h^{16} s^6 t_4 t_3 t_2$$
$$+ 6470668800000\, h^{14} t_4$$
$$+ 78798134880000\, h^{26} s^6 t_4^2 t_3^2 t_2^2 - 218883708000\, h^{26} s^6 t_4^2 t_3^2 t_2$$
$$- 1080907200\, h^{20} s^6 t_4 t_3 - 113523379200000\, h^{14} t_4 t_3 t_2$$
$$- 17874561600000\, h^{10} s^2 t_4 + 13414584960000\, h^{10} s^4 t_4$$
$$- 18920563200000\, h^{12} t_4 t_3$$
$$- 12180510720000\, h^8 - 1960858368000000\, h^{10} t_4 t_3$$

$$
\begin{aligned}
&- 11765150208000000\,h^{12}\,t_4\,t_3\,t_2\\
&+ 352338336000000\,h^{8}\,s^{2}\,t_4\\
&+ 2114030016000000\,h^{10}\,s^{2}\,t_4\,t_3 + 63009515520000\,h^{6}\,s^{2}\\
&- 3153427200000\,h^{10}\,t_4\\
&- 326809728000000\,h^{8}\,t_4 - 107247369600000\,h^{12}\,s^{2}\,t_4\,t_3\\
&+ 9361210880000\,h^{8}\,s^{2}\\
&- 723989145600000\,h^{10}\,s^{4}\,t_4\,t_3 - 1884507136000\,h^{8}\,s^{4}\\
&+ 589159680000\,h^{10}\,s^{4}\\
&- 18240309000\,h^{24}\,s^{6}\,t_4^{2}\,t_3^{2} - 26063609241600000\,h^{14}\,s^{4}\,t_4\,t_3\,t_2\,t_1\\
&- 643484217600000\,h^{14}\,s^{2}\,t_4\,t_3\,t_2 + 482925058560000\,h^{14}\,s^{4}\,t_4\,t_3\,t_2\\
&- 6485443200\,h^{22}\,s^{6}\,t_4\,t_3\,t_2 + 80487509760000\,h^{12}\,s^{4}\,t_4\,t_3\\
&- 70590901248000000\,h^{14}\,t_4\,t_3\,t_2\,t_1\\
&+ 12684180096000000\,h^{12}\,s^{2}\,t_4\,t_3\,t_2\\
&- 1176483840000\,h^{10}\,s^{2} + 6102835200000\,h^{4}\\
&- 4343934873600000\,h^{12}\,s^{4}\,t_4\,t_3\,t_2\\
&+ 715322880000\,h^{12}\,t_4 - 120664857600000\,h^{8}\,s^{4}\,t_4\\
&- 1824030900000\,h^{16}\,s^{6}\,t_4^{2}\\
&+ 125103690000\,h^{16}\,s^{8}\,t_4^{2} + 7413552000\,h^{16}\,s^{8}\,t_4\\
&+ 42255360000\,h^{14}\,s^{8}\,t_4\\
&- 8036064000\,h^{12}\,s^{8}\,t_4 - 4170123000\,h^{18}\,s^{8}\,t_4^{2}\\
&+ 12355920\,h^{18}\,s^{8}\,t_4\\
&- 627374592000\,h^{14}\,s^{6}\,t_4 + 142611840000\,h^{10}\,s^{8}\,t_4\\
&- 21999762000000\,h^{16}\,s^{2}\,t_4^{2}\\
&+ 3374075520000\,h^{14}\,s^{4}\,t_4 + 9666430650000\,h^{16}\,s^{4}\,t_4^{2}\\
&+ 218385072000000\,h^{18}\,t_4^{2}\,t_3\\
&+ 655155216000000\,h^{20}\,t_4^{2}\,t_3^{2}\\
&- 2363944046400000\,h^{24}\,s^{6}\,t_4^{2}\,t_3^{2}\,t_2^{2}\\
&- 7279502400000\,h^{20}\,t_4^{2}\,t_3^{2} - 21838507200000\,h^{22}\,t_4^{2}\,t_3^{2}\\
&+ 10784448000\,h^{20}\,t_4\,t_3\\
&+ 162134382240000\,h^{24}\,s^{8}\,t_4^{2}\,t_3^{2}\,t_2^{2}\\
&+ 54044794080000\,h^{22}\,s^{8}\,t_4^{2}\,t_3\,t_2\,t_1
\end{aligned}
$$

$$+ 1945612586880000\, h^{26} s^8 t_4^2 t_3^2 t_2^2 t_1$$
$$+ 30804157440000\, h^{16} s^8 t_4 t_3 t_2 t_1$$
$$+ 5134026240000\, h^{14} s^8 t_4 t_3 t_2$$
$$+ 9007465680000\, h^{20} s^8 t_4^2 t_3 t_2 + 1098304\, h^{16} s^8$$
$$+ 587304960000\, h^{10} - 95038971840000\, h^{30} s^2 t_4^2 t_3^2 t_2^2 t_1$$
$$+ 1159971678000\, h^{26} s^4 t_4^2 t_3 t_2 t_1$$
$$- 218883708000\, h^{26} s^6 t_4^2 t_3 t_2 t_1$$
$$- 15839828640000\, h^{28} s^2 t_4^2 t_3^2 t_2 t_1$$
$$- 469328256000\, h^{24} s^2 t_4 t_3 t_2 t_1$$
$$+ 1900779436800000\, h^{26} s^2 t_4^2 t_3^2 t_2 t_1$$
$$+ 3558169600\, h^{12} s^8$$
$$+ 11404676620800000\, h^{28} s^2 t_4^2 t_3^2 t_2^2 t_1$$
$$+ 1621343822400\, h^{32} s^8 t_4^2 t_3^2 t_2^2 t_1^2$$
$$+ 2836732855680000\, h^{30} s^6 t_4^2 t_3^2 t_2^2 t_1^2$$
$$- 578812469760000\, h^{16} s^6 t_4 t_3 t_2 t_1$$
$$+ 41758980408000\, h^{30} s^4 t_4^2 t_3^2 t_2^2 t_1$$
$$+ 125276941224000\, h^{32} s^4 t_4^2 t_3^2 t_2^2 t_1^2$$
$$- 23639440464000\, h^{32} s^6 t_4^2 t_3^2 t_2^2 t_1^2$$
$$- 15033232946880000\, h^{30} s^4 t_4^2 t_3^2 t_2^2 t_1^2$$
$$- 285116915520000\, h^{32} s^2 t_4^2 t_3^2 t_2^2 t_1^2$$
$$- 281596953600000\, h^{22} s^2 t_4 t_3 t_2 t_1$$
$$+ 575170560000\, h^{12} + 306443886336000\, h^{18} s^4 t_4 t_3 t_2 t_1$$
$$+ 154509742080000\, h^{18} t_4 t_3 t_2 t_1$$
$$- 613828730880000\, h^{18} s^2 t_4 t_3 t_2 t_1$$
$$- 88600780800000\, s^4 h^2 + 9002649600000\, s^4 h^4$$
$$+ 3642009600\, h^{10} s^8 - 22290831360000\, h^6 s^4$$
$$- 3225600000\, s^8 h^6 + 26094592000\, s^8 h^8$$
$$+ 40642560000\, s^8 h^4$$
$$+ 117863424000000\, s^2 h^2 + 294328704000\, h^{12} s^4$$
$$+ 20244453120000\, h^{16} s^4 t_4 t_3$$
$$- 8334950400000\, s^2 h^4 + 347991503400000\, h^{20} s^4 t_4^2 t_3^2$$

$$
\begin{aligned}
&+ 1310310432000000\, h^{20}\, t_4^2\, t_3\, t_2 \\
&- 279450984960000\, h^{18}\, t_4\, t_3\, t_2\, s^2 \\
&+ 115997167800000\, h^{18}\, s^4\, t_4^2\, t_3 \\
&+ 7861862592000000\, h^{22}\, t_4^2\, t_3^2\, t_2 \\
&- 263997144000000\, h^{18}\, t_4^2\, t_3\, s^2 \\
&- 791991432000000\, h^{20}\, t_4^2\, t_3^2\, s^2 \\
&+ 23585587776000000\, h^{24}\, t_4^2\, t_3^2\, t_2^2 \\
&- 1583982864000000\, h^{20}\, t_4^2\, t_3\, t_2\, s^2 \\
&- 9503897184000000\, h^{22}\, t_4^2\, t_3^2\, t_2\, s^2 \\
&- 254943744000\, h^{14}\, s^2 + 1797408000\, h^{18}\, t_4 \\
&+ 159769600\, h^{16} + 26399714400000\, h^{22}\, t_4^2\, t_3^2\, s^2 \\
&- 7822137600000\, h^{18}\, t_4\, t_3\, s^2 \\
&+ 60662520000\, h^{22}\, t_4^2\, t_3 + 32221435500\, h^{22}\, s^4\, t_4^2\, t_3 \\
&- 23199433560000\, h^{22}\, s^4\, t_4^2\, t_3\, t_2 \\
&+ 729612360000\, h^{20}\, s^6\, t_4^2\, t_3 \\
&- 43677014400000\, h^{22}\, t_4^2\, t_3\, t_2 \\
&- 73332540000\, h^{22}\, s^2\, t_4^2\, t_3 \\
&+ 8799904800000\, h^{20}\, s^2\, t_4^2\, t_3 - 3866572260000\, h^{20}\, s^4\, t_4^2\, t_3 \\
&+ 6551552160000\, h^{28}\, t_4^2\, t_3^2\, t_2^2 + 2183850720000\, h^{26}\, t_4^2\, t_3^2\, t_2 \\
&- 46575164160000\, h^{16}\, s^2\, t_4\, t_3 + 232944076800000\, h^{18}\, t_4\, t_3\, t_2 \\
&- 439995240000\, h^{24}\, t_4^2\, t_3\, t_2\, s^2 + 193328613000\, h^{24}\, t_4^2\, t_3\, t_2\, s^4 \\
&+ 64706688000\, h^{22}\, t_4\, t_3\, t_2 - 262062086400000\, h^{24}\, t_4^2\, t_3^2\, t_2 \\
&- 786186259200000\, h^{26}\, t_4^2\, t_3^2\, t_2^2 + 52799428800000\, h^{22}\, t_4^2\, t_3\, t_2\, s^2 \\
&+ 316796572800000\, h^{24}\, t_4^2\, t_3^2\, t_2\, s^2 - 46932825600000\, h^{20}\, t_4\, t_3\, t_2\, s^2 \\
&+ 363975120000\, h^{24}\, t_4^2\, t_3\, t_2 + 13103104320000\, h^{28}\, t_4^2\, t_3^2\, t_2\, t_1 \\
&+ 388240128000\, h^{24}\, t_4\, t_3\, t_2\, t_1 - 1572372518400000\, h^{26}\, t_4^2\, t_3^2\, t_2\, t_1 \\
&- 9434235110400000\, h^{28}\, t_4^2\, t_3^2\, t_2^2\, t_1 + 2183850720000\, h^{26}\, t_4^2\, t_3\, t_2\, t_1 \\
&- 262062086400000\, h^{24}\, t_4^2\, t_3\, t_2\, t_1 + 38824012800000\, h^{20}\, t_4\, t_3\, t_2 \\
&+ 210895872000\, h^{14} + 728800312320000\, h^{20}\, s^4\, t_4\, t_3\, t_2\, t_1 \\
&- 9503897184000000\, h^{22}\, s^2\, t_4^2\, t_3\, t_2\, t_1 \\
&+ 25055388244800000\, h^{24}\, s^4\, t_4^2\, t_3^2\, t_2\, t_1
\end{aligned}
$$

$$
\begin{aligned}
&+ 78618625920000\, h^{30} t_4^2\, t_3^2\, t_2^2\, t_1 + 1467196416000000 \\
&- 57023383104000000\, h^{24}\, s^2\, t_4^2\, t_3^2\, t_2\, t_1 \\
&- 342140298624000000\, h^{26}\, s^2\, t_4^2\, t_3^2\, t_2^2\, t_1 \\
&+ 4175898040800000\, h^{22}\, s^4\, t_4^2\, t_3\, t_2\, t_1 \\
&+ 1449761280\, h^{14} s^8 + 51073981056000\, h^{16}\, s^4\, t_4\, t_3\, t_2 \\
&- 102304788480000\, h^{16}\, s^2\, t_4\, t_3\, t_2 \\
&+ 1418721696000\, h^{12}\, s^4\, t_4 \\
&+ 26266044960000\, h^{24}\, s^6\, t_4^2\, t_3\, t_2\, t_1 \\
&+ 157596269760000\, h^{26}\, s^6\, t_4^2\, t_3^2\, t_2\, t_1 \\
&+ 232944076800000\, h^{22}\, t_4\, t_3\, t_2\, t_1 \\
&+ 6959830068000\, h^{28}\, s^4\, t_4^2\, t_3^2\, t_2\, t_1 \\
&+ 206217187200\, h^{24}\, s^4\, t_4\, t_3\, t_2\, t_1 \\
&+ 15012442800\, h^{26}\, s^8\, t_4^2\, t_3\, t_2\, t_1 \\
&- 5011077648960000\, h^{28}\, s^4\, t_4^2\, t_3^2\, t_2^2\, t_1 \\
&- 23347595520000\, h^{22}\, s^6\, t_4\, t_3\, t_2\, t_1 \\
&+ 450996988406400000\, h^{28}\, s^4\, t_4^2\, t_3^2\, t_2^2\, t_1^2 \\
&+ 34214029862400000\, h^{30}\, s^2\, t_4^2\, t_3^2\, t_2^2\, t_1^2 \\
&- 1676705909760000\, h^{20}\, s^2\, t_4\, t_3\, t_2\, t_1 \\
&+ 235855877760000\, h^{32}\, t_4^2\, t_3^2\, t_2^2\, t_1^2 \\
&- 139196601360000\, h^{24}\, s^4\, t_4^2\, t_3\, t_2\, t_1 \\
&- 835179608160000\, h^{26}\, s^4\, t_4^2\, t_3^2\, t_2\, t_1 \\
&+ 123730312320000\, h^{22}\, s^4\, t_4\, t_3\, t_2\, t_1 \\
&- 2639971440000\, h^{26}\, s^2\, t_4^2\, t_3\, t_2\, t_1 \\
&+ 316796572800000\, h^{24}\, s^2\, t_4^2\, t_3\, t_2\, t_1 \\
&- 7879813488000\, h^{30}\, s^6\, t_4^2\, t_3^2\, t_2^2\, t_1 \\
&- 38912659200\, h^{24}\, s^6\, t_4\, t_3\, t_2\, t_1 \\
&- 1313302248000\, h^{28}\, s^6\, t_4^2\, t_3^2\, t_2\, t_1 \\
&- 30496227840000\, h^{18}\, s^6\, t_4\, t_3\, t_2\, t_1 \\
&- 135512911872000\, h^{20}\, s^6\, t_4\, t_3\, t_2\, t_1 \\
&+ 18198756000000\, h^{16}\, t_4^2 \\
&+ 5055210000\, h^{20}\, t_4^2 - 606625200000\, h^{18}\, t_4^2
\end{aligned}
$$

$$
\begin{aligned}
&- 36480618000\, h^{24} s^6 t_4^2 t_3 t_2 \\
&- 6080103000\, h^{22} s^6 t_4^2 t_3 \\
&+ 4377674160000\, h^{22} s^6 t_4^2 t_3 t_2 \\
&- 78221376000\, h^{22} t_4 t_3 t_2 s^2 \\
&- 139196601360000\, h^{24} t_4^2 t_3^2 t_2 s^4 \\
&+ 34369531200\, h^{22} t_4 t_3 t_2 s^4 \\
&- 7919914320000\, h^{28} t_4^2 t_3^2 t_2^2 s^2 \\
&+ 3479915034000\, h^{28} t_4^2 t_3^2 t_2^2 s^4 \\
&- 2639971440000\, h^{26} t_4^2 t_3^2 t_2 s^2 \\
&+ 1159971678000\, h^{26} t_4^2 t_3^2 t_2 s^4 \\
&+ 950389718400000\, h^{26} t_4^2 t_3^2 t_2^2 s^2 \\
&- 417589804080000\, h^{26} t_4^2 t_3^2 t_2^2 s^4 \\
&+ 77010393600000\, s^6 h^{10} t_4 t_3 \\
&+ 2772374169600000\, s^6 h^{14} t_4 t_3 t_2 t_1 \\
&- 96468744960000\, s^6 h^{14} t_4 t_3 t_2 \\
&- 16078124160000\, s^6 h^{12} t_4 t_3 \\
&+ 462062361600000\, s^6 h^{12} t_4 t_3 t_2 \\
&+ 12835065600000\, s^6 h^8 t_4 - 28407296000\, s^6 h^8 \\
&+ 7315660800000\, s^6 h^2 \\
&- 1103155200000\, s^6 h^4 + 2427586560000\, s^6 h^6 \\
&+ 20621718720000\, h^{20} s^4 t_4 t_3 t_2 \\
&+ 3436953120000\, h^{18} s^4 t_4 t_3 \\
&+ 121466718720000\, h^{18} s^4 t_4 t_3 t_2 \\
&+ 112019212800\, h^{14} s^4 \\
&+ 1397664460800000\, h^{20} t_4 t_3 t_2 t_1 \\
&- 28302705331200000\, h^{30} t_4^2 t_3^2 t_2^2 t_1^2 \\
&- 787981348800000\, h^{22} s^6 t_4^2 t_3 t_2 t_1 \\
&- 1026420895872000000\, h^{28} s^2 t_4^2 t_3^2 t_2^2 t_1^2 \\
&+ 150332329468800000\, h^{26} s^4 t_4^2 t_3^2 t_2^2 t_1 \\
&- 28367328556800000\, h^{26} s^6 t_4^2 t_3^2 t_2^2 t_1 \\
&- 4727888092800000\, h^{24} s^6 t_4^2 t_3^2 t_2 t_1
\end{aligned}
$$

$$
\begin{aligned}
&- 85101985670400000\, h^{28} s^6 t_4^2 t_3^2 t_2^2 t_1^2 \\
&+ 90074656800\, h^{28} s^8 t_4^2 t_3^2 t_2 t_1 \\
&- 10808958816000\, h^{26} s^8 t_4^2 t_3^2 t_2 t_1 \\
&+ 2668878720\, h^{24} s^8 t_4 t_3 t_2 t_1 \\
&- 194561258688000\, h^{30} s^8 t_4^2 t_3^2 t_2^2 t_1^2 \\
&+ 540447940800\, h^{30} s^8 t_4^2 t_3^2 t_2^2 t_1 \\
&- 64853752896000\, h^{28} s^8 t_4^2 t_3^2 t_2^2 t_1 \\
&- 1801493136000\, h^{24} s^8 t_4^2 t_3 t_2 t_1 \\
&- 1735789824000\, h^{18} s^8 t_4 t_3 t_2 t_1 \\
&+ 9127157760000\, h^{20} s^8 t_4 t_3 t_2 t_1 \\
&+ 1601327232000\, h^{22} s^8 t_4 t_3 t_2 t_1 \\
&+ 945577618560000\, h^{28} s^6 t_4^2 t_3^2 t_2^2 t_1 \\
&- 300248856000\, h^{22} s^8 t_4^2 t_3 t_2 \\
&- 219997620000\, h^{24} t_4^2 t_3^2 s^2 \\
&- 13036896000\, h^{20} t_4 t_3 s^2 \\
&- 11599716780000\, h^{22} t_4^2 t_3^2 s^4 \\
&+ 5728255200\, h^{20} t_4 t_3 s^4 \\
&- 50041476000\, h^{20} s^8 t_4^2 t_3 + 2502073800\, h^{24} s^8 t_4^2 t_3 t_2 \\
&+ 417012300\, h^{22} s^8 t_4^2 t_3 \\
&- 131330224800000\, h^{20} s^6 t_4^2 t_3 t_2 \\
&+ 12527694122400000\, h^{24} t_4^2 t_3^2 t_2^2 s^4 \\
&+ 695983006800000\, h^{20} t_4^2 t_3 t_2 s^4 \\
&+ 283027053312000000\, h^{26} t_4^2 t_3^2 t_2^2 t_1 \\
&- 28511691552000000\, h^{24} t_4^2 t_3^2 t_2^2 s^2 \\
&- 218883870800000\, h^{18} s^6 t_4^2 t_3 \\
&+ 47171175552000000\, h^{24} t_4^2 t_3^2 t_2 t_1 \\
&+ 4175898040800000\, h^{22} t_4^2 t_3^2 s^4 t_2 \\
&+ 84863040\, h^{16} s^4 + 96664306500\, h^{24} t_4^2 t_3^2 s^4 \\
&- 193139200\, h^{16} s^2 \\
&- 94662144000\, h^{10} s^6 - 53884876800\, h^{12} s^6 \\
&- 3891265920000\, h^{20} s^6 t_4 t_3 t_2
\end{aligned}
$$

$$
\begin{aligned}
& - 787981348800000\, h^{22} s^6 t_4^2 t_3^2 t_2 \\
& - 847117440000\, h^{14} s^6 t_4 t_3 \\
& - 3764247552000\, h^{16} s^6 t_4 t_3 \\
& - 22585485312000\, h^{18} s^6 t_4 t_3 t_2 \\
& - 21137740800\, h^{14} s^6 \\
& + 26266044960000\, h^{24} s^6 t_4^2 t_3^2 t_2 \\
& + 2188837080000\, h^{22} s^6 t_4^2 t_3^2 \\
& - 65665112400000\, h^{20} s^6 t_4^2 t_3^2 - 648544320000\, h^{18} s^6 t_4 t_3 \\
& + 7861862592000000\, h^{22} t_4^2 t_3 t_2 t_1)/(465 s^2 - 139)^2 \qquad (66)
\end{aligned}
$$

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