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Construction of trigonometrically and exponentially fitted Runge–Kutta–Nyström methods for the numerical solution of the Schrödinger equation and related problems – a method of 8th algebraic order

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General conditions are presented for an m-stage Runge–Kutta–Nyström fitting to exponential and trigonometric functions. As an example an 8th order Runge–Kutta–Nyström method is constructed. Numerical results on the numerical solution of the Schrödinger equation and related problems indicate that the new method is more accurate than the classical one (we call classical Runge–Kutta–Nyström method the corresponding method with constant coefficients).

KEY WORDS: trigonometrically-fitted, exponentially-fitted, Runge–Kutta–Nyström, Schrödinger equation, scattering problems, resonance problem, periodic solutions, oscillating solutions

AMS subject classification: 65L05

1. Introduction

An investigation of special Runge–Kutta–Nyström (RKN) method of Dormand et al. [1] for the investigation of systems of ODEs of the form

$$\frac{\mathrm{d}^2 u(t)}{\mathrm{d}t^2} = f\big(t, u(t)\big), \tag{1}$$

for which it is known in advance that their solution is periodic or oscillating, is presented in this paper. Special attention to the numerical solution of the Schrödinger equation is given.

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For the numerical solution of the above problem many categories of methods have been constructed (see, for example, [2–8] and references therein). Lyche [9] has described a procedure for the construction of exponentially and trigonometrically fitted multistep methods.

For the numerical solution of the Schrödinger equation many research has taken place the last decade (see [4,5,10–15]).

We write in a compact (matrix) form conditions that should be satisfied in order to construct a modified Runge–Kutta–Nyström method of any order fitting to exponential and trigonometric functions. Modified Runge–Kutta–Nyström methods are presented in section 2. In section 3 the conditions for the exponentially-fitted Runge–Kutta–Nyström Dormand et al. method [1,16] are presented. In section 4 the conditions for the trigonometrically-fitted method are described. In section 5 a modified RKN method is constructed (both trigonometrically and exponentially fitted versions) based on the 8th order method of Dormand et al. [17]. In section 6 an error analysis is presented. Some numerical illustrations are presented in section 7. We note here that the procedure for the construction of the exponentially-fitted and trigonometrically-fitted Runge–Kutta–Nyström methods is different from that described by Lyche [9] for multistep methods.

2. Exponentially and trigonometrically fitted Runge–Kutta–Nyström methods

The general form of the modified m stage method for the equation (1) is:

$$u_n^{(0)} = u_{n-1},$$
$$u_n^{(i)} = u_{n-1} + a_i g_i h \dot{u}_{n-1} + h^2 \sum_{j=0}^{i-1} \gamma_{ij} f_j,$$

where

$$f_i = f\left(t_{n-1} + a_i h, u_n^{(i)}\right)$$

and

$$u_n = u_{n-1} + h\dot{u}_{n-1} + h^2 \sum_{j=0}^{m} c_j f_j,$$
$$\dot{u}_n = \dot{u}_{n-1} + h \sum_{j=0}^{m} \dot{c}_j f_j,$$

$a_0 = 0$ and $a_m = 1$.

Table 1
The m-stage modified Runge–Kutta–Nyström method.

$$\begin{array}{c|c|ccccc}
0 & & & & & & \\
a_1 & g_1 & \gamma_{10} & & & & \\
a_2 & g_2 & \gamma_{20} & \gamma_{21} & & & \\
\vdots & \vdots & \vdots & \vdots & \ddots & & \\
a_m & g_m & \gamma_{m0} & \gamma_{m1} & \cdots & \gamma_{m,m-1} & \\
\hline
 & & c_0 & c_1 & \cdots & c_{m-1} & c_m \\
 & & \dot{c}_0 & \dot{c}_1 & \cdots & \dot{c}_{m-1} & \dot{c}_m
\end{array}$$

The above expression is equivalent with the well-known Butcher table (see table 1). The new parameters $g_i,\ i = 1(1)m$ are to be estimated. One can see that for g_i, $i = 1, \dots, m$, equal to 1 the method is the classical RKN method. The condition

$$\sum_{j=0}^{i-1} \gamma_{ij} = \frac{1}{2} a_i^2$$

for the classical RKN method is no longer valid, so we also have to estimate $\gamma_{i,i-1}$, $i = 1(1)m$. Also the FSAL assumption is not made here so we have to estimate c_0, c_{m-1} and $\dot{c}_{m-2}$, $\dot{c}_{m-1}$.

In order to write the method in matrix form, we define the following matrices of size $(m+1) \times (m+1)$:

$$\Gamma = \begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ \gamma_{10} & 0 & \dots & 0 & 0 \\ \gamma_{20} & \gamma_{21} & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \gamma_{m0} & \gamma_{m1} & \dots & \gamma_{m,m-1} & 0 \end{pmatrix},$$
$$A = \operatorname{diag}(0, a_1, \dots, a_m);$$

and vectors of length $(m+1)$:

$$g = (0, g_1, \dots, g_m)^{\mathrm{T}},$$
$$c = (c_0, c_1, \dots, c_m)^{\mathrm{T}},$$
$$\dot{c} = (\dot{c}_0, \dot{c}_1, \dots, \dot{c}_m)^{\mathrm{T}},$$
$$e = (1, 1, \dots, 1)^{\mathrm{T}};$$

also define the stages vectors of length $(m+1)$:

$$\underline{u}_n = \left(u_n^{(0)}, u_n^{(1)}, \dots, u_n^{(m)}\right)^{\mathrm{T}}, \qquad \underline{f} = (f_0, f_1, \dots, f_m)^{\mathrm{T}}.$$

Now the method can be written as follows:

$$\underline{u}_n = u_{n-1} e + Agh\dot{u}_{n-1} + h^2 \Gamma \underline{f}, \tag{2}$$
$$\underline{f} = f\left(t_{n-1} e + Aeh, \tilde{u}_n\right) \tag{3}$$

and

$$u_n = u_{n-1} + h\dot{u}_{n-1} + h^2 c^{\mathrm{T}} \underline{f}, \tag{4}$$
$$\dot{u}_n = \dot{u}_{n-1} + h\dot{c}^{\mathrm{T}} \underline{f}. \tag{5}$$

This formulation of the modified RKN method is the one that we are going to use in the rest of the paper.

3. Exponentially-fitted RKN method

Definition 1. A modified RKN method of the form (2)–(5) is called exponentially fitted if all stages of the method integrate the functions

$$u(t) = \exp(\pm vt).$$

Theorem 1. The modified RKN method of the form (2)–(5) is exponentially fitted if the following conditions are satisfied:

$$\exp(Aew) = G(e + Agw), \tag{6}$$
$$\exp(-Aew) = G(e - Agw), \tag{7}$$
$$\exp w = 1 + w + w^2 cG(e + Agw), \tag{8}$$
$$\exp(-w) = 1 - w + w^2 cG(e - Agw), \tag{9}$$
$$\exp w = 1 + w\dot{c}G(e + Agw), \tag{10}$$
$$\exp(-w) = 1 + w\dot{c}G(e - Agw), \tag{11}$$

where $G = (I - w^2\Gamma)^{-1}$ and $w = vh$.

Proof. We shall prove first (6), (8) and (10) the rest follows similarly.
Let

$$u(t) = \exp(vt)$$

then

$$\frac{\mathrm{d}u}{\mathrm{d}t} = vu(t),$$
$$\frac{\mathrm{d}^2 u(t)}{\mathrm{d}t^2} = v^2 u(t).$$

Assume that the method is exact for $u(t)$ at $t = t_{n-1}$, that is,

$$u_{n-1} = u(t),$$
$$\dot{u}_{n-1} = vu(t).$$

From equation (3) we have that

$$\underline{f} = f(t_{n-1}e + Aeh, \underline{u}_n) = v^2 \underline{u}_n.$$

Substitution in (2) gives

$$\begin{aligned}\underline{u}_n &= u_{n-1}e + Agh\dot{u}_{n-1} + h^2\Gamma\big(v^2\underline{u}_n\big) \quad \Rightarrow \\ \underline{u}_n &= u(t)e + Agwu(t) + w^2(\Gamma\underline{u}_n);\end{aligned} \tag{12}$$

on the other hand, we want the method to be exact for $u(t)$ at $t = t_n$ at all stages, that is,

$$\begin{aligned}\underline{u}_n &= u\big(v(te + Aeh)\big) = \exp\big(v(te + Aeh)\big) \\ &= \exp(vt)\exp\big(Ae)vh\big) = u(t)\exp(Aew).\end{aligned}$$

Substitution in (12) results

$$\begin{aligned}u(t)\exp(Aew) &= u(t)e + Agwu(t) + w^2\Gamma u(t)\exp(Aew) \quad \Rightarrow \\ \exp(Aew) &= e + Agw + w^2\Gamma\exp(Aew) \quad \Rightarrow \\ \big(I - w^2\Gamma\big)\exp(Aew) &= e + Agw \quad \Rightarrow \\ \exp(Aew) &= \big(I - w^2\Gamma\big)^{-1}(e + Agw).\end{aligned}$$

The matrix $(I - w^2\Gamma)$ is unitary low triangular hence invertable. This proves (6). In order to prove (8) we substitute the function $u(t)$ in (4)

$$\begin{aligned}u(t + h) &= u(t) + wu(t) + w^2u(t)\big(c\exp(Aew)\big) \quad \Rightarrow \\ u(t)\exp w &= u(t) + wu(t) + w^2u(t)\big(c\exp(Aew)\big) \quad \Rightarrow \\ \exp w &= 1 + w + w^2\big(c\exp(Ae)w\big).\end{aligned}$$

Applying similar arguments to (5) we have

$$\begin{aligned}vu(t + h) &= vu(t) + hv^2u(t)\big(\dot{c}\exp\big((Ae)w\big)\big), \\ \exp w &= 1 + w\big(\dot{c}\exp\big((Ae)w\big)\big),\end{aligned}$$

and (10) follows.

The proof of (7), (9) and (11) follows if we apply the same arguments for the function $u(t) = \exp(-vt)$. □

It is not obvious how we construct the method from equations (6)–(11). Evaluation of the matrix G involves matrix inversion, though this can be avoided by noticing that Γ is strictly low triangular so it has all eigenvalues equal to zero. It is well known then that

$$G = \big(I - w^2\Gamma\big)^{-1} = I + w^2\Gamma + w^4\Gamma^2 + \cdots + w^{2n}\Gamma^n + \cdots.$$

Also notice that since

$$\Gamma^{m+1} = 0 \quad \text{and} \quad \Gamma^m A = 0$$

we can write

$$G = \big(I - w^2\Gamma\big)^{-1} = I + w^2\Gamma + w^4\Gamma^2 + \cdots + w^{2m}\Gamma^m = \sum_{i=0}^{m} w^{2i}\Gamma^i. \tag{13}$$

Then equation (6) can be written as

$$\begin{aligned}\exp(Aew) &= G(e + Agw)\\ &= \left(\sum_{i=0}^{m} w^{2i}\Gamma^i\right)(e + Agw)\\ &= \sum_{i=0}^{m} w^{2i}\big(\Gamma^i e\big) + \sum_{i=0}^{m-1} w^{2i+1}\big(\Gamma^i Ag\big).\end{aligned}$$

Working similarly equations (7)–(11) can be written as

$$\exp(-Aew) = \sum_{i=0}^{m} w^{2i}\big(\Gamma^i e\big) - \sum_{i=0}^{m-1} w^{2i+1}\big(\Gamma^i Ag\big),$$

$$\exp w = 1 + w + w^2 \sum_{i=0}^{m} \big(c^{\mathrm{T}}\Gamma^i e\big)w^{2i} + w^2 \sum_{i=0}^{m-1} \big(c^{\mathrm{T}}\Gamma^i Ag\big)w^{2i+1},$$

$$\exp w = 1 + w \sum_{i=0}^{m} \big(\dot{c}^{\mathrm{T}}\Gamma^i e\big)w^{2i} + w \sum_{i=0}^{m-1} \big(\dot{c}^{\mathrm{T}}\Gamma^i Ag\big)w^{2i+1},$$

$$\exp(-w) = 1 - w + w^2 \sum_{i=0}^{m} \big(c^{\mathrm{T}}\Gamma^i e\big)w^{2i} - w^2 \sum_{i=0}^{m-1} \big(c^{\mathrm{T}}\Gamma^i Ag\big)w^{2i+1},$$

$$\exp(-w) = 1 - w \sum_{i=0}^{m} \big(\dot{c}^{\mathrm{T}}\Gamma^i e\big)w^{2i} + w \sum_{i=0}^{m-1} \big(\dot{c}^{\mathrm{T}}\Gamma^i Ag\big)w^{2i+1}.$$

Equation (6) is a vector of equations with m components and so is (7). Since the matrix G is a unitary low triangular matrix of the form (13) it follows that line i of G involves the parameters $\gamma_{k,j}$ with $j < k < i$ only. That is, g_1 and γ_{10} appear alone in the second component of each (6) and (7) and we can solve the two equations for these parameters. Then in the third component of each of (6) and (7) the parameters that appear are g_1, g_2 and γ_{10}, γ_{21} from which we can evaluate g_2 and γ_{21}. We procced similarly until all g_i and $\gamma_{i,j}$ are evaluated.

Equations (8) and (9) are solved for c_0 and c_{m-1}. Finally, $\dot{c}_{m-2}$ and $\dot{c}_{m-1}$ are evaluated from equations (10) and (11).

4. Trigonometrically-fitted RKN method

Definition 2. A modified RKN method of the form (2)–(5) is called trigonometrically fitted if all stages of the method integrate the function

$$u(t) = \exp(\mathrm{i}vt), \quad \text{where } \mathrm{i} = \sqrt{-1}.$$

Theorem 2. The modified RKN method of the form (2)–(5) is trigonometrically fitted if the following conditions are satisfied:

$$\cos\bigl((Ae)w\bigr) = Ge, \tag{14}$$

$$\frac{\sin\,((Ae)w)}{w} = GAg, \tag{15}$$

$$\cos w = 1 - w^2 cGe, \tag{16}$$

$$\frac{\sin w}{w} = 1 - w^2 cGAg, \tag{17}$$

$$\cos w = 1 - w^2 \dot{c}GAg, \tag{18}$$

$$\frac{\sin w}{w} = \dot{c}Ge, \tag{19}$$

where $G = (I - w^2\Gamma)^{-1}$ and $w = vh$.

Proof. Let

$$u(t) = \exp(\mathrm{i}vt) = \cos(vt) + \mathrm{i}\sin(vt)$$

then

$$\begin{aligned}\frac{\mathrm{d}u}{\mathrm{d}t} &= \mathrm{i}vu(t) = -v\sin(vt) + \mathrm{i}v\cos(vt),\\ \frac{\mathrm{d}^2u(t)}{\mathrm{d}t^2} &= -v^2u(t) = -v^2\cos(vt) - \mathrm{i}v^2\sin(vt).\end{aligned}$$

Assume that the method is exact for $u(t)$ at $t = t_{n-1}$, that is,

$$u_{n-1} = u(t), \qquad \dot{u}_{n-1} = (\mathrm{i}v)u(t).$$

Working similarly with the exponentially fitted case we have that

$$\begin{aligned} u(t)\exp(\mathrm{i}Aew) = u(t)e + \mathrm{i}Agwu(t) - w^2\Gamma u(t)\exp(Aew) \quad &\Rightarrow\\ \cos(Aew) + \mathrm{i}\sin(Aew) = e + \mathrm{i}Agw - w^2\Gamma\bigl(\cos(Aew) + \mathrm{i}\sin(Aew)\bigr).&\end{aligned}$$

From this we have the following two equations:

$$\begin{aligned}\cos(Aew) &= e - w^2\Gamma\cos(Aew),\\ \sin(Aew) &= Agw - w^2\Gamma\sin(Aew),\end{aligned}$$

and

$$\begin{aligned}\bigl(I + w^2\Gamma\bigr)\cos(Aew) &= e,\\ \bigl(I + w^2\Gamma\bigr)\sin(Aew) &= Agw,\end{aligned}$$

so equations (14) and (15) follow. Equations (16)–(19) follow by applying similar arguments. □

We can write similarly that

$$G = \left(I + w^2\Gamma\right)^{-1} = \sum_{i=0}^{m} (-1)^i w^{2i} \Gamma^i. \tag{20}$$

Then equation (14) can be written as

$$\cos(Aew) = Ge = \sum_{i=0}^{m} (-1)^i w^{2i} \Gamma^i e.$$

Working similarly equations (15)–(19) can be written as

$$\sum_{i=0}^{m} (-1)^i w^{2i} \left(\Gamma^i Ag\right) = \frac{1}{w} \sin\left((Ae)w\right),$$

$$1 - w^2 \sum_{i=0}^{m} (-1)^i w^{2i} \left(c\Gamma^i e\right) = \cos w,$$

$$1 - w^2 \sum_{i=0}^{m-1} (-1)^i w^{2i} \left(c\Gamma^i Ag\right) = \frac{\sin w}{w},$$

$$\sum_{i=0}^{m} (-1)^i w^{2i} \left(\dot{c}\Gamma^i e\right) = \frac{\sin w}{w},$$

$$1 - w^2 \sum_{i=0}^{m-1} (-1)^i w^{2i} \left(\dot{c}\Gamma^i Ag\right) = \cos w.$$

5. The modified RKN method of 8th order

We will construct exponentially and trigonometrically fitted eight-stage RKN methods based on the well-known RKN method by Dormand et al. [17] of algebraic order 8 as shown in table 2.

The coefficients of the modified trigonometrically and exponentially fitted methods as well as their Taylor expansions are given in appendices A and B at the end of the paper. The coefficients of the 8th order modified method would also be available on the following URL address: http://kastoria.teikoz.gr/gr/tei/de/ep/kalogiratou

6. Error analysis

Substituting the coefficients obtained to the order condition equations for the 8th order Runge–Kutta–Nyström method (see for more details [1]) and taking Taylor expansions we have the results given in appendix C. We note that the order conditions are the same with the order conditions of a classical Runge–Kutta–Nyström method if $w = 0$.

Table 2
The 8-stage 8th algebraic order Runge–Kutta–Nyström (Dormand et al.) method.

$\frac{1}{20}$	$\frac{1}{800}$								
$\frac{1}{10}$	$\frac{1}{600}$	$\frac{1}{300}$							
$\frac{3}{10}$	$\frac{9}{200}$	$\frac{-9}{100}$	$\frac{9}{100}$						
$\frac{1}{2}$	$\frac{-66701}{197352}$	$\frac{28325}{32892}$	$\frac{-2665}{5482}$	$\frac{2170}{24669}$					
$\frac{7}{10}$	$\frac{227015747}{304251000}$	$\frac{-54897451}{304251000}$	$\frac{12942349}{10141700}$	$\frac{-9499}{304251}$	$\frac{539}{9250}$				
$\frac{9}{10}$	$\frac{-1131891597}{901789000}$	$\frac{41964921}{12882700}$	$\frac{-6663147}{3220675}$	$\frac{270954}{644135}$	$\frac{-108}{5875}$	$\frac{114}{1645}$			
1	$\frac{13836959}{3667458}$	$\frac{-17731450}{1833729}$	$\frac{1063919505}{156478208}$	$\frac{-33213845}{39119552}$	$\frac{13335}{28544}$	$\frac{-705}{14272}$	$\frac{1645}{57088}$		
1	$\frac{223}{7938}$	0	$\frac{1175}{8064}$	$\frac{925}{6048}$	$\frac{41}{448}$	$\frac{925}{14112}$	$\frac{1175}{72576}$	0	
	$\frac{223}{7938}$	0	$\frac{1175}{8064}$	$\frac{925}{6048}$	$\frac{41}{448}$	$\frac{925}{14112}$	$\frac{1175}{72576}$	0	0
	$\frac{223}{7938}$	0	$\frac{5875}{36288}$	$\frac{4625}{21168}$	$\frac{41}{224}$	$\frac{4625}{21168}$	$\frac{5875}{36288}$	$\frac{223}{7938}$	0

7. Numerical results

In this section we present numerical results of the application of the new proposed method in the resonance problem of the radial Schrödinger equation and in some related problems. The method used for numerical comparison is the Runge–Kutta–Nyström of eigth order by Dormand et al. [17], we refer to this method by RKN8.

7.1. Resonance problem of the radial Schrödinger equation

We consider the numerical integration of the radial Schrödinger equation

$$y''(x) = \left[\frac{l(l+1)}{x^2} + V(x) - k^2\right] y(x). \tag{21}$$

Equations of this type occur very frequently in theoretical physics and quantum chemistry (see, for example, [18,19]). In (21) the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k^2 is a real number denoting *the energy*, l is a given integer, related to the angular momentum and V is a given function representing the potential. The boundary conditions are:

$$y(0) = 0 \tag{22}$$

and a second boundary condition, for large values of x, determined by physical considerations.

In the asymptotic region the equation (21) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{23}$$

for x greater than some value X, where X defines the asymptotic region.

The above equation (23) has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$, $n_l(kx)$ are the *spherical Bessel* and *Neumann functions*, respectively. Thus the solution of equation (21) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\sim Akxj_l(kx) - Bn_l(kx) \\ &\sim D\left[\sin\frac{kx - \pi l}{2} + \tan\delta_l \cos\frac{kx - \pi l}{2}\right], \end{aligned} \tag{24}$$

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

$$\tan\delta_l = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})} \tag{25}$$

for x_i and x_{i+1} distinct points on the asymptotic region (for which we have that x_{i+1} is the right-hand endpoint of the interval of integration and $x_i = x_{i+1} - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

We evaluate the phase shift δ_l from the above relation at x_i in the asymptotic region.

7.1.1. The Woods–Saxon potential

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (21) with $l = 0$ in the case where $V(x)$ is the Woods–Saxon potential:

$$V(x) = V_{\mathrm{W}}(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{a(1+z)^2} \tag{26}$$

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

For positive energies one has the so-called resonance problem. For this problem and for the potential mentioned above it is known (see [10]) that $\delta = \pi/2$. So, in our case and for each of the four known energies (resonances) we calculate the phase-shift using the two numerical methods. In the following table we present the absolute error which is the absolute value of the difference of the computed phase-shift and the theoretical value (which is equal to $\pi/2$). The empty area in the table indicates that the error is greater than 1. The boundary conditions for this problem are:

$$\begin{aligned} &y(0) = 0, \\ &y(x) \sim \cos\left[\sqrt{E}x\right] \quad \text{for large } x. \end{aligned}$$

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

E	h	RKN8	New
53.588872	$\frac{1}{8}$	$4.6 \cdot 10^{-5}$	$6.4 \cdot 10^{-6}$
	$\frac{1}{16}$	$7.0 \cdot 10^{-7}$	$8.2 \cdot 10^{-8}$
	$\frac{1}{32}$	$2.6 \cdot 10^{-8}$	$9.1 \cdot 10^{-10}$
163.215341	$\frac{1}{8}$	$9.6 \cdot 10^{-4}$	$8.4 \cdot 10^{-6}$
	$\frac{1}{16}$	$1.8 \cdot 10^{-5}$	$6.5 \cdot 10^{-8}$
	$\frac{1}{32}$	$2.7 \cdot 10^{-7}$	$7.3 \cdot 10^{-10}$
341.495874	$\frac{1}{8}$	$1.8 \cdot 10^{-2}$	$2.6 \cdot 10^{-5}$
	$\frac{1}{16}$	$1.9 \cdot 10^{-4}$	$3.7 \cdot 10^{-7}$
	$\frac{1}{32}$	$2.8 \cdot 10^{-6}$	$7.1 \cdot 10^{-9}$
989.701916	$\frac{1}{8}$		$3.3 \cdot 10^{-4}$
	$\frac{1}{16}$	$5.8 \cdot 10^{-3}$	$4.1 \cdot 10^{-6}$
	$\frac{1}{32}$	$7.7 \cdot 10^{-5}$	$1.8 \cdot 10^{-8}$

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [10]):

$$v = \begin{cases} \sqrt{-50+E} & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E} & \text{for } x = 6.5-h, \\ \sqrt{-25+E} & \text{for } x = 6.5, \\ \sqrt{-12.5+E} & \text{for } x = 6.5+h, \\ \sqrt{E} & \text{for } x \in [6.5+2h, 15]. \end{cases} \tag{27}$$

7.2. *Related problems*

We consider two problems with periodic behaviour. Results are presented with stepsizes from $h = 1.0$ to $h = 5.0$. For each stepsize h the maximum absolute error is given.

7.2.1. An orbit problem studied by Stiefel and Bettis

We consider the following "almost" periodic orbit problem studied by Stiefel and Bettis [20]:

$$z'' + z = 0.001\mathrm{e}^{\mathrm{i}x}, \qquad z(0) = 1,\ z'(0) = 0.9995\mathrm{i},\ z \in \mathbb{C}, \tag{28}$$

whose analytical solution is given by

$$\begin{aligned} z(x) &= u(x) + \mathrm{i}v(x), \qquad u, v \in \mathbb{R}, \\ u(x) &= \cos x + 0.0005x \sin x, \\ v(x) &= \sin x - 0.0005x \cos x. \end{aligned}$$

The solution represents motion on a perturbation of a circular orbit in the complex plane.
We write the above equation in the equivalent form

$$u'' + u = 0.001\cos x, \quad u(0) = 1,\ u'(0) = 0,$$
$$v'' + v = 0.001\sin x, \quad v(0) = 0,\ v'(0) = 0.9995.$$

The equivalent system of equations has been solved numerically for $0 \leqslant x \leqslant 100$. For this problem $v = 1$.

Results for component y:

h	RKN8	New
1.0	$2.1230 \cdot 10^{-6}$	$4.3881 \cdot 10^{-8}$
2.0	$4.9200 \cdot 10^{-4}$	$1.3276 \cdot 10^{-4}$
3.0	0.0108	0.0012
4.0	0.1846	0.0016
5.0		0.0559

The results for the component z:

h	RKN8	New
1.0	$2.0066 \cdot 10^{-6}$	$4.2502 \cdot 10^{-8}$
2.0	$5.1183 \cdot 10^{-4}$	$1.3896 \cdot 10^{-4}$
3.0	0.0105	0.0013
4.0	0.1696	0.0014
5.0		0.0632

7.2.2. Two-body problem

We consider the following system of coupled differential equations which is well known as two-body problem:

$$y'' = -\frac{y}{(y^2 + z^2)^{3/2}}, \qquad z'' = -\frac{z}{(y^2 + z^2)^{3/2}},$$
$$y(0) = 1,\ y'(0) = 0,\ z(0) = 0,\ z'(0) = 1,$$

whose analytical solution is given by

$$y(x) = \cos(x), \qquad z(x) = \sin(x). \tag{29}$$

The above system of equations has been solved numerically for $0 \leqslant x \leqslant 100$. For this problem $v = \sqrt{1/r}$, where $r = \sqrt{(y^2 + z^2)^3}$.

Results for component y:

h	RKN8	New
1.0	$6.8394 \cdot 10^{-4}$	$2.0507 \cdot 10^{-13}$
2.0	0.2533	$1.8027 \cdot 10^{-13}$
3.0		$1.4003 \cdot 10^{-12}$
4.0		$9.0836 \cdot 10^{-6}$

Results for component z:

h	RKN8	New
1.0	$6.1083 \cdot 10^{-4}$	$2.0040 \cdot 10^{-13}$
2.0	0.2333	$2.0589 \cdot 10^{-13}$
3.0		$5.4501 \cdot 10^{-13}$
4.0		$1.7736 \cdot 10^{-6}$

We note here that the empty areas in the previous tables indicate that the error is greater than 1.

Appendix A. Coefficients of the trigonometrically fitted method

$$
\begin{aligned}
g_1 &= 20\sin(w/20)/w,\\
g_2 &= \left(1200 - w^2\right)\tan(w/20)/(60w),\\
g_3 &= \sec(w/10)\left(18w^2\sin(w/20) + \left(200 - 9w^2\right)\sin(w/10) + 200\sin(w/5)\right)/(60w),\\
g_4 &= \sec(3w/10)\left(\left(197352 + 95940w^2\right)\sin(w/5) + \left(197352 + 66701w^2\right)\sin(3w/10)\right.\\
&\quad \left. - 169950w^2\sin(w/4)\right)/(98676w),\\
g_5 &= \sec(w/2)\left(\left(304251000 + 9499000w^2\right)\sin(w/5)\right.\\
&\quad - 388270470w^2\sin(2w/5) + 548974510w^2\sin(9w/20)\\
&\quad \left. + \left(304251000 - 227015747w^2\right)\sin(w/2)\right)/(212975700w),\\
g_6 &= \sec(7w/10)\left(\left(901789000 + 16577568w^2\right)\sin(w/5) - 379335600w^2\sin(2w/5)\right.\\
&\quad + \left(901789000 + 1131891597w^2\right)\sin(7w/10) + 1865681160w^2\sin(3w/5)\\
&\quad \left. - 2937544470w^2\sin(13w/20)\right)/(811610100w),\\
g_7 &= \sec(9w/10)\left(469434624\sin(w/10) + \left(469434624 - 1771130752w^2\right)\sin(9w/10)\right.\\
&\quad + w^2\left(23188860\sin(w/5) - 219307410\sin(2w/5) + 398566140\sin(3w/5)\right.\\
&\quad \left.\left. - 3191758515\sin(4w/5) + 4539251200\sin(17w/20)\right)\right)/(469434624w),
\end{aligned}
$$

$$
\begin{aligned}
g_8 = {} & -\sec w\big(w^2\big(8225\sin(w/10) + 33300\sin(3w/10) + 46494\sin(w/2) \\
& + 77700\sin(7w/10) + 74025\sin(9w/10)\big) \\
& + \big(-508032 + 14272w^2\big)\sin w\big)/(508032w), \\
\gamma_{10} = {} & \big(1 - \cos(w/20)\big)/w^2, \\
\gamma_{21} = {} & \sec(w/20)\big(\big(1 - \cos(w/10)\big)/w^2 - 1/600\big), \\
\gamma_{32} = {} & \sec(w/10)\big(\big(1 - \cos(3w/10)\big)/w^2 + \big(-9 + 18\cos(w/20)\big)/200\big), \\
\gamma_{43} = {} & \sec(3w/10)\big(\big(1 - \cos(w/2)\big)/w^2 \\
& + \big(66701 - 169950\cos(w/20) + 95940\cos(w/10)\big)/197352\big), \\
\gamma_{54} = {} & \sec(w/2)\big(\big(1 - \cos(7w/10)\big)/w^2 \\
& + \big(-227015747 + 548974510\cos(w/20) \\
& - 388270470\cos(w/10) + 9499000\cos(3w/10)\big)/304251000\big), \\
\gamma_{65} = {} & \sec(7w/10)\big(\big(1 + \cos(9w/10)\big)/w^2 \\
& + \big(1131891597 + 2937544470\cos(w/20) \\
& + 1865681160\cos(w/10) + 379335600\cos(3w/10) \\
& + 16577568\cos(w/2)\big)/901789000\big), \\
\gamma_{76} = {} & \sec(9w/10)\big((1 - \cos w)/w^2 + \big(-1771130752 + 4539251200\cos(w/20) \\
& - 3191758515\cos(w/10) + 398566140\cos(3w/10) - 219307410\cos(w/2) \\
& + 23188860\cos(7w/10) - 469434624\cos w\big)/469434624\big), \\
\gamma_{87} = {} & \sec w\big((1 - \cos w)/w^2 - \big(14272 + 74025\cos(w/10) + 77700\cos(3w/10) \\
& + 46494\cos(5w/10) + 33300\cos(7w/10) + 8225\cos(9w/10)\big)/508032\big), \\
c_0 = {} & \csc w\big(-\cos w/w + \sin w/w^2 - w^2\big(8225\sin(w/10) + 33300\sin(3w/10) \\
& + 46494\sin(5w/10) + 77700\sin(7w/10) + 74025\sin(9w/10)\big)/508032\big), \\
c_8 = {} & \csc w\big(1/w - \sin w/w^2 - \big(74025\sin(w/10) + 77700\sin(3w/10) \\
& + 46494\sin(5w/10) + 33300\sin(7w/10) + 8225\sin(9w/10)\big)/508032\big), \\
\dot{c}_6 = {} & \csc(w/10)\big(1/w - \cos w/w - w\big(55500\sin(3w/10) + 46494w\sin(5w/10) \\
& + 55500\sin(7w/10) + 41125\sin(9w/10) + 7136\sin w\big)/254016\big), \\
\dot{c}_7 = {} & \csc(w/10)\big(\big(-\cos(w/10) + \cos(9w/10)\big)/w + w\big(55500\sin(w/5) \\
& + 46494\sin(2w/5) + 55500\sin(3w/5) + 41125\sin(4w/5) \\
& + 7136\sin(9w/10)\big)/254016\big).
\end{aligned}
$$

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

$$g_1 = 1 - \tfrac{w^2}{2400} + \tfrac{w^4}{19210^5} + \mathrm{O}(w^6), \qquad \gamma_{10} = \tfrac{1}{800} - \tfrac{w^2}{3840000} + \tfrac{w^4}{460810^7} + \mathrm{O}(w^6),$$
$$g_2 = 1 + \tfrac{w^4}{7210^5} + \mathrm{O}(w^6), \qquad \gamma_{21} = \tfrac{1}{300} + \tfrac{w^4}{19210^7} + \mathrm{O}(w^6),$$
$$g_3 = 1 + \tfrac{19w^4}{810^5} + \mathrm{O}(w^6), \qquad \gamma_{32} = \tfrac{9}{100} + \tfrac{423w^4}{6410^7} + \mathrm{O}(w^6),$$
$$g_4 = 1 - \tfrac{22843w^4}{157881600} + \mathrm{O}(w^6), \qquad \gamma_{43} = \tfrac{2170}{24669} - \tfrac{17361w^4}{2806784000} + \mathrm{O}(w^6),$$
$$g_5 = 1 + \tfrac{158570927w^4}{730202410^5} + \mathrm{O}(w^6), \qquad \gamma_{54} = \tfrac{539}{9250} + \tfrac{1125844951w^4}{649068810^7} + \mathrm{O}(w^6),$$
$$g_6 = 1 - \tfrac{94109471w^4}{309184810^5} + \mathrm{O}(w^6), \qquad \gamma_{65} = \tfrac{114}{1645} - \tfrac{3422444871w^4}{824492810^7} + \mathrm{O}(w^6),$$
$$g_7 = 1 + \tfrac{7149859w^4}{8801899200} + \mathrm{O}(w^6), \qquad \gamma_{76} = \tfrac{1645}{57088} + \tfrac{6547403w^4}{46943462400} + \mathrm{O}(w^6),$$
$$g_8 = 1 + \mathrm{O}(w^8), \qquad \gamma_{87} = \mathrm{O}(w^8),$$
$$c_0 = \tfrac{223}{7938} + \mathrm{O}(w^6), \qquad c_8 = \mathrm{O}(w^6),$$
$$\dot{c}_6 = \tfrac{5875}{36288} + \mathrm{O}(w^8), \qquad \dot{c}_7 = \tfrac{223}{7938} + \mathrm{O}(w^8).$$

Appendix B. Coefficients of the exponentially fitted method

$$g_1 = \frac{10\mathrm{e}^{-w/20}(-1 + \mathrm{e}^{w/10})}{w},$$
$$\gamma_{10} = \frac{\mathrm{e}^{-w/20}(-1 + \mathrm{e}^{w/20})^2}{2w^2},$$
$$g_2 = \frac{(-1 + \mathrm{e}^{w/10})(1200 + w^2)}{60(1 + \mathrm{e}^{w/10})w},$$
$$\gamma_{21} = \frac{\mathrm{e}^{-w/20}(300 - 600\mathrm{e}^{w/10} + 300\mathrm{e}^{w/5} - \mathrm{e}^{w/10}w^2)}{300(1 + \mathrm{e}^{w/10})w^2},$$
$$g_3 = \frac{1}{60(1 + \mathrm{e}^{w/5})w}\big(\mathrm{e}^{-w/10}(-1 + \mathrm{e}^{w/10})(200 + 400\mathrm{e}^{w/10} + 400\mathrm{e}^{w/5} + 200\mathrm{e}^{3w/10} + 9\mathrm{e}^{w/10}w^2 - 18\mathrm{e}^{3w/20}w^2 + 9\mathrm{e}^{w/5}w^2)\big),$$
$$\gamma_{32} = -\left(\frac{3}{10}w\left(1 - \mathrm{e}^{-3w/10} + \frac{9}{200}(1 - 2\mathrm{e}^{-w/20})w^2\right) + \frac{3}{10}w\left(1 - \mathrm{e}^{3w/10} + \frac{1}{200}(9 - 18\mathrm{e}^{w/20})w^2\right)\right)\left(\frac{3}{10}\mathrm{e}^{-w/10}w^3 + \frac{3}{10}\mathrm{e}^{w/10}w^3\right),$$

$$g_4 = \frac{1}{98676(1+e^{3w/5})w}\Big(197352\big(-1-e^{w/10}+e^{w/2}+e^{3w/5}\big) + \big(66701 - 169950e^{w/20} + 95940e^{w/10} - 95940e^{w/2} + 169950e^{11w/20} - 66701e^{3w/5}\big)w^2\Big),$$

$$\gamma_{43} = \frac{1}{98676(1+e^{3w/5})w^2}\big(e^{-w/5}\big(98676\big(-1+e^{w/2}\big)^2 + e^{2w/5}\big(47970 - 84975e^{w/20} + 66701e^{w/10} - 84975e^{3w/20} + 47970e^{w/5}\big)w^2\big)\big),$$

$$g_5 = \frac{1}{212975700(1+e^{w})w}\big(304251000\big(-1-e^{3w/10}+e^{7w/10}+e^{w}\big) + 7\big(-32430821\big(1-e^{w}\big) + 78424930\big(e^{w/20}-e^{19w/20}\big) - 55467210\big(e^{w/10}-e^{9w/10}\big) + 1357000\big(e^{3w/10}-e^{7w/10}\big)\big)w^2\big),$$

$$\gamma_{54} = \frac{1}{152125500(1+e^{w})w^2}\big(e^{-w/5}\big(152125500\big(-1+e^{7w/10}\big)^2 + 7e^{2w/5}\big(678500\big(1+e^{3w/5}\big) - 27733605\big(e^{w/5}+e^{2w/5}\big) + 39212465\big(e^{w/4}+e^{7w/20}\big) - 32430821e^{3w/10} + \big)w^2\big)\big),$$

$$g_6 = \frac{1}{811610100(1+e^{7w/5})w}\big(901789000\big(-1-e^{w/2}+e^{9w/10}+e^{7w/5}\big) - 3\big(-377297199\big(1-e^{7w/5}\big) + 979181490\big(e^{w/20}-e^{27w/20}\big) - 621893720\big(e^{w/10}-e^{13w/10}\big) + 126445200\big(e^{3w/10}-e^{11w/10}\big) - 5525856\big(e^{w/2}-e^{9w/10}\big)\big)w^2\big),$$

$$\gamma_{65} = \frac{1}{450894500(1+e^{7w/5})w^2}\big(450894500e^{-w/5}\big(-1+e^{9w/10}\big)^2 + 3e^{w/5}\big(2762928\big(1+e^{w}\big) - 63222600\big(e^{w/5}+e^{4w/5}\big) + 310946860\big(e^{2w/5}+e^{3w/5}\big) - 489590745\big(e^{9w/20}+e^{11w/20}\big) + 377297199e^{w/2}\big)w^2\big),$$

$$g_7 = \frac{1}{469434624(1+e^{9w/5})w}\big(469434624\big(-1-e^{4w/5}+e^{w}+e^{9w/5}\big) + \big(-1771130752(1-e^{9w/5}) + 4539251200\big(e^{w/20}-e^{7w/4}\big) - 3191758515\big(e^{w/10}-e^{17w/10}\big) + 398566140\big(e^{3w/10}-e^{3w/2}\big) - 219307410\big(e^{w/2}-e^{13w/10}\big) + 23188860\big(e^{7w/10}-e^{11w/10}\big)\big)w^2\big),$$

$$\gamma_{76} = \frac{1}{469434624(1+e^{9w/5})w^2}\big(469434624e^{-w/10}\big(-1+e^{w}\big)^2 + e^{w/5}\big(23188860\big(1+e^{7w/5}\big) - 219307410\big(e^{w/5}+e^{6w/5}\big) + 398566140\big(e^{2w/5}+e^{w}\big) - 3191758515\big(e^{3w/5}+e^{4w/5}\big) + 4539251200\big(e^{13w/20}+e^{3w/4}\big) - 3542261504e^{7w/10}\big)w^2\big),$$

$$g_8 = \frac{1}{508032(1+e^{2w})w}\big(508032\big(-1+e^{2w}+\big(-14272\big(1-e^{2w}\big)$$
$$-74025\big(e^{w/10}-e^{19w/10}\big)-77700\big(e^{3w/10}-e^{17w/10}\big)-46494\big(e^{w/2}-e^{3w/2}\big)$$
$$-33300\big(e^{7w/10}+e^{13w/10}\big)-8225\big(e^{9w/10}-e^{11w/10}\big)\big)w^2\big),$$

$$\gamma_{87} = \frac{1}{508032(1+e^{2w})w^2}\big(508032\big(-1+e^{w}\big)^2-e^{w/10}\big(8225\big(1+e^{9w/5}\big)$$
$$+33300\big(e^{w/5}+e^{8w/5}\big)+46494\big(e^{2w/5}+e^{7w/5}\big)+77700\big(e^{3w/5}+e^{6w/5}\big)$$
$$+74025\big(e^{4w/5}+e^{w}\big)+28544e^{9w/10}\big)w^2\big),$$

$$c_0 = -\frac{1}{508032(-1+e^{2w})w^2}\big(508032\big(-1+e^{2w}\big)-508032w\big(1+e^{2w}\big)$$
$$+e^{w/10}\big(-1+e^{w/5}\big)\big(74025\big(1+e^{8w/5}\big)+151725\big(e^{w/5}+e^{7w/5}\big)$$
$$+198219\big(e^{2w/5}+e^{6w/5}+231519\big(e^{3w/5}+e^{w}\big)+239744e^{4w/5}\big)w^2\big),$$

$$c_8 = -\frac{1}{508032(-1+e^{2w})w^2}\big(-508032\big(-1+e^{2w}\big)+1016064we^{w}$$
$$+e^{w/10}\big(-1+e^{w/5}\big)\big(8225\big(1+e^{8w/5}\big)+41525\big(e^{w/5}+e^{7w/5}\big)$$
$$+88019\big(e^{2w/5}+e^{6w/5}\big)+165719\big(e^{3w/5}+e^{w}\big)+239744e^{4w/5}\big)w^2\big),$$

$$\dot{c}_6 = \frac{e^{-9w/10}}{254016(-1+e^{w/5})w}\big(-254016\big(-1+e^{2w}\big)+\big(7136\big(1-e^{2w}\big)$$
$$+41125\big(e^{w/10}-e^{19w/10}\big)+55500\big(e^{3w/10}+e^{7w/10}-e^{13w/10}-e^{17w/10}\big)$$
$$+46494\big(e^{w/2}+e^{3w/2}\big)\big)w\big),$$

$$\dot{c}_7 = \frac{1}{127008w}\left(254016+3568w+198619w\cosh\left(\frac{w}{10}\right)+143119w\cosh\left(\left(\frac{3w}{10}\right)\right.\right.$$
$$+96625w\cosh\left(\frac{w}{2}\right)+32(7938+223w)\left(\cosh\left(\frac{w}{5}\right)+\cosh\left(\frac{2w}{5}\right)\right.$$
$$\left.\left.+\cosh\left(\frac{3w}{5}\right)+\cosh\left(\frac{4w}{5}\right)\right)+41125w\cosh\left(\frac{7w}{10}\right)\right).$$

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

$$g_1 = 1+\frac{w^2}{2400}+\frac{w^4 10^{-5}}{192}+O\big(w^6\big),$$
$$g_2 = 1+\frac{w^4 10^{-5}}{72}+O\big(w^6\big),$$
$$g_3 = 1+\frac{19w^4 10^{-5}}{8}+O\big(w^6\big),$$
$$g_4 = 1-\frac{22843w^4}{157881600}+O\big(w^6\big),$$

$$
\begin{aligned}
g_5 &= 1 + \frac{158570927 w^4 10^{-5}}{7302024} + \mathrm{O}(w^6),\\
g_6 &= 1 - \frac{94109471 w^4 10^{-5}}{3091848} + \mathrm{O}(w^6),\\
g_7 &= 1 + \frac{7149859 w^4}{8801899200} + \mathrm{O}(w^6),\\
g_8 &= 1 - \mathrm{O}(w^6),\\
c_0 &= \frac{223}{7938} + \mathrm{O}(w^6),\\
\dot{c}_6 &= \frac{5875}{36288} + \mathrm{O}(w^8),\\
\gamma_{10} &= \frac{1}{800} + \frac{w^2}{3840000} + \frac{w^4}{460810^7} + \mathrm{O}(w^6),\\
\gamma_{21} &= \frac{1}{300} + \frac{w^4 10^{-7}}{192} + \mathrm{O}(w^6),\\
\gamma_{32} &= \frac{9}{100} + \frac{423 w^4 10^{-7}}{64} + \mathrm{O}(w^6),\\
\gamma_{43} &= \frac{2170}{24669} - \frac{17361 w^4}{2806784000} + \mathrm{O}(w^6),\\
\gamma_{54} &= \frac{539}{9250} + \frac{1125844951 w^4 10^{-7}}{6490688} + \mathrm{O}(w^6),\\
\gamma_{65} &= \frac{114}{1645} - \frac{3422444871 w^4 10^{-7}}{8244928} + \mathrm{O}(w^6),\\
\gamma_{76} &= \frac{1645}{57088} + \frac{6547403 w^4}{46943462400} + \mathrm{O}(w^6),\\
\gamma_{87} &= \mathrm{O}(w^8),\\
c_8 &= \mathrm{O}(w^6),\\
\dot{c}_7 &= \frac{223}{7938} + \mathrm{O}(w^8).
\end{aligned}
$$

Appendix C. Error analysis

$$
\begin{aligned}
\sum \dot{c}_i &= 1 + \mathrm{O}(w^8),\\
\sum \dot{c}_i a_i &= \frac{1}{2} + \mathrm{O}(w^8),\\
\sum \dot{c}_i a_i^2 &= \frac{1}{3} + \mathrm{O}(w^8),\\
\sum \dot{c}_i a_i^3 &= \frac{1}{4} + \mathrm{O}(w^8),
\end{aligned}
$$

$$\sum \dot{c}_i \gamma_{ij} a_j = \frac{1}{24} + \frac{83809463767 w^4}{213890413363200000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i^4 = \frac{1}{5} + \mathrm{O}(w^8),$$
$$\sum \dot{c}_i a_i \gamma_{ij} a_j = \frac{1}{30} + \frac{969983523799 w^4}{2138904133632000000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma_{ij} a_j^2 = \frac{1}{60} + \frac{3113253549097 w^4}{4277808267264000000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i^5 = \frac{1}{6} - \mathrm{O}(w^8),$$
$$\sum \dot{c}_i a_i^2 \gamma_{ij} a_j = \frac{1}{36} + \frac{11995524793303 w^4}{21389041336320000000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i \gamma i j a_j^2 = \frac{1}{72} + \frac{35196334708777 w^4}{42778082672640000000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma_{ij} a_j^3 = \frac{1}{120} + \frac{12156149664019 w^4}{12222309335040000000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma_{ij} \gamma_{jk} a_k = \frac{1}{720} + \frac{76837027837 w^4}{407410311168000000} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i^6 = \frac{1}{7} - \mathrm{O}(w^8),$$
$$\sum \dot{c}_i a_i^3 \gamma_{ij} a_j = \frac{1}{42} + \frac{150763836787927 w^4 10^{-8}}{2138904133632} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i^2 \gamma_{ij} a_i^2 = \frac{1}{84} + \frac{404397742228009 w^4 10^{-8}}{4277808267264} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i \gamma i j a_j^3 = \frac{1}{140} + \frac{19174368276373 w^4 10^{-8}}{174604419072} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma i j a_j^4 = \frac{1}{210} + \frac{2027476918186189 w^4 10^{-8}}{17111233069056} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma i j \gamma_{jk} a_k^2 = \frac{1}{2520} + \frac{10697178649891 w^4 10^{-8}}{950624059392} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i \gamma_{ij} \gamma j k a_k = \frac{1}{840} + \frac{38028004665197 w^4 10^{-8}}{1884272689152} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma_{ij} a_j \gamma_{jk} a_k = \frac{1}{1260} + \frac{10258877576513 w^4 10^{-8}}{475312029696} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i (\gamma_{ij} a_j)^2 = \frac{1}{252} + \frac{150763836787927 w^4 10^{-8}}{6416712400896} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i^7 = \frac{1}{8} + \mathrm{O}(w^8),$$
$$\sum \dot{c}_i a_i^3 \gamma_{ij} a_j^2 = \frac{1}{96} + \frac{4643305320576553 w^4 10^{-9}}{4277808267264} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i a_i \gamma_{ij} a_j^4 = \frac{1}{240} + \frac{21898151264637133 w^4 10^{-9}}{17111233069056} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma_{ij} \gamma_{jk} a_k^3 = \frac{1}{6720} + \frac{25756277107923379042 7 w^4 10^{-9}}{3020829127249231872} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i \gamma_{ij} \gamma_{jk} a_k^2 = \frac{1}{2880} + \frac{1032721373184727 w^4 10^{-9}}{8793272549376} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i a_i \gamma_{ij} a_j \gamma_{jk} a_k = \frac{1}{1440} + \frac{500883763381891 w^4 10^{-9}}{2198318137344} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i \gamma_{ij} a_j \gamma_{jk} a_k^2 = \frac{1}{4032} + \frac{333911962354493 w^4 10^{-9}}{2851872178176} + \mathrm{O}(w^6),$$
$$\sum \dot{c}_i (\gamma_{ij} a_j)(\gamma_{ij} a_j^2) = \frac{1}{576} + \frac{203507025859 w^4}{802089050112000000} + \mathrm{O}(w^6),$$
$$\sum c_i = \frac{1}{2} + \mathrm{O}(w^8),$$
$$\sum c_i a_i = \frac{1}{6} + \mathrm{O}(w^6),$$
$$\sum c_i a_i^2 = \frac{1}{12} + \mathrm{O}(w^6),$$
$$\sum c_i a_i^3 = \frac{1}{20} + \mathrm{O}(w^6),$$
$$\sum c_i \gamma_{ij} a_j = \frac{1}{120} - \frac{109109 w^4}{1769472000000} + \mathrm{O}(w^6),$$
$$\sum c_i a_i^4 = \frac{1}{30} + \mathrm{O}(w^6),$$
$$\sum c_i a_i \gamma_{ij} a_j = \frac{1}{180} - \frac{36439516751 w^4}{339508592640000000} + \mathrm{O}(w^6),$$
$$\sum c_i \gamma_{ij} a_j^2 = \frac{1}{360} - \frac{21501583163 w^4}{226339061760000000} + \mathrm{O}(w^6),$$
$$\sum c_i a_i^5 = \frac{1}{42} + \mathrm{O}(w^6),$$
$$\sum c_i a_i^2 \gamma_{ij} a_j = \frac{1}{252} - \frac{489025219919 w^4 10^{-8}}{33950859264} + \mathrm{O}(w^6),$$
$$\sum c_i a_i \gamma_{ij} a_j^2 = \frac{1}{504} - \frac{832291986353 w^4 10^{-8}}{67901718528} + \mathrm{O}(w^6),$$
$$\sum c_i \gamma_{ij} a_j^3 = \frac{1}{840} - \frac{1406564588269 w^4 10^{-8}}{135803437056} + \mathrm{O}(w^6),$$
$$\sum c_i \gamma_{ij} \gamma\, jk a_k = \frac{1}{5040} - \frac{553528731241 w^4 10^{-8}}{418727264256} + \mathrm{O}(w^6),$$
$$\sum c_i a_i^6 = \frac{1}{56} + \mathrm{O}(w^6),$$

$$\sum c_i a_i^3 \gamma_{ij} a_j = \frac{1}{336} - \frac{5734621254479 w^4 10^{-9}}{33950859264} + \mathrm{O}(w^6),$$

$$\sum c_i a_i^2 \gamma_{ij} a_j^2 = \frac{1}{672} - \frac{1359020177543 w^4 10^{-9}}{9700245504} + \mathrm{O}(w^6),$$

$$\sum c_i a_i \gamma_{ij} a_j^3 = \frac{1}{1120} - \frac{15697114153709 w^4 10^{-9}}{135803437056} + \mathrm{O}(w^6),$$

$$\sum c_i \gamma_{ij} a_j^4 = \frac{1}{1680} - \frac{8589323189287 w^4 10^{-9}}{90535624704} + \mathrm{O}(w^6),$$

$$\sum c_i \gamma_{ij} \gamma\, jk a_k^2 = \frac{1}{20160} - \frac{4117366482839 w^4 10^{-9}}{837454528512} + \mathrm{O}(w^6),$$

$$\sum c_i a_i \gamma_{ij} \gamma\, jk a_k = \frac{1}{6720} - \frac{6027300838841 w^4 10^{-9}}{418727264256} + \mathrm{O}(w^6),$$

$$\sum c_i \gamma_{ij} a_j \gamma\, jk a_k = \frac{1}{10080} - \frac{1676868283693 w^4 10^{-9}}{139575754752} + \mathrm{O}(w^6),$$

$$\sum c_i (\gamma_{ij} a_j)^2 = \frac{1}{2016} - \frac{5734621254479 w^4 10^{-9}}{101852577792} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i a_i^4 \gamma_{ij} a_j = \frac{1}{48} + \frac{1868919506911447 w^4 10^{-9}}{2138904133632} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i a_i^2 \gamma_{ij} a_j^3 = \frac{1}{160} + \frac{1483479806729491 w^4 10^{-9}}{1222230933504} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i \gamma_{ij} a_j^5 = \frac{1}{336} + \frac{44484093129033277 w^4 10^{-9}}{34222466138112} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i a_i^2 \gamma_{ij} \gamma_{jk} a_k = \frac{1}{960} + \frac{814805800853509 w^4 10^{-9}}{3768545378304} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i \gamma_{ij} a_j^2 \gamma_{jk} a_k = \frac{1}{2016} + \frac{326649063550871 w^4 10^{-9}}{1425936089088} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i \gamma_{ij} \gamma_{jk} \gamma\, kr a_r = \frac{1}{40320} + \frac{8977379092005611457 w^4 10^{-9}}{6796865536310771712} + \mathrm{O}(w^6),$$

$$\sum \dot{c}_i a_i (\gamma_{ij} a_j)^2 = \frac{1}{288} + \frac{1868919506911447 w^4 10^{-9}}{6416712400896} + \mathrm{O}(w^6).$$

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