J Math Chem (2012) 50:1736–1746
DOI 10.1007/s10910-012-0003-0

ORIGINAL PAPER

Phase fitted symplectic partitioned Runge–Kutta methods for the numerical integration of the Schrödinger equation

Th. Monovasilis

Received: 4 January 2012 / Accepted: 24 March 2012 / Published online: 5 April 2012

Abstract In this work we consider explicit symplectic partitioned Runge–Kutta methods with five stages for problems with separable Hamiltonian. We construct three new methods, one with constant coefficients of eight phase-lag order and two phase-fitted methods.

Keywords Partitioned Runge Kutta methods · Symplectic methods · Schrödinger equation · Phase-lag · Phase-fitted

1 Introduction

In the last decade there has been a lot of research on the construction of numerical methods specially designed for the integration of problems with oscillatory or periodic solution. ([2,5–7,10,11,14,13,16–23]). Also a lot of research has been performed in the area of numerical integration of Hamiltonian systems. Hamiltonian systems appear in many areas of mechanics, physics, chemistry, and elsewhere.

Symplecticity is a characteristic property of Hamiltonian systems and many authors developed and applied symplectic schemes for the numerical integration of such systems. Many authors constructed symplectic numerical methods based on the theory of Runge–Kutta methods these are symplectic Runge–Kutta (SRK) methods, symplectic Runge–Kutta–Nyström (SRKN) methods and symplectic partitioned Runge–Kutta (SRRK) methods. The theory of these methods can be found in the books of Hairer et al. [4] and Sanz-Serna and Calvo [15].

Th. Monovasilis (✉)
Department of International Trade, Technological Educational Institution of Western Macedonia at Kastoria, P.O. Box. 30, 52100 Kastoria, Greece
e-mail: monoba@kastoria.teikoz.gr

Additionally the solution of Hamiltonian systems often has an oscillatory behavior and have been solved in the literature with methods which take into account the nature of the problem. There are two categories of such methods with coefficients depending on the problem and with constant coefficients. For the first category a good estimate of the period or of the dominant frequency is needed, such methods are exponetially and trigonometrically fitted methods, phase-fitted and amplification fitted methods. In the second category are methods with minimum phase-lag, P-stable methods and are suitable for every oscillatory problem. The phase-lag (or dispersion) property was introduced by Brusa and Nigro [3] and was extended to RK(N) methods by van der Houwen and Sommeijer [24]. The idea of phase-fitting was introduced by Rapris and Simos [12].

In this work we consider SPRK methods with five stages and we present three new methods. A method with constant coefficients, third algebraic order and eight phase-lag order. Two phase fitted methods one of third algebraic order and a modified method based on the fourth algebraic order SPRK method of [8]. In Sect. 2 we present the basic theory of SPRK methods and phase-lag analysis. In Sect. 3 the new methods are developed. Section 4 presents numerical evidence and conclusions are given in Sect. 5.

2 General theory

2.1 Symplectic partitioned Runge–Kutta methods

We shall consider Hamiltonian systems with separable Hamiltonian

$$H(p,q,x) = T(p,x) + V(q,x)$$

where T is the kinetic energy and V is the potential energy. Then the Hamiltonian system can be written as:

$$p' = f(q,x), \quad q' = g(p,x) \tag{1}$$

where

$$f(q,x) = -\frac{\partial H}{\partial q}(p,q,x) \;=\; -\frac{\partial V}{\partial q}(q,x),$$
$$g(p,x) = \frac{\partial H}{\partial p}(p,q,x) \;=\; \frac{\partial T}{\partial p}(p,x)$$

Partitioned Runge Kutta methods are appropriate methods for the numerical integration of Hamiltonian systems with separable Hamiltoniann.

A partitioned Runge–Kutta (PRK) scheme is specified by two tableaux

$$\begin{array}{c|c} C & a \\ \hline & c \end{array} \qquad \begin{array}{c|c} D & A \\ \hline & d \end{array}$$

where a, A are $s \times s$ matrices and c, d, C, D are s size vectors. Let $e = (1, 1, \ldots, 1)$ then $C = a.e$ and $D = A.e$. The first tableau is used for the integration of p

components and the second tableau is used for the integration of the q components as follows:

$$P_i = p^n + h \sum_{j=1}^{s} a_{ij} f(Q_j, x + C_j h),$$

$$Q_i = q^n + h \sum_{j=1}^{s} A_{ij} g(P_j, x + c_j h), \tag{2}$$

$i = 1, 2, \ldots, s$, and

$$p^{n+1} = p^n + h \sum_{j=1}^{s} c_i f(Q_i, x + C_i h),$$

$$q^{n+1} = q^n + h \sum_{j=1}^{s} d_i g(P_i, x + c_i h).$$

The above method is symplectic if the coefficients satisfy

$$c_i A_{ij} + d_j a_{ji} - c_i d_j = 0, \quad i, j = 1, 2, \ldots, s. \tag{3}$$

The advantage of using SPRK is that there exist explicit SPRK methods, while SRK methods can not be explicit. Assume the following explicit form $a_{ij} = 0$ for $i < j$ and $A_{ij} = 0$ for $i \leq j$. Then due to the symplecticness requirement (3) the coefficients a_{ij} and A_{ij} are fully determined in terms of the coefficients c_i and d_i.

$$a_{ij} = c_j, \quad A_{ij} = d_j, \quad i = 1, 2, \ldots, s. \tag{4}$$

The SPRK method can be denoted by

$$[c_1, c_2, \ldots, c_s](d_1, d_2, \ldots, d_s)$$

Abia and Sanz-Serna [1] considered symplectic PRK methods and gave the order conditions. The order conditions for SPRK methods up to order 3 are the following.

first order

$$c.e = 1, \quad d.e = 1,$$

second order

$$c.A.e = \frac{1}{2},$$

third order

$$c.A.a.e = \frac{1}{6}, \quad d.a.A.e = \frac{1}{6},$$

fourth order

$$c.A.a.A.e = \frac{1}{24}, \quad d.a.A.a.e = \frac{1}{12}, \quad c.A.((a.e)(a.e)) = \frac{1}{12}.$$

2.2 Phase-lag analysis

Phase-lag analysis of numerical methods for second order equations is based on the scalar test equation $q'' = -w^2 q$, where w is a real constant. For the numerical solution of this equation we can write

$$\begin{pmatrix} q_n \\ h\ p_n \end{pmatrix} = M_n \begin{pmatrix} q_0 \\ h\ p_0 \end{pmatrix}, \quad M = \begin{pmatrix} A_s(v^2) & B_s(v^2) \\ C_s(v^2) & D_s(v^2) \end{pmatrix}, \quad v = wh$$

The eigenvalues of the M are called amplification factors of the method and are the roots of the characteristic equation

$$\xi^2 - tr(M(v^2))\xi + \det(M(v^2)) = 0$$

The phase-lag (dispersion) of the method is

$$\phi(v) = v - \arccos\left(\frac{tr(M(v^2))}{2\sqrt{\det(M(v^2))}}\right),$$

and the dissipation (amplification error) is

$$\alpha(v) = 1 - \sqrt{\det(M(v^2))}.$$

A PRK method is said to have phase-lag order q and dissipation order r if

$$\phi(v) = O(^{q+1}) \quad \text{and} \quad \alpha(v) = O(v^{r+1})$$

The method is called zero-dissipative if $\alpha(v) = 0$. For a symplectic PRK method the determinant of the amplification matrix is zero, so the methods we construct here are zero dissipative. Then the phase-lag of the method is

$$\phi(v) = v - \arccos\left(\frac{tr(M(v^2))}{2}\right),$$

The trace $tr(M(v^2))$ is a polynomial of order $2s$ where s is the number of stages of the PRK method.

A phase-fitted method is a method with phase-lag order infinity. Then the coefficients of the method satisfy $\phi(v) = 0$ and depend on the frequency v.

3 Construction of the new methods

We shall construct methods with five stages then the trace is a polynomial of degree ten.

$$tr(M(v^2)) = 2 - pl_2 v^2 + pl_4 v^4 - pl_6 v^6 + pl_8 v^8 - pl_{10} v^{10}$$

where

$$pl_2 = (c_1 + c_2 + c_3 + c_4 + c_5)(d_1 + d_2 + d_3 + d_4 + d_5),$$

$$
\begin{aligned}
pl_4 = {} & c_1c_2d_1d_2 + c_2c_3d_1d_2 + c_2c_4d_1d_2 + c_2c_5d_1d_2 + c_1c_2d_1d_3 \\
& + c_1c_3d_1d_3 + c_2c_4d_1d_3 + c_3c_4d_1d_3 \\
& + c_2c_5d_1d_3 + c_3c_5d_1d_3 + c_1c_3d_2d_3 + c_2c_3d_2d_3 + c_3c_4d_2d_3 \\
& + c_3c_5d_2d_3 + c_1c_2d_1d_4 + c_1c_3d_1d_4 \\
& + c_1c_4d_1d_4 + c_2c_5d_1d_4 + c_3c_5d_1d_4 + c_4c_5d_1d_4 + c_1c_3d_2d_4 \\
& + c_2c_3d_2d_4 + c_1c_4d_2d_4 + c_2c_4d_2d_4 \\
& + c_3c_5d_2d_4 + c_4c_5d_2d_4 + c_1c_4d_3d_4 + c_2c_4d_3d_4 + c_3c_4d_3d_4 \\
& + c_4c_5d_3d_4 + c_1c_2d_1d_5 + c_1c_3d_1d_5 \\
& + c_1c_4d_1d_5 + c_1c_5d_1d_5 + c_1c_3d_2d_5 + c_2c_3d_2d_5 + c_1c_4d_2d_5 \\
& + c_2c_4d_2d_5 + c_1c_5d_2d_5 + c_2c_5d_2d_5 \\
& + c_1c_4d_3d_5 + c_2c_4d_3d_5 + c_3c_4d_3d_5 + c_1c_5d_3d_5 + c_2c_5d_3d_5 \\
& + c_3c_5d_3d_5 + c_1c_5d_4d_5 + c_2c_5d_4d_5 \\
& + c_3c_5d_4d_5 + c_4c_5d_4d_5, \\
pl_6 = {} & c_1c_2c_3d_1d_2d_3 + c_2c_3c_4d_1d_2d_3 + c_2c_3c_5d_1d_2d_3 + c_1c_2c_3d_1d_2d_4 \\
& + c_1c_2c_4d_1d_2d_4 + c_2c_3c_5d_1d_2d_4 \\
& + c_2c_4c_5d_1d_2d_4 + c_1c_2c_4d_1d_3d_4 + c_1c_3c_4d_1d_3d_4 + c_2c_4c_5d_1d_3d_4 \\
& + c_3c_4c_5d_1d_3d_4 + c_1c_3c_4d_2d_3d_4 \\
& + c_2c_3c_4d_2d_3d_4 + c_3c_4c_5d_2d_3d_4 + c_1c_2c_3d_1d_2d_5 + c_1c_2c_4d_1d_2d_5 \\
& + c_1c_2c_5d_1d_2d_5 + c_1c_2c_4d_1d_3d_5 \\
& + c_1c_3c_4d_1d_3d_5 + c_1c_2c_5d_1d_3d_5 + c_1c_3c_5d_1d_3d_5 + c_1c_3c_4d_2d_3d_5 \\
& + c_2c_3c_4d_2d_3d_5 + c_1c_3c_5d_2d_3d_5 \\
& + c_2c_3c_5d_2d_3d_5 + c_1c_2c_5d_1d_4d_5 + c_1c_3c_5d_1d_4d_5 + c_1c_4c_5d_1d_4d_5 \\
& + c_1c_3c_5d_2d_4d_5 + c_2c_3c_5d_2d_4d_5 \\
& + c_1c_4c_5d_2d_4d_5 + c_2c_4c_5d_2d_4d_5 + c_1c_4c_5d_3d_4d_5 + c_2c_4c_5d_3d_4d_5 \\
& + c_3c_4c_5d_3d_4d_5 \\
pl_8 = {} & c_1c_2c_3c_4d_1d_2d_3d_4 + c_2c_3c_4c_5d_1d_2d_3d_4 + c_1c_2c_3c_4d_1d_2d_3d_5 \\
& + c_1c_2c_3c_5d_1d_2d_3d_5 + c_1c_2c_3c_5d_1d_2d_4d_5 \\
& + c_1c_2c_4c_5d_1d_2d_4d_5 + c_1c_2c_4c_5d_1d_3d_4d_5 + c_1c_3c_4c_5d_1d_3d_4d_5 \\
& + c_1c_3c_4c_5d_2d_3d_4d_5 + c_2c_3c_4c_5d_2d_3d_4d_5, \\
pl_{10} = {} & c_1c_2c_3c_4c_5d_1d_2d_3d_4d_5
\end{aligned}
$$

We consider three different methods:

Method I A method with constant coefficients third algebraic order and eight phase-lag order.
Method II A modified phase-fitted method of third algebraic order.
Method III A modified phase-fitted method based on a fourth algebraic SPRK method.

3.1 Construction of Method I

To ensure third algebraic order the coefficients of the method must satisfy five order conditions. We take the coefficients c_i

$$c_1 = \frac{1}{2} - z, \quad c_2 = z - \frac{1}{3}, \quad c_3 = \frac{2}{3}, \quad c_4 = c_2, \quad c_5 = c_1$$

then the first order condition for c_i is satisfied. We solve the other four order conditions for the coefficients d_1, d_2, d_3 and d_4.

$$\begin{aligned} d_1 &= \frac{-9z^2 + 3z - p + 3d_5(2z-1)(3z-1)(9z+2)}{24(1-3z)^2 z(3z+1)}, \\ d_2 &= \frac{p - 9z - 9(3z-1)(4(d_5-1)z^2 - d_5) + 3}{8(1-3z)^2(3z+1)}, \\ d_3 &= -\frac{p + 9z + 9(3z-1)(4(d_5-1)z^2 - d_5) - 3}{8(1-3z)^2(3z+1)}, \\ d_4 &= \frac{-9z^2 + 3z + p + 3d_5(z(-54z^2 + 3z + 11) - 2)}{24(1-3z)^2 z(3z+1)} \end{aligned}$$

where

$$p = (1-3z) \times \sqrt{3(z(-72z^2+7) + 6d_5 z(72z^3 - 24z^2 - 8z + 1) + 3d_5^2(144z^4 + 60z^3 - 52z^2 - 15z + 4))}.$$

Since the method has third algebraic order the trace agree with the Taylor series of $2cos(v)$ for terms up to v^4, that is

$$pl_2 = -1, \quad pl_4 = 1/12.$$

In order to increase the phase-lag order we require the following conditions to hold

$$pl_6 = -1/360, \quad pl_8 = 1/20160.$$

We solve these two equations for z and d_5

$$z = 0.7907481189777148, \quad d_5 = 0.7037095181303595.$$

3.2 Construction of Method II

This is a method with variable coefficients. We want the five conditions of third algebraic order to hold together with the phase fitting condition. We let

$$c_1 = c_5 = 0, \quad c_2 = c_4, \quad d_5 = 0$$

and solve for c_2, c_3 and d_i for $i = 1, 2, 3, 4$.

These coefficients are complicated and their Taylor expansions are given here.

$$
\begin{aligned}
c_2 &= 0.5755919111469455 - 0.006552769020205345\, v^2 \\
&\quad - 0.00001830478271674793\, v^4 - 4.055537776210506\, 10^{-6}\, v^6 \\
&\quad + 2.81863169165949\, 10^{-8}\, v^8, \\
c_3 &= -0.151183822293891 + 0.01310553804041069\, v^2 \\
&\quad + 0.00003660956543349587\, v^4 + 8.111075552421013\, 10^{-6}\, v^6 \\
&\quad - 5.637263383318979\, 10^{-8}\, v^8, \\
d_1 &= 0.24041204616533 - 0.003789825915522\, v^2 - 0.000063636842587\, v^4 \\
&\quad - 4.92256296593\, 10^{-6}\, v^6 - 1.96594965267\, 10^{-7}\, v^8, \\
d_2 &= 0.880489976205 + 0.01115335865068\, v^2 + 0.001266315074214\, v^4 \\
&\quad + 0.00009622891235\, v^6 + 8.6293569801\, 10^{-6}\, v^8, \\
d_3 &= -0.1982291828831 - 0.0139201872815\, v^2 - 0.00114290069064\, v^4 \\
&\quad - 0.000098226801417\, v^6 - 8.4354539829\, 10^{-6}\, v^8, \\
d_4 &= 0.07732716051274 + 0.006556654546339\, v^2 - 0.0000597775409872\, v^4 \\
&\quad + 6.92045203331\, 10^{-6}\, v^6 + 2.691968031\, 10^{-9}\, v^8.
\end{aligned}
$$

3.3 Construction of Method III

We modify the fourth order symplectic partitioned Runge–Kutta method of McLachlan [8]. The coefficients of the method are

$$
\begin{aligned}
&c_1 = \frac{1}{2} - z, c_2 = z - \frac{1}{3}, c_3 = \frac{2}{3},\ c_4 = c_2,\ c_5 = c_1, \\
&d_1 = 1, d_2 = -\frac{1}{2}, d_3 = d_2,\ d_4 = d_1,\ d_5 = 0.
\end{aligned}
$$

The first and second order conditions are satisfied as well as two conditions from orders three and four ($d.a.A.e = 1/6$, $d.a.A.a.e = 1/12$). For the remaining three equations we have

$$
c.A.a.e = \frac{13}{36} - 2z^2, \quad c.A.a.A.e = \frac{5}{36} - z^2, \quad c.A.((a.e)(a.e)) = \frac{13}{72} - z^2.
$$

McLachlan used

$$
z = \frac{1}{3}\sqrt{\frac{7}{8}}
$$

to achieve fourth order. Here we obtain z from the phase fitting equation

$$
z = \frac{(-36 + 24\, v^2 + 7\, v^4)\, v^4 \ + \ a_1^{-1/3} a_3\, v^8 + a_1^{-1/3}}{18\, (6 + v^2)\, v^6}
$$

where

$$a_1 = (a_2 + \cos(v)(-629856 - 209952\,v^2 - 17496\,v^4))\,v^{12} + \sqrt{a_4},$$
$$a_4 = (-a_3^3 + (a_2 - 17496 * (6 + v^2)^2\,\cos(v))^2)\,v^{24},$$
$$a_2 = 583200 - 11664\,v^2 - 23328\,v^4 - 3996\,v^6 - 162\,v^8 + 18\,v^{10} + v^{12},$$
$$a_3 = 1296 - 1728\,v^2 - 144\,v^4 + 12\,v^6 + v^8.$$

For the order conditions that are not satisfied we have

$$c.A.a.e = \frac{1}{6} + O(v^2), \quad c.A.a.A.e = \frac{1}{24} + O(v^2),$$
$$c.A.((a.e)(a.e)) = \frac{1}{12} + O(v^2).$$

4 Numerical results

We shall use our new methods for the computation of the eigenvalues of the one-dimensional time-independent Schrödinger equation. The Schrödinger equation may be written in the form

$$-\frac{1}{2}\psi'' + V(x)\psi = E\psi \tag{5}$$

where E is the energy eigenvalue, $V(x)$ the potential, and $y(x)$ the wave function.

We present numerical results obtained by the three new methods (Meth1, Meth2, Meth3), as well as several SPRK methods the third order three stage method of Ruth, fourth order methods with 4–7 stages, the sixth order ten stage method of Yoshida and the well known fourth order Numerov method (Num). The coefficients of all methods can be found in [9].

We consider two potentials the harmonic oscillator potential and the doubly anharmonic oscillator.

4.1 The harmonic oscillator

The potential is

$$V(x) = \frac{1}{2}kx^2$$

with boundary conditions $\psi(-R) = \psi(R) = 0$. We consider $k = 1$.

The exact eigenvalues are given by

$$E_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \ldots$$

In Table 1 we give the absolute error ($\times 10^{-6}$) of the eigenvalues of the harmonic oscillator with step size $h = 0.05$.

Table 1 Absolute error ($\times 10^{-6}$) of the eigenvalues of the harmonic oscillator ($h = 0.05$)

	R	Meth1	Meth2	Meth3	Y4	Ruth	Num	4,5	4,6	4,7
E_0	5	0	0	0	0	0	0	0	0	0
E_5	6	0	0	0	174	2	6	0	0	0
E_{10}	7	2	0	0	1,209	13	71	0	0	5
E_{30}	10	4	2	1	–	294	930	20	18	6
E_{50}	12	6	3	2	–	–	–	94	84	27
E_{100}	16	9	6	5	–	–	–	745	691	213
E_{150}	19	166	8	7	–	–	–	–	2,425	716
E_{200}	22	795	9	10	–	–	–	–	–	1,697
E_{300}	26	–	34	16	–	–	–	–	–	–
E_{400}	30	–	375	20	–	–	–	–	–	–
E_{500}	33	–	–	27	–	–	–	–	–	–

Table 2 Absolute error ($\times 10^{-6}$) of the eigenvalues of the doubly anharmonic oscillator with step size $h = 1/40$ ($R = 3$)

	Meth1	Meth2	Meth3	Y4	Y6	Num	4,5	4,6	4,7
0.807447	0	0	0	0	0	0	0	0	0
5.553677	1	1	1	19	0	1	1	0	0
12.534335	3	0	1	235	0	8	1	0	0
21.118364	7	1	2	1,141	7	37	1	1	0
31.030942	14	2	5	3,665	40	118	2	3	1
42.104446	24	4	9	–	144	295	2	8	1
54.222484	35	5	12	–	410	630	4	14	2
67.29805	51	8	18	–	1,004	1,207	10	26	7
81.262879	71	12	25	–	2,191	–	24	46	12
96.061534	94	15	32	–	–	–	48	74	21
111.647831	121	19	42	–	–	–	84	115	33
127.982510	152	24	53	–	–	–	138	173	51
145.031661	184	27	63	–	–	–	216	248	78
162.765612	213	36	64	–	–	–	328	340	121
181.158105	448	43	77	–	–	–	523	413	223
200.185694	621	51	111	–	–	–	980	300	560
219.827273	838	60	131	–	–	–	2,388	673	1,815

4.2 The doubly anharmonic oscillator

The potential is

$$V(x) = \frac{1}{2}x^2 + \lambda_1 x^4 + \lambda_2 x^6$$

we take $\lambda_1 = \lambda_2 = 1/2$ The integration interval is $[-R, R]$.

In Table 2 we give the absolute error ($\times 10^{-6}$) of the eigenvalues of the doubly anharmonic oscillator with step size $h = 1/40$.

5 Conclusions

In this work three new SPRK methods were constructed and their efficiency has been tested on the computation of the eigenvalues of the Schrödinger equation. For both potentials used the new methods have superior performance when compared with other SPRK methods even with the seven stages fourth order method. The phase fitted methods give more accurate results than the minimum phase-lag method.

References

1. L. Abia, J.M. Sanz-Serna, Partitioned Runge–Kutta methods for separable Hamiltonian problems. Math. Comput. **60**, 617–634 (1993)
2. Z.A. Anastassi, T.E. Simos, An optimized Runge–Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**, 1–9 (2005)
3. L. Brusa, L. Nigro, A one-step method for direct integration of structural dynamic equations. Int. J. Numer. Methods Eng. **14**, 685–699 (1980)
4. E. Hairer, Ch. Lubich, G. Wanner, *Geometric Numerical Integration* (Springer, Berlin, 2002)
5. Z. Kalogiratou, Th. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**, 83–92 (2003)
6. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**, 75–82 (2003)
7. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**, 93–106 (2003)
8. R.I. McLachlan, On the numerical integration of ordinary differential equations by symmetric composition methods. SIAM J. Sci. Comput. **16**, 151–168 (1995)
9. Th. Monovasilis, T.E. Simos, Symplectic methods for the numerical of the Schrödinger equation. Comput. Mater. Sci. **38**, 526–532 (2007)
10. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**, 135–144 (2003)
11. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**, 137–147 (2005)
12. A.D. Raptis, T.E. Simos, A four step phase-fitted method for the numerical integration of second order initial-value problems. BIT **31**, 160–168 (1991)
13. T.E. Simos, A fourth algebraic order exponentially-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. IMA J. Numer. Anal. **21**(4), 919–931 (2001)
14. D. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. J. Comput. Appl. Math. **175**, 161–172 (2005)
15. J.M. Sanz-Serna, M.P. Calvo, *Numerical Hamiltonian Problem* (Chapman and Hall, London, 1994)
16. T.E. Simos, Exponentially-fitted Runge–Kutta–Nystrom method for the numerical solution of initial-value problems with oscillating solutions. Appl. Math. Lett. **15**(2), 217–225 (2002)
17. T.E. Simos, I.T. Famelis, Ch. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions. Numer. Algorithms **34**, 27–40 (2003)
18. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. Appl. Math. Lett. **17**(5), 601–607 (2004)
19. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems. Appl. Math. Lett. **22**(10), 1616–1621 (2009)
20. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. Applicandae Mathematicae **110**(3), 1331–1352 (2010)
21. S. Stavroyiannis, T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs. Appl. Numer. Math. **59**(10), 2467–2474 (2009)

22. Ch. Tsitouras, T.E. Simos, Optimized Runge–Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
23. K. Tselios, T.E. Simos, Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**, 173–181 (2005)
24. P.J. Van Der Houwen, B.P. Sommeijer, Explicit Runge–Kutta (-Nyström) methods with reduced phase errors for computing oscillating solutions. SIAM J. Numer. Anal. **24**, 595–617 (1987)