



New modified Runge–Kutta–Nyström methods for the numerical integration of the Schrödinger equation

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ABSTRACT

In this work we construct new Runge–Kutta–Nyström methods especially designed to integrate exactly the test equation $y'' = -w^2y$. We modify two existing methods: the Runge–Kutta–Nyström methods of fifth and sixth order. We apply the new methods to the computation of the eigenvalues of the Schrödinger equation with different potentials such as the harmonic oscillator, the doubly anharmonic oscillator and the exponential potential.

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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 when the frequency is known in advance. Such methods include exponentially/trigonometrically fitted methods, phase fitted methods and amplification fitted methods.

We consider systems of second-order ODEs of the form

$$y''(x) = f(x, y(x)), \quad x \in [x_0, X], \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad (1)$$

with periodic or oscillating solution. Such problems arise in different fields such as celestial mechanics, astrophysics and molecular dynamics.

Many categories of numerical methods have been developed for the numerical solution of the special problem (1) among them are the well known Runge–Kutta–Nyström (RKN) methods.

Exponentially fitted RKN methods have been studied by Simos [1], Van de Vyver [2], Franco [3], Kalogiratou and Simos [4].

Here we construct new trigonometrically fitted RKN methods following the approach introduced by Simos [5] for Runge–Kutta methods. These methods integrate exactly the test equation $y'' = -w^2y$.

In Section 2 we give the necessary conditions for such methods. In Sections 3 and 4 we modify two existing RKN methods of fifth and sixth order and derive four new methods. Numerical results are presented in Section 5 where we apply the new methods as well as the classical methods for the computation of the eigenvalues of the Schrödinger equation with different potentials such as the harmonic oscillator, the doubly anharmonic oscillator and the exponential potential.

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2. Trigonometrically fitted RKN methods

A RKN method is defined by

$$\begin{aligned} y_{n+1} &= y_n + hy'_n + h^2 \sum_{i=1}^s b_i f_i, \\ y'_{n+1} &= y'_n + h \sum_{i=1}^s b'_i f_i, \end{aligned} \quad (2)$$

where

$$f_i = f \left(x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f_j \right)$$

with the following associated Butcher tableau:

c_1				
c_2	a_{21}			
c_3	a_{31}	a_{32}		
\vdots	\vdots	\vdots		
c_s	a_{s1}	a_{s2}	\cdots	$a_{s,s-1}$
	b_1	b_2	\cdots	b_{s-1}
	b'_1	b'_2	\cdots	b'_{s-1}
				b'_s

or in matrix form

$$\begin{array}{c|c} c & A \\ \hline & b \\ \hline & b' \end{array}$$

where A is $s \times s$ matrix c , b , b' and e are s size vectors, with $e = (1, 1, \dots, 1)$.

We define the operators $L(x)$ and $Lp(x)$ as follows:

$$L(x) = y(x+h) - y(x) - hy'(x) - h^2 \sum_{i=1}^s b_i Y''_i(x), \quad (3)$$

$$Lp(x) = y'(x+h) - y'(x) - h \sum_{i=1}^s b'_i Y''_i(x), \quad (4)$$

where

$$Y_i(x) = y(x) + c_i h y'(x) + h^2 \sum_{j=1}^{i-1} a_{ij} Y''_j(x), \quad i = 1, 2, \dots, s.$$

The following definitions of quadrature order and exponential order can be found in [6].

Definition 1. The method has exponential order p if the associated operator L vanishes for any linear combination of the functions

$$\exp(w_0 x), \exp(w_1 x), \dots, \exp(w_p x),$$

where w_i are real or complex numbers.

The following remark is due to Lyche [7].

Remark. If $w_i = w$ for $i = 0, 1, \dots, n$, $n \leq p$, then the operator vanishes for any linear combination of

$$\exp(wx), x \exp(wx), x^2 \exp(wx), \dots, x^n \exp(wx), \exp(w_{n+1} x), \dots, \exp(w_p x).$$

Conditions for the modified RKN methods are given in the following theorem.

Theorem 1. Method (2) is of exponential order p if the following conditions are satisfied:

$$\begin{aligned}\cos v - 1 &= -v^2 \sum_{k=0}^{s-1} (-1)^k (b.A^k.e) v^{2k}, \\ \frac{\sin v}{v} - 1 &= -v^2 \sum_{k=0}^{s-2} (-1)^k (b.A^k.C.e) v^{2k}, \\ \cos v - 1 &= -v^2 \sum_{k=0}^{s-2} (-1)^k (b'.A^k.C.e) v^{2k}, \\ \frac{\sin v}{v} &= \sum_{k=0}^{s-1} (-1)^i (b'.A^i.e) v^{2k}\end{aligned}\tag{5}$$

where $v = w_i h$ for $i = 0, 1, \dots, p$.

Remark. If $w_q = w_r = w$ for $q, r \in 0, 1, \dots, p$ then the following additional conditions are required:

$$\begin{aligned}\cos v - 1 &= -v^2 \sum_{k=0}^{s-2} (-1)^k (2k+3)(b.A^k.C.e) v^{2k}, \\ \frac{\sin v}{v} &= \sum_{k=0}^{s-1} (-1)^k (2k+2)(b.A^k.e) v^{2k}, \\ \cos v - 1 - v \sin v &= -v^2 \sum_{k=0}^{s-2} (-1)^k (2k+3)(b'.A^k.C.e) v^{2k}, \\ \cos v + \frac{\sin v}{v} &= \sum_{k=0}^{s-1} (-1)^i (2k+2)(b'.A^i.e) v^{2k}.\end{aligned}\tag{6}$$

On the basis of the above result we construct four specific methods: two methods based on the fifth-order method [8] and two methods based on the sixth-order method [9] developed by Dormand et al.

3. Methods based on the RKN method of fifth algebraic order

We shall consider the following fifth-order method with four stages (Hairer [8], p. 285)

$$c_2 = \frac{1}{5}, \quad c_3 = \frac{2}{3}, \quad c_4 = 1, \quad a_{31} = -\frac{1}{27}, \quad a_{41} = \frac{3}{10}, \quad a_{42} = -\frac{2}{35}.$$

We shall construct two methods with first and second exponential order.

3.1. The first trigonometrically fitted method

The conditions of first exponential order are

$$\begin{aligned}\cos v - 1 &= -(b.e)v^2 + (b.A.e)v^4 - (b.A.A.e)v^6 + (b.A.A.A.e)v^8, \\ \frac{\sin v}{v} &= 1 - (b.C.e)v^2 + (b.A.C.e)v^4 - (b.A.A.C.e)v^6, \\ \cos v - 1 &= -(b'.C.e)v^2 + (b'.A.C.e)v^4 - (b'.A.A.C.e)v^6, \\ \frac{\sin v}{v} &= (b'.e) - (b'.A.e)v^2 + (b'.A.A.e)v^4 - (b'.A.A.A.e)v^6,\end{aligned}\tag{7}$$

we also impose the following algebraic order conditions

$$b.e = \frac{1}{2}, \quad b.c.e = \frac{1}{6}, \quad b'.e = 1, \quad b'.c.e = \frac{1}{2}.$$

Then the method integrates exactly the functions

$$\{1, x, x^2, x^3, \cos(wx), \sin(wx)\}.$$

The coefficients b and b' of the method are

$$\begin{aligned} b_1 &= \frac{1}{12v^5} (v(5v^4 - 138v^2 + 420) - 30v(3v^2 - 16)\cos(v) + (-9v^4 + 318v^2 - 900)\sin(v)), \\ b_2 &= \frac{5}{84v^5} (-4v^5 + 291v^3 + 30(6v^2 - 37)\cos(v)v - 1140v + 3(6v^4 - 217v^2 + 750)\sin(v)), \\ b_3 &= \frac{9}{28v^5} (v(v^4 - 22v^2 + 180) - 10v(v^2 - 12)\cos(v) - (v^4 - 42v^2 + 300)\sin(v)), \\ b_4 &= \frac{5}{4v^5} (v(v^2 - 20) - 10v\cos(v) - (v^2 - 30)\sin(v)) \end{aligned}$$

and

$$\begin{aligned} b'_1 &= \frac{-1}{4v^4} (-300 + 96v^2 - 12v^4 + (300 - 106v^2 + 3v^4)\cos(v) + (160 - 30v^2)v\sin(v)), \\ b'_2 &= \frac{5}{28v^4} (-750 + 222v^2 - 22v^4 + (750 - 217v^2 + 6v^4)\cos(v) + (370 - 60v^2)v\sin(v)), \\ b'_3 &= \frac{-9}{28v^4} (-300 + 72v^2 - 6v^4 + (300 - 42v^2 + v^4)\cos(v) + (120 - 10v^2)v\sin(v)), \\ b'_4 &= \frac{-5}{4v^4} (30 - 6v^2 + (-30 + v^2)\cos(v) - 10v\sin(v)). \end{aligned}$$

We shall refer to this method as *New5a*.

3.2. The second trigonometrically fitted method

For second exponential order we require Eq. (7) to be satisfied and the following additional conditions should hold:

$$\begin{aligned} \cos v - 1 &= -3(b.C.e)v^2 + 5(b.A.C.e)v^4 - 7(b.A.A.C.e)v^6, \\ \frac{\sin v}{v} &= 2(b.e) - 4(b.A.e)v^2 + 6(b.A.A.e)v^4 - 8(b.A.A.A.e)v^6, \end{aligned}$$

and

$$\begin{aligned} \cos v - 1 - v\sin v &= -3(b'.C.e)v^2 + 5(b'.A.C.e)v^4 - 7(b'.A.A.C.e)v^6, \\ \frac{\sin v}{v} + \cos v &= 2(b'.e) - 4(b'.A.e)v^2 + 6(b'.A.A.e)v^4 - 8(b'.A.A.A.e)v^6. \end{aligned}$$

Then the method integrates exactly the functions

$$\{1, x, \cos(wx), \sin(wx), x\cos(wx), x\sin(wx)\}.$$

The coefficients of this method are

$$\begin{aligned} b_1 &= \frac{-1}{60v^5} (2100v - 1320v^3 + 34v^5 + (4650v - 2100v^3 + 92v^5 - v^7)\cos(v) \\ &\quad + (-6750 + 4620v^2 - 546v^4 + 11v^6)\sin(v)) \\ b_2 &= \frac{-1}{168v^5} (-11400v + 5520v^3 - 280v^5 + (-22350v + 9135v^3 - 530v^5 + 7v^7)\cos(v) \\ &\quad + (33750 - 20205v^2 + 2610v^4 - 77v^6)\sin(v)) \\ b_3 &= \frac{-9}{28v^5} (180v - 40v^3 + (270v - 56v^3 + v^5)\cos(v) + (-450 + 156v^2 - 11v^4)\sin(v)) \\ b_4 &= \frac{-5}{8v^5} (-40v + (-50v + v^3)\cos(v) + (90 - 11v^2)\sin(v)) \end{aligned}$$

and

$$\begin{aligned} b'_1 &= \frac{-1}{60v^4} (4500 - 2100v^2 + 54v^4 + (-4500 + 3300v^2 - 474v^4 + 10v^6)\cos(v) \\ &\quad + (-3450v + 1680v^3 - 82v^5 + v^7)\sin(v)) \\ b'_2 &= \frac{-1}{168v^4} (-22500 + 9120v^2 - 420v^4 + (22500 - 14670v^2 + 2220v^4 - 70v^6)\cos(v) \\ &\quad + (16800v - 7335v^3 + 460v^5 - 7v^7)\sin(v)) \end{aligned}$$

$$b'_3 = \frac{9}{28v^4} (-300 + 60v^2 + (300 - 120v^2 + 10v^4) \cos(v) + (210v - 46v^3 + v^5) \sin(v))$$

$$b'_4 = \frac{5}{8v^4} (60 + (-60 + 10v^2) \cos(v) + (-40v + v^3) \sin(v)).$$

We shall refer to this method as *New5b*.

4. Methods based on an RKN method of sixth algebraic order

Also we shall consider the sixth order with six stages method developed by Dormand et al. [9]:

$$c_2 = \frac{1}{10}, \quad c_3 = \frac{3}{10}, \quad c_4 = \frac{7}{10}, \quad c_5 = \frac{17}{25}, \quad c_6 = 1, \quad a_{31} = \frac{-1}{2200},$$

$$a_{41} = \frac{637}{6600}, \quad a_{42} = \frac{-7}{110}, \quad a_{51} = \frac{225437}{1968750}, \quad a_{52} = \frac{-30073}{281250}, \quad a_{53} = \frac{65569}{281250},$$

$$a_{61} = \frac{151}{2142}, \quad a_{62} = \frac{5}{116}, \quad a_{63} = \frac{385}{1368}, \quad a_{64} = \frac{55}{168}$$

and we shall construct two methods with first and second exponential order.

4.1. The first trigonometrically fitted method

In this case the conditions of first exponential order are

$$\begin{aligned} \cos v - 1 &= -(b.e)v^2 + (b.A.e)v^4 - (b.A.A.e)v^6 + (b.A.A.A.e)v^8 - (b.A.A.A.A.e)v^{10} + (b.A.A.A.A.A.e)v^{12}, \\ \frac{\sin v}{v} &= 1 - (b.C.e)v^2 + (b.A.C.e)v^4 - (b.A.A.C.e)v^6 + (b.A.A.A.C.e)v^8 - (b.A.A.A.A.C.e)v^{10}, \\ \cos v - 1 &= -(b'.C.e)v^2 + (b'.A.C.e)v^4 - (b'.A.A.C.e)v^6 + (b'.A.A.A.C.e)v^8 - (b'.A.A.A.A.C.e)v^{10}, \\ \frac{\sin v}{v} &= (b'.e) - (b'.A.e)v^2 + (b'.A.A.e)v^4 - (b'.A.A.A.e)v^6 + (b'.A.A.A.A.e)v^8 - (b'.A.A.A.A.A.e)v^{10} \end{aligned} \tag{8}$$

we also impose the following algebraic order conditions

$$\begin{aligned} b.e &= \frac{1}{2}, & b.c.e &= \frac{1}{6}, & b.c.c.e &= \frac{1}{12}, & b'.e &= 1, & b'.c.e &= \frac{1}{2}, \\ b'.c.c.e &= \frac{1}{3}, & b'.c.c.c.e &= \frac{1}{4} \end{aligned}$$

and we set $b_6 = 0$.

Then the method integrates exactly the functions

$$\{1, x, x^2, x^3, x^4, \cos(wx), \sin(wx)\}.$$

The coefficients of the method are

$$\begin{aligned} b_1 &= \frac{1}{6426v^6} (1980000 + 524520v^2 - 10834v^4 + 527v^6 - 40(49500 - 27477v^2 + 680v^4) \cos(v) \\ &\quad - 2v(1306800 - 117237v^2 + 680v^4) \sin(v)), \\ b_2 &= \frac{1}{783v^6} (-495000 - 94530v^2 + 1676v^4 + 29v^6 + 40(12375 - 5928v^2 + 145v^4) \cos(v) \\ &\quad + 2v(289575 - 25068v^2 + 145v^4) \sin(v)), \\ b_3 &= \frac{1}{1026v^6} (495000 + 21330v^2 + 389v^4 + 266v^6 - 20(24750 - 8091v^2 + 190v^4) \cos(v) \\ &\quad - v(430650 - 33171v^2 + 190v^4) \sin(v)), \\ b_4 &= \frac{1}{378v^6} (495000 - 125070v^2 + 4519v^4 + 46v^6 + 20(-24750 + 561v^2 + 10v^4) \cos(v) \\ &\quad + v(-133650 - 759v^2 + 10v^4) \sin(v)), \\ b_5 &= \frac{-15625}{28101v^6} (2640 - 628v^2 + 23v^4 + 20(-132 + 5v^2) \cos(v) + v(-792 + 5v^2) \sin(v)), \\ b_6 &= 0 \end{aligned}$$

$$\begin{aligned}
b'_1 &= (443361600v - 45758124v^3 + 525717v^5 - 6074v^7 \\
&\quad + (-383961600v + 41729004v^3 + 75615v^5 - 2000v^7) \cos(v) \\
&\quad + 20(-2970000 - 9892584v^2 + 188385v^4 + 2000v^6) \sin(v)) / 1071/p, \\
b'_2 &= 5(v(-165369600 + 17019864v^2 - 199782v^4 + 2687v^6) \\
&\quad + 2v(70804800 - 7661772v^2 - 19155v^4 + 400v^6) \cos(v) \\
&\quad - 40(-594000 - 1826712v^2 + 33645v^4 + 400v^6) \sin(v)) / 1044/p \\
b'_3 &= -5(v(-131155200 + 13353048v^2 - 127494v^4 + 839v^6) \\
&\quad + 2v(53697600 - 5707404v^2 - 30675v^4 + 400v^6) \cos(v) \\
&\quad - 40(-594000 - 1392984v^2 + 22125v^4 + 400v^6) \sin(v)) / 1368/p \\
b'_4 &= -5(74131200v - 8647848v^3 + 176634v^5 - 2329v^7 \\
&\quad + 2v(-48945600 + 6018804v^2 - 99795v^4 + 400v^6) \cos(v) \\
&\quad - 40(-594000 + 1209384v^2 - 46995v^4 + 400v^6) \sin(v)) / 504/p \\
b'_5 &= 3125(v(-7543800 + 947250v^2 - 18447v^4 + 80v^6) \cos(v) - 2v(-2583900 + 312075v^2 - 6741v^4 + 73v^6) \\
&\quad + 20(-118800 + 184950v^2 - 7887v^4 + 80v^6) \sin(v)) / 28101/p \\
b'_6 &= v(59400 - 6366v^2 + 73v^4 + (-59400 + 6786v^2 - 40v^4) \cos(v) \\
&\quad + 40v(-753 + 20v^2) \sin(v)) / p, \\
p &= v^5(-180 + 11v^2).
\end{aligned}$$

We shall refer to this method as *New6a*.

4.2. The second trigonometrically fitted method

For second exponential order we require Eq. (8) to be satisfied and the following additional conditions should hold:

$$\begin{aligned}
\cos v - 1 &= -3(b.C.e)v^2 + 5(b.A.C.e)v^4 - 7(b.A.A.C.e)v^6 + 9(b.A.A.A.C.e)v^8 - 11(b.A.A.A.A.C.e)v^{10}, \\
\frac{\sin v}{v} &= 2(b.e) - 4(b.A.e)v^2 + 6(b.A.A.e)v^4 - 8(b.A.A.A.e)v^6 + 10(b.A.A.A.A.e)v^8 - 12(b.A.A.A.A.A.e)v^{10}, \\
\cos v - 1 - v \sin v &= -3(b'.C.e)v^2 + 5(b'.A.C.e)v^4 - 7(b'.A.A.C.e)v^6 \\
&\quad + 9(b'.A.A.A.C.e)v^8 - 11(b'.A.A.A.A.C.e)v^{10}, \\
\frac{\sin v}{v} + \cos v &= 2(b'.e) - 4(b'.A.e)v^2 + 6(b'.A.A.e)v^4 - 8(b'.A.A.A.e)v^6 \\
&\quad - 10(b'.A.A.A.A.e)v^8 - 12(b'.A.A.A.A.A.e)v^{10}
\end{aligned}$$

we also impose the following algebraic order conditions

$$b.e = \frac{1}{2}, \quad b'.e = 1, \quad b'.c.e = \frac{1}{2}$$

and we set $b_6 = 0$.

Then the method integrates exactly the functions

$$\{1, x, \cos(wx), \sin(wx), x \cos(wx), x \sin(wx)\}.$$

The coefficients of this method are

$$\begin{aligned}
b_1 &= \frac{1}{2120580v^6}(8(-163350000 + 14211450v^2 - 3942810v^4 + 101269v^6) \\
&\quad + (1306800000 - 1080723600v^2 + 81675090v^4 - 1312859v^6 + 4760v^8) \cos(v) \\
&\quad - 3v(-540144000 + 124957470v^2 - 4117519v^4 + 33320v^6) \sin(v)) \\
b_2 &= \frac{1}{172260v^6}(217800000 - 28584600v^2 + 5283800v^4 - 101094v^6 \\
&\quad + (-217800000 + 165254100v^2 - 13143410v^4 + 229883v^6 - 870v^8) \cos(v) \\
&\quad + 3v(-81856500 + 19544470v^2 - 687503v^4 + 6090v^6) \sin(v)) \\
b_3 &= \frac{1}{67716v^6}(4(-16335000 + 2920995v^2 - 379962v^4 + 11932v^6) \\
&\quad + (65340000 - 3798330v^2 + 2934261v^4 - 50236v^6 + 190v^8) \cos(v) \\
&\quad - 3v(-19656450 + 4433451v^2 - 151316v^4 + 1330v^6) \sin(v))
\end{aligned}$$

$$\begin{aligned}
b_4 &= \frac{1}{756v^6} (4(-495000 + 54615v^2 + 1256v^4) + (1980000 - 124410v^2 - 3143v^4 + 20v^6) \cos(v) \\
&\quad + (895950v + 2739v^3 - 420v^5) \sin(v)) \\
b_5 &= \frac{-15625}{56202v^6} (-10560 + 1256v^2 + (10560 - 992v^2 + 5v^4) \cos(v) + (5016v - 105v^3) \sin(v)) \\
b_6 &= 0
\end{aligned}$$

and

$$\begin{aligned}
b'_1 &= \frac{-1}{7775460v^6} (6(101721312000 - 5645391840v^2 + 3465000v^4 + 2615773v^6) \\
&\quad + 2(-305163936000 + 54903111120v^2 - 393277500v^4 - 60536619v^6 + 965600v^8) \cos(v) \\
&\quad + v(-381097807200 + 17582902920v^2 + 394914990v^4 - 19141729v^6 + 96560v^8) \sin(v)) \\
b'_2 &= \frac{1}{3789720v^6} (6(93174840000 - 5007736800v^2 - 9830700v^4 + 2827993v^6) \\
&\quad + 2(-279524520000 + 49649252400v^2 - 204444900v^4 - 63736299v^6 + 997600v^8) \cos(v) \\
&\quad + v(-348776604000 + 15281402400v^2 + 445718640v^4 - 19880609v^6 + 99760v^8) \sin(v)) \\
b'_3 &= \frac{-1}{2482920v^6} (6(35218260000 - 1714957200v^2 - 16924050v^4 + 1110569v^6) \\
&\quad + 2(-105654780000 + 18013584600v^2 + 70423650v^4 - 29812167v^6 + 440800v^8) \cos(v) \\
&\quad + v(-131392206000 + 4880145600v^2 + 236061420v^4 - 8941397v^6 + 44080v^8) \sin(v)) \\
b'_4 &= \frac{1}{20790v^6} (3(1143450000 - 85437000v^2 + 1626975v^4 + 8488v^6) \\
&\quad + (-3430350000 + 744133500v^2 - 28049175v^4 + 212616v^6 + 1600v^8) \cos(v) \\
&\quad + v(-2202997500 + 171000000v^2 - 3151605v^4 - 172v^6 + 80v^8) \sin(v)) \\
b'_5 &= \frac{-3125}{618222v^6} (12(2277000 - 184275v^2 + 4244v^4) \\
&\quad + 4(-6831000 + 1551825v^2 - 68067v^4 + 800v^6) \cos(v) \\
&\quad + v(-17658000 + 1520490v^2 - 35219v^4 + 160v^6) \sin(v)) \\
b'_6 &= \frac{1}{11v^6} (-118800 + 6366v^2 + 2(59400 - 10923v^2 + 200v^4) \cos(v) \\
&\quad + v(74880 - 3793v^2 + 20v^4) \sin(v)).
\end{aligned}$$

We shall refer to this method as *New6b*.

5. 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

$$-\frac{1}{2}y'' + V(x)y = Ey, \quad x \in [a, b], \quad y(a) = y(b) = 0 \quad (9)$$

where E is the energy eigenvalue, $V(x)$ the potential, and $y(x)$ the wave function. The problems used are the harmonic oscillator, the doubly anharmonic oscillator and exponential potential. For all problems we use $w = \sqrt{B(x)}$. We compare the numerical results produced by the new trigonometrically fitted methods *New5a*, *New5b*, *New6a* and *New6b* with those obtained from the corresponding classical RKN methods *Meth5* and *Meth6* and the eighth-order RKN method [10] as well as the trigonometrically fitted methods constructed by the authors [7] *Trig5* and *Trig6*. The last two methods are developed using each stage integration of the trigonometric functions.

5.0.1. The harmonic oscillator

The potential of the one-dimensional harmonic oscillator is

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

we consider $k = 1$. The integration interval is $[-R, R]$.

The exact eigenvalues are given by

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

Table 1Absolute error ($\times 10^{-6}$) of the eigenvalues of the harmonic oscillator with step size $h = 0.1$.

	Meth5	Trig5	New5a	New5b	Meth6	Trig6	New6a	New6b	Meth8
E_{10}	8	0	0	0	0	0	0	0	0
E_{50}	4140	4	5	6	46	0	0	1	0
E_{100}	–	12	20	21	768	2	0	5	6
E_{150}	–	12	45	48	–	6	2	9	12
E_{200}	–	27	77	84	–	18	4	15	79
E_{250}	–	99	114	131	–	342	7	20	590
E_{300}	–	–	154	187	–	1173	12	28	2209
E_{350}	–	–	192	248	–	3849	18	34	6126
E_{400}	–	–	223	312	–	2744	26	40	–
E_{450}	–	–	228	368	–	4552	38	48	–
E_{500}	–	–	4472	3795	–	–	381	273	–
E_{550}	–	–	–	–	–	–	719	486	–
E_{600}	–	–	–	–	–	–	461	279	–
E_{650}	–	–	–	–	–	–	1013	680	–
E_{700}	–	–	–	–	–	–	2185	1254	–

Table 2Absolute error ($\times 10^{-6}$) of the eigenvalues of the harmonic oscillator with step size $h = 0.05$.

	Trig5	New5a	New5b	Meth6	Trig6	New6a	New6b	Meth8
E_{400}	5	5	5	7564	0	2	2	25
E_{500}	21	8	8	7564	0	0	5	47
E_{600}	59	11	10	–	1	2	12	50
E_{700}	134	15	16	–	2	0	0	30
E_{800}	268	22	24	–	2	3	0	308
E_{900}	497	24	27	–	9	13	0	983
E_{1000}	857	28	33	–	73	2	8	–

Table 3The absolute error ($\times 10^{-6}$) of the eigenvalues of the doubly anharmonic oscillator with step size $h = 0.1$.

	Meth5	Trig5	New5a	New5b	Meth6	Trig6	New6a	New6b	Meth8
E_4	41	13	4	2	0	0	1	0	0
E_6	294	38	10	7	2	5	1	0	0
E_8	1298	88	10	17	11	6	3	1	0
E_{10}	4306	180	25	36	42	4	7	1	0
E_{12}	–	336	160	68	122	0	15	1	0
E_{14}	–	588	513	110	299	8	29	10	3
E_{16}	–	950	1278	160	657	31	49	29	6
E_{18}	–	1414	1690	269	–	71	80	65	11
E_{20}	–	–	–	248	–	130	122	130	17
E_{22}	–	–	–	255	–	130	177	234	21
E_{24}	–	–	–	209	–	442	246	393	17

In [Table 1](#) we give the absolute error of several eigenvalues up to E_{240} computed with step size $h = 0.1$. The integration interval ranges from $R = 5$ to $R = 24$. Both new methods give very accurate eigenvalues. In [Table 2](#) we proceed with the computation of higher state eigenvalues up to E_{1000} with $h = 0.05$ again for the new methods, especially Trig6, while the classical methods failed. For [Table 2](#) the integration interval ranges from $R = 22$ to $R = 46$.

5.0.2. The doubly anharmonic oscillator

The potential is

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

and we take $\lambda_1 = \lambda_2 = 1/2$. The integration interval is $[-R, R]$. In the following [Tables 3](#) and [4](#) we give the computed eigenvalues up to E_{16} with step $h = 0.1$ and up to E_{34} with step $h = 0.05$. The integration interval is $[-3, 3]$. Performance of all methods considered is similar with that of the harmonic oscillator.

5.0.3. The exponential potential

The exponential potential is

$$V(x) = \exp(x)$$

with boundary conditions $\psi(x_{\min}) = 0$ and $\psi(x_{\max}) = 0$. We have used 50 points in the interval of integration $[0, \pi]$.

Table 4

The absolute error ($\times 10^{-6}$) of the eigenvalues of the exponential potential.

	Meth5	Trig5	New5a	Meth6	Trig6	New6a
E_6	97	22	11	1	5	0
E_8	757	66	31	8	15	0
E_{10}	3817	153	67	41	36	2
E_{12}	–	313	116	164	80	1
E_{14}	–	564	193	511	141	6
E_{16}	–	967	270	1418	254	7
E_{18}	–	1566	352	3512	419	21
E_{20}	–	2447	381	7963	678	38

6. Conclusions

In this work we have produced conditions for modified RKN methods following Simo's approach for first and second exponential order. On the basis of these conditions we constructed four new modified methods based on classical RKN methods of fifth and sixth algebraic order. We have applied the new methods to the computation of the eigenvalues of the Schrödinger equation. The numerical evidence is that our new methods have superior performance in comparison to the corresponding classical RKN methods as well as the eighth-order RKN method. Additionally we note that in these problems the new methods are more accurate than the methods produced by the authors using at each stage integration of the trigonometric functions.

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