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Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation

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The solution of the one-dimensional time-independent Schrödinger equation is considered by exponentially fitted symplectic integrators. The Schrödinger equation is first transformed into a Hamiltonian canonical equation. Numerical results are obtained for the one-dimensional harmonic oscillator and the doubly anharmonic oscillator.

KEY WORDS: eigenvalue problem, Schrödinger equation, symplectic methods, exponentially and trigonometrically fitted

1. Introduction

The time-independent Schrödinger equation is one of the basic equations of quantum mechanics. Its solutions are required in the studies of atomic and molecular structure and spectra, molecular dynamics and quantum chemistry. In the literature many numerical methods have been developed to solve the time-independent Schrödinger equation [1–31]. Symplectic integrators are suitable methods for the numerical solution of the Schrödinger equation, among their properties is the energy preservation, which is an important property in quantum mechanics [32–36]. Also, exponentially fitted methods have been very widely used for the numerical integration of the Schrödinger equation [37]. Simos and Aguiar [38] developed a symplectic integrator with the exponential-fitting property based on the idea of Runge–Kutta–Nyström methods. In this work, we develope

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a symplectic integrator with the exponential-fitting property based on the fourth order symplectic method of Yoshida [35]. Our new method is tested on the computation of the eigenvalues of the one-dimensional harmonic oscillator and the doubly anharmonic eoscillator.

2. The time-independent Schrödinger equation

The one-dimensional time-independent Schrödinger equation may be written in the form

$$-\frac{1}{2}\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} + V(x)\Psi = E\Psi, \tag{1}$$

where E is the energy eigenvalue, $V(x)$ the potential, and $\psi(x)$ the wave function. Equation (1) can be rewritten in the form

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = -B(x)\Psi,$$

where $B(x) = 2(E - V(x))$, or

$$\begin{aligned} \Phi' &= -B(x)\Psi, \\ \Psi' &= \Phi. \end{aligned} \tag{2}$$

3. Numerical methods

3.1. Symplectic numerical schemes

Given an interval $[a, b]$ and a partition with N points

$$x_0 = a, \qquad x_n = x_0 + nh, \quad n = 1, 2, \ldots, N.$$

Yoshida's [35] fourth-order, four stages method is of the form

$$\begin{aligned} p_1 &= b_1\Phi_n - c_1hB\Psi_n, \\ q_1 &= a_1\Psi_n + d_1hp_1, \\ p_2 &= b_2p_1 - c_2hBq_1, \\ q_2 &= a_2q_1 + d_2hp_2, \\ p_3 &= b_3p_2 - c_3hBq_2, \\ q_3 &= a_3q_2 + d_3hp_3, \\ \Phi_{n+1} &= b_4p_3 - c_4hBq_3, \\ \Psi_{n+1} &= a_4q_3 + d_4h\Phi_{n+1}, \end{aligned}$$

where

$$
\begin{aligned}
&b_i = 1, \quad a_i = 1, \quad \text{for} \quad i = 1,2,3,4,\\
&c_1 = 0, \quad c_2 = 2x+1, \quad c_3 = -4x-1, \quad c_4 = c_2,\\
&d_1 = x+\frac{1}{2}, \quad d_2 = -x, \quad d_3 = d_2, \quad d_4 = d_1, \quad x = (2^{\frac{1}{3}} - 2^{-\frac{1}{3}} - 1)/6.
\end{aligned}
$$

We assume that the coefficients c_i, d_i for $i = 1,2,3,4$ are the same as and a_2, a_3, b_2 and b_3 equal to 1. Then we solve the following equations for a_1, a_4, b_1 and b_4.

$$
\begin{aligned}
&e^v - (b_1b_2b_3b_4) - (b_2b_3b_4c_1 + a_1b_3b_4c_2 + a_1a_2b_4c_3 + a_1a_2a_3c_4)v\\
&-(b_1b_3b_4c_2d_1 + a_2b_1b_4c_3d_1 + a_2a_3b_1c_4d_1 + b_1b_2b_4c_3d_2 + a_3b_1b_2c_4d_2\\
&\quad +b_1b_2b_3c_4d_3)v^2\\
&-(b_3b_4c_1c_2d_1 + a_2b_4c_1c_3d_1 + a_2a_3c_1c_4d_1 + b_2b_4c_1c_3d_2 + a_1b_4c_2c_3d_2 +\\
&a_3b_2c_1c_4d_2 + a_1a_3c_2c_4d_2 + b_2b_3c_1c_4d_3 + a_1b_3c_2c_4d_3 + a_1a_2c_3c_4d_3)v^3\\
&-(b_1b_4c_2c_3d_1d_2 + a_3b_1c_2c_4d_1d_2 + b_1b_3c_2c_4d_1d_3 + a_2b_1c_3c_4d_1d_3 + b_1b_2c_3c_4d_2d_3)v^4\\
&-(b_4c_1c_2c_3d_1d_2 + a_3c_1c_2c_4d_1d_2 + b_3c_1c_2c_4d_1d_3 + a_2c_1c_3c_4d_1d_3 +\\
&b_2c_1c_3c_4d_2d_3 + a_1c_2c_3c_4d_2d_3)v^5\\
&-b_1c_2c_3c_4d_1d_2d_3v^6 - c_1c_2c_3c_4d_1d_2d_3v^7 = 0,\\
&e^v - (a_1a_2a_3a_4) - (a_2a_3a_4b_1d_1 + a_3a_4b_1b_2d_2 + a_4b_1b_2b_3d_3 + d_4e^v)v\\
&-(a_2a_3a_4c_1d_1 + a_3a_4b_2c_1d_2 + a_1a_3a_4c_2d_2 + a_4b_2b_3c_1d_3 + a_1a_4b_3c_2d_3\\
&\quad +a_1a_2a_4c_3d_3)v^2\\
&-(a_3a_4b_1c_2d_1d_2 + a_4b_1b_3c_2d_1d_3 + a_2a_4b_1c_3d_1d_3 + a_4b_1b_2c_3d_2d_3)v^3\\
&-(a_3a_4c_1c_2d_1d_2 + a_4b_3c_1c_2d_1d_3 + a_2a_4c_1c_3d_1d_3 + a_4b_2c_1c_3d_2d_3 + a_1a_4c_2c_3d_2d_3)v^4\\
&-a_4b_1c_2c_3d_1d_2d_3v^5 - a_4c_1c_2c_3d_1d_2d_3v^6 = 0,\\
&e^{-v} - (b_1b_2b_3b_4) + (b_2b_3b_4c_1 + a_1b_3b_4c_2 + a_1a_2b_4c_3 + a_1a_2a_3c_4)v\\
&-(b_1b_3b_4c_2d_1 + a_2b_1b_4c_3d_1 + a_2a_3b_1c_4d_1 + b_1b_2b_4c_3d_2 + a_3b_1b_2c_4d_2\\
&\quad +b_1b_2b_3c_4d_3)v^2\\
&+(b_3b_4c_1c_2d_1 + a_2b_4c_1c_3d_1 + a_2a_3c_1c_4d_1 + b_2b_4c_1c_3d_2 + a_1b_4c_2c_3d_2 +\\
&a_3b_2c_1c_4d_2 + a_1a_3c_2c_4d_2 + b_2b_3c_1c_4d_3 + a_1b_3c_2c_4d_3 + a_1a_2c_3c_4d_3)v^3\\
&-(b_1b_4c_2c_3d_1d_2 + a_3b_1c_2c_4d_1d_2 + b_1b_3c_2c_4d_1d_3 + a_2b_1c_3c_4d_1d_3 + b_1b_2c_3c_4d_2d_3)v^4\\
&+(b_4c_1c_2c_3d_1d_2 + a_3c_1c_2c_4d_1d_2 + b_3c_1c_2c_4d_1d_3 +\\
&a_2c_1c_3c_4d_1d_3 + b_2c_1c_3c_4d_2d_3 + a_1c_2c_3c_4d_2d_3)v^5\\
&-b_1c_2c_3c_4d_1d_2d_3v^6 + c_1c_2c_3c_4d_1d_2d_3v^7 = 0,\\
&e^{-v} - (a_1a_2a_3a_4) + (a_2a_3a_4b_1d_1 + a_3a_4b_1b_2d_2 + a_4b_1b_2b_3d_3 + d_4e^{-v})v\\
&-(a_2a_3a_4c_1d_1 + a_3a_4b_2c_1d_2 + a_1a_3a_4c_2d_2 + a_4b_2b_3c_1d_3 + a_1a_4b_3c_2d_3\\
&\quad +a_1a_2a_4c_3d_3)v^2
\end{aligned}
$$

$$+(a_3a_4b_1c_2d_1d_2 + a_4b_1b_3c_2d_1d_3 + a_2a_4b_1c_3d_1d_3 + a_4b_1b_2c_3d_2d_3)v^3$$
$$-(a_3a_4c_1c_2d_1d_2 + a_4b_3c_1c_2d_1d_3 + a_2a_4c_1c_3d_1d_3 + a_4b_2c_1c_3d_2d_3 + a_1a_4c_2c_3d_2d_3)v^4$$
$$+a_4b_1c_2c_3d_1d_2d_3v^5 - a_4c_1c_2c_3d_1d_2d_3v^6 = 0$$

and

$$a_1a_2a_3b_1b_2b_3 = 1,$$

where $v = wh$. We solve the above equations for a_1, a_4, b_1 and b_4. And we find:

$$a_1 = \frac{s_7}{3ve^v(s_3 + e^{2v}s_4)}, \qquad a_4 = \frac{-6v(s_1 + e^{2v}s_2)(s_3 + e^{2v}s_4)}{s_5s_6},$$
$$b_1 = \frac{-2s_6}{v^2e^v(s_1 + e^{2v}s_2)}, \qquad b_4 = \frac{v^2e^{2v}s_5}{4s_7},$$

where

$$\begin{aligned}
s_1 &= 144t_1 + 72(3 + 2\kappa + \lambda)v - 24(4 + 5\kappa + 4\lambda)v^2 - 12(7 + 6\kappa + 5\lambda)v^3 \\
&\quad -6(6 + 5\kappa + 4\lambda)v^4 - (25 + 20\kappa + 16\lambda)v^5, \\
s_2 &= 144t_1 - 72(3 + 2\kappa + \lambda)v - 24(4 + 5\kappa + 4\lambda)v^2 + 12(7 + 6\kappa + 5\lambda)v^3 \\
&\quad -6(6 + 5\kappa + 4\lambda)v^4 + (25 + 20\kappa + 16\lambda)v^5, \\
s_3 &= -3456t_3 - 1728(4+3\kappa+2\lambda)v + 1728(-1+\kappa+\lambda)v^2 \\
&\quad +144(2 + 4\kappa + 5\lambda)v^3 \\
&\quad -144(16+8\kappa+7\lambda)v^4 - 72(18 + 13\kappa + 10\lambda)v^5 + 24(19+17\kappa+13\lambda)v^6 \\
&\quad +6(54 + 44\kappa + 35\lambda)v^7 + 6(30 + 24\kappa + 19\lambda)v^8 + (122 + 97\kappa + 77\lambda)v^9, \\
s_4 &= 3456t_3 - 1728(4+3\kappa+2\lambda)v - 1728(-1+\kappa+\lambda)v^2 + 144(2+4\kappa+5\lambda)v^3 \\
&\quad +144(16+8\kappa+7\lambda)v^4 - 72(18+13\kappa+10\lambda)v^5 - 24(19 + 17\kappa + 13\lambda)v^6 \\
&\quad +6(54 + 44\kappa + 35\lambda)v^7 - 6(30 + 24\kappa + 19\lambda)v^8 + (122 + 97\kappa + 77\lambda)v^9, \\
s_5 &= 41472t_1 - 10368(-2 + 6\kappa + 5\lambda)v^2 + 1728(14 - 2\kappa + \lambda)v^4 \\
&\quad -576(14 + 16\kappa + 11\lambda)v^6 - 48(28 + 26\kappa + 19\lambda)v^8 \\
&\quad +6(218 + 172\kappa + 137\lambda)v^{10} + (208 + 165\kappa + 131\lambda)v^{12}, \\
s_6 &= 36e^{4v}((-12 + t_3v) + 36(12 + t_3v) \\
&\quad +e^{2v}(-864 + 144(-4 + 3\kappa + \lambda)v^2 - 72(3 + \lambda)v^4 \\
&\quad +6(4 + 5\kappa + 3\lambda)v^6 + (11 + 9\kappa + 7\lambda)v^8)), \\
s_7 &= -(72 - 6(-2 + \kappa)v^2 + (7 + 5\kappa + 4\lambda)v^4)s_6
\end{aligned}$$

and

$$t_1 = 4 + \kappa, \qquad t_2 = -44 + 8\kappa + 13\lambda, \qquad t_3 = 4 + 2\kappa + \lambda, \quad \kappa = 2^{\frac{1}{3}}, \quad \lambda = 2^{\frac{2}{3}}.$$

For small values of v, the above formulas are subject to heavy cancelations. In this case, the following Taylor series expansions must be used:

$$a_1 = 1+t_4v^4+\frac{(378+297\kappa+239\lambda)}{1680{t_1}^2}v^6+\frac{(202163+161386\kappa+127460\lambda)}{302400{t_1}^3}v^8+O(v^9)$$
$$a_4 = 1-t_4v^4-\frac{(658+533\kappa+418\lambda)}{2520{t_1}^2}v^6-\frac{(86083+67712\kappa+54025\lambda)}{151200{t_1}^3}v^8+O(v^9)$$
$$b_1 = 1+t_5v^4+\frac{(3340+2672\kappa+2101\lambda)}{5040{t_1}^2}v^6+\frac{(808327+640356\kappa+508982\lambda)}{302400{t_1}^3}v^8+O(v^9)$$
$$b_4 = 1-t_5v^4-\frac{(3158+2497\kappa+1982\lambda)}{5040{t_1}^2}v^6-\frac{(251036+199725\kappa+158272\lambda)}{151200{t_1}^3}v^8+O(v^9),$$

where

$$t_4 = (12+9\kappa+7\lambda)/(120t_1) \quad \text{and} \quad t_5 = (30+23\kappa+19\lambda)/(120t_1)$$

Requiring the modified method to integrate exactly $\cos(wx)$ and $\sin(wx)$ we obtain the following equations

$$\begin{aligned}
&\cos(v)-(b_1b_2b_3b_4)+(b_1b_3b_4c_2d_1+a_2b_1b_4c_3d_1+a_2a_3b_1c_4d_1\\
&+b_1b_2b_4c_3d_2+a_3b_1b_2c_4d_2+b_1b_2b_3c_4d_3)v^2\\
&-(b_1b_4c_2c_3d_1d_2+a_3b_1c_2c_4d_1d_2+b_1b_3c_2c_4d_1d_3+a_2b_1c_3c_4d_1d_3+b_1b_2c_3c_4d_2d_3)v^4\\
&+b_1c_2c_3c_4d_1d_2d_3v^6=0,\\
&\sin(v)-(b_2b_3b_4c_1+a_1b_3b_4c_2+a_1a_2b_4c_3+a_1a_2a_3c_4)v\\
&+(b_3b_4c_1c_2d_1+a_2b_4c_1c_3d_1+a_2a_3c_1c_4d_1+b_2b_4c_1c_3d_2+a_1b_4c_2c_3d_2\\
&+a_3b_2c_1c_4d_2+a_1a_3c_2c_4d_2+b_2b_3c_1c_4d_3+a_1b_3c_2c_4d_3+a_1a_2c_3c_4d_3)v^3\\
&-(b_4c_1c_2c_3d_1d_2+a_3c_1c_2c_4d_1d_2+b_3c_1c_2c_4d_1d_3\\
&+a_2c_1c_3c_4d_1d_3+b_2c_1c_3c_4d_2d_3+a_1c_2c_3c_4d_2d_3)v^5\\
&+c_1c_2c_3c_4d_1d_2d_3v^7=0,\\
&\cos(v)-(a_1a_2a_3a_4)+d_4v\sin(v)\\
&+(a_2a_3a_4c_1d_1+a_3a_4b_2c_1d_2+a_1a_3a_4c_2d_2+a_4b_2b_3c_1d_3+a_1a_4b_3c_2d_3+a_1a_2a_4c_3d_3)v^2\\
&-(a_3a_4c_1c_2d_1d_2+a_4b_3c_1c_2d_1d_3+a_2a_4c_1c_3d_1d_3+a_4b_2c_1c_3d_2d_3+a_1a_4c_2c_3d_2d_3)v^4\\
&\quad+a_4c_1c_2c_3d_1d_2d_3v^6=0,\\
&\quad\sin(v)-(a_2a_3a_4b_1d_1+a_3a_4b_1b_2d_2+a_4b_1b_2b_3d_3+d_4\cos(v))v\\
&\quad+(a_3a_4b_1c_2d_1d_2+a_4b_1b_3c_2d_1d_3+a_2a_4b_1c_3d_1d_3+a_4b_1b_2c_3d_2d_3)v^3\\
&\quad-a_4b_1c_2c_3d_1d_2d_3v^5=0.
\end{aligned}$$

Assuming that

$$a_2=a_3=1 \quad \text{and} \quad b_1=b_2=1$$

and solving the above system we obtain the following coefficients

$$a_1=\frac{-(s_4+s_5)}{6vs_3}, \qquad a_4=\frac{s_6}{s_1}, \qquad b_1=\frac{2s_1s_2}{s_7}, \qquad b_4=\frac{-v^2s_3}{2s_1s_2},$$

where

$$
\begin{aligned}
s_1 = {} & -20736\ (-8+2\kappa+\lambda)+10368\ (-14+12\kappa+3\lambda)\ v^2 \\
& +864s\,(56-32\kappa+11\lambda)\ v^4+3456\ (1+3\kappa+\lambda)\ v^6 \\
& -288\ (3+4\kappa+2\lambda)\ v^8-36\ (27+21\kappa+17\lambda)\ v^{10}+(154+122\kappa+97\lambda)\ v^{12} \\
& +864\ \left(24\ (-8+2\kappa+\lambda)-12\kappa\ (2+\kappa)\ v^2+(4+4\kappa+3\lambda)\ v^4\right)\ \cos(2v)+ \\
& +432\,v\ \left(-24\ (4+\kappa)-4\ (4+5\kappa+4\lambda)\ v^2+(6+5\kappa+4\lambda)\ v^4\right)\ \sin(2v), \\
s_2 = {} & v\ \left(24\ (4+2\kappa+\lambda)-12\,v^2+(18+14\kappa+11\lambda)\ v^4\right)\ \cos(v) \\
& -4\ \left(72+6\ (-2+\kappa)\ v^2+(7+5\kappa+4\lambda)\ v^4\right)\ \sin(v), \\
s_3 = {} & v(995328\,(4+\kappa)^2+497664\,(9+19\kappa+20\lambda)\,v^2+41472\,(116+34\kappa+23\lambda)\,v^4 \\
& +6912\ (77+127\kappa+92\lambda)\ v^6+3456\ (107+71\kappa+60\lambda)\ v^8 \\
& -288\ (1557+1225\kappa+976\lambda)\ v^{10}-72\ (464+370\kappa+293\lambda)\ v^{12} \\
& +12\,(3181+2525\kappa+2004\lambda)\,v^{14}-(3878+3078\kappa+2443\lambda)\ v^{16})\,\cos(v) \\
& +4(2985984\,(-5+\lambda)-248832\,(-22+29\kappa+21\lambda)\,v^2-124416\,(31-8\kappa+2\lambda)\,v^4 \\
& -10368\ (-10+59\kappa+19\lambda)\ v^6-1728\ (94+35\kappa+49\lambda)\ v^8 \\
& +144\ (1162+893\kappa+727\lambda)\ v^{10}+216\ (57+46\kappa+36\lambda)\ v^{12} \\
& -6\ (2354+1869\kappa+1483\lambda)\ v^{14}+(1435+1139\kappa+904\lambda)\ v^{16})\ \sin(v), \\
s_4 = {} & 35831808\,(-12+5\kappa+2\lambda)-2985984\,(-184+154\kappa+17\lambda)\,v^2 \\
& -1492992\,(178-157\kappa+43\lambda)\,v^4+746496\,(34-112\kappa+17\lambda)\,v^6 \\
& -62208\,(170-91\kappa+144\lambda)\,v^8+5184\,(88-170\kappa+139\lambda)\,v^{10} \\
& -864\,(458+275\kappa+333\lambda)\,v^{12}+432\,(1242+978\kappa+787\lambda)\,v^{14} \\
& +72\,(1403+1115\kappa+883\lambda)\,v^{16}-12\,(5837+4633\kappa+3677\lambda)\,v^{18} \\
& +(6956+5521\kappa+4382\lambda)\,v^{20}, \\
s_5 = {} & 864\,(-41472\,(-12+52^{\frac{1}{3}}+2\lambda)+3456\,(-44+50\kappa+7\lambda)\,v^2 \\
& +1728\,(20-13\kappa+5\lambda)\,v^4+576\,(4+11\kappa+4\lambda)\,v^6+24\,(44+25\kappa+26\lambda)\,v^8 \\
& -6\,(256+202\kappa+161\lambda)\,v^{10}+(208+165\kappa+131\lambda)\,v^{12})\ \cos(2v) \\
& +432\,v\,(-41472\,(-5+\lambda)+3456\,(-8+21\kappa+14\lambda)\,v^2+576\,(37-\kappa+7\lambda)\,v^4 \\
& +576\,(9+10\kappa+7\lambda)\,v^6+24\,(55+40\kappa+33\lambda)\,v^8 \\
& -2\,(1036+821\kappa+652\lambda)\,v^{10}+(281+223\kappa+177\lambda)\,v^{12})\ \sin(2v), \\
s_6 = {} & 36\,v\,(8\,v\,(-72\,(3+2\kappa+\lambda)-12\,(7+6\kappa+5\lambda)\,v^2+(25+20\kappa+16\lambda)v^4)\,\cos(2v) \\
& +(576\,(4+\kappa)+24\,(-4+4\kappa+5\lambda)\,v^2-12\,(32+26\kappa+21\lambda)\,v^4 \\
& +(68+54\kappa+43\lambda)\,v^6)\ \sin(2v)), \\
s_7 = {} & 6\,v^2\,(4\,v\,(41472\,(4+\kappa)^2+20736\,(11+16\kappa+15\lambda)\,v^2+s1728\,(58+28\kappa+21\lambda)\,v^4 \\
& +1728\,(28+24\kappa+19\lambda)\,v^6+72\,(144+112\kappa+89\lambda)\,v^8
\end{aligned}
$$

$$-12\,(1399 + 1110\,\kappa + 881\,\lambda)\,v^{10} + (2278 + 1808\,\kappa + 1435\,\lambda)\,v^{12})\,\cos(2\,v)$$
$$+(995328\,(-5+\lambda) - 41472\,(-30 + 31\,\kappa + 22\,\lambda)\,v^2 + 10368\,(-4 + 40\,\kappa + 25\,\lambda)\,v^4$$
$$-1728\,(10 + 35\,\kappa + 23\,\lambda)\,v^6 + 576\,(63 + 55\,\kappa + 43\,\lambda)\,v^8$$
$$+24\,(2650 + 2099\,\kappa + 1666\,\lambda)\,v^{10} - 6\,(4904 + 3892\,\kappa + 3089\,\lambda)\,v^{12}$$
$$+(3078 + 2443\,\kappa + 1939\,\lambda)\,v^{14})\,\sin(2\,v)).$$

The Taylor expansions of the coefficients are

$$\begin{aligned}
a_1 &= 1 + \frac{(-2933 - 61\kappa + 1090\lambda)}{10{t_2}^3}v^4 - \frac{3(33682 - 58903\kappa + 47823\lambda)}{140{t_2}^4}v^6 \\
&\quad + \frac{(49695084 - 98597115\kappa + 36871016\lambda)}{2800{t_2}^5}v^8 + O(v^9), \\
a_4 &= 1 + \frac{(25 + 17\kappa + 13\lambda)}{360(-5+\lambda)}v^4 + \frac{(528 + 478\kappa + 345\lambda)}{5040(-5+\lambda)^2}v^6 \\
&\quad + \frac{(148805 + 101548\kappa + 91106\lambda)}{907200(-5+\lambda)^3}v^8 + O(v^9) \\
b_1 &= 1 - \frac{(78 + 50\kappa + 53\lambda)}{120t_2}v^4 - \frac{(3504 + 3487\kappa + 1750\lambda)}{840{t_2}^2}v^6 \\
&\quad - \frac{(2372351 + 1145366\kappa + 1694892\lambda)}{50400{t_2}^3}v^8 + O(v^9) \\
b_4 &= 1 + \frac{(3055 - 2119\kappa + 1843\lambda)}{10{t_2}^3}v^4 + \frac{(326414 - 16967\kappa - 6010\lambda)}{140{t_2}^4}v^6 \\
&\quad + \frac{(-89982340 + 150753736\kappa - 25461361\lambda)}{4200{t_2}^5}v^8 + O(v^9)
\end{aligned}$$

4. Numerical results

We consider the one-dimesional eigenvalue problem with boundary conditions

$$\Psi(a) = 0, \qquad \Psi(b) = 0.$$

We use the shooting scheme in the implementation of the above methods. The shooting method converts the boundary value problem into an initial value problem where the boundary value at the end point b is tranformed into an initial value $\Psi'(a)$, the results are independent of $\Psi'(a)$ if $\Psi'(a) \neq 0$. The eigenvalue E is a parameter in the computation, the value of E that makes $\Psi(b) = 0$ is the eigenvalue computed.

We have tested our new method (*MethNew*) as well as the fourth and sixth order methods of Yoshida [35] (*Meth4, Meth6*) on two potentials, the harmonic oscillator and doubly anharmonic oscillator.

Table 1
Errors ($\times 10^{-6}$) for the harmonic oscillator.

	Meth4	*Meth6*	*MethNew*	R
E_0	417	416	416	5.5
E_1	467	415	416	
E_2	668	412	415	
E_3	1122	400	415	
E_4	1931	373	414	
E_5	3199	272	414	6.5
E_6	5036	229	414	
E_7	7548	174	414	
E_8	10846	139	414	
E_9	15045	48	414	
E_{10}	20263	894	412	
E_{11}	26606	1489	412	7.5
E_{12}	34209	2264	411	
E_{13}	43190	3259	410	
E_{14}	53679	4510	409	

4.1. *The harmonic oscillator*

The potential of the one dimensional harmonic oscillator is

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

we consider $k = 1$. The exact eigenvalues are given by

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

For the computation of the eigenavlues we used step $h = 0.1$, the interval $[-R, R]$ is given in table 1. Also in table 1, we present the errors of the three methods up to the 14th eigenvalue. For both Yoshida's methods the error increases as we compute higher state eigenvalues, while the new modified fourth order method gives almost constant error. (see figure 1).

4.2. *Doubly anharmonic oscillator*

The exponential potential is

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

with interval of integration $[a, b]$, and boundary conditions $\Psi(a) = 0$ and $\Psi(b) = 0$.

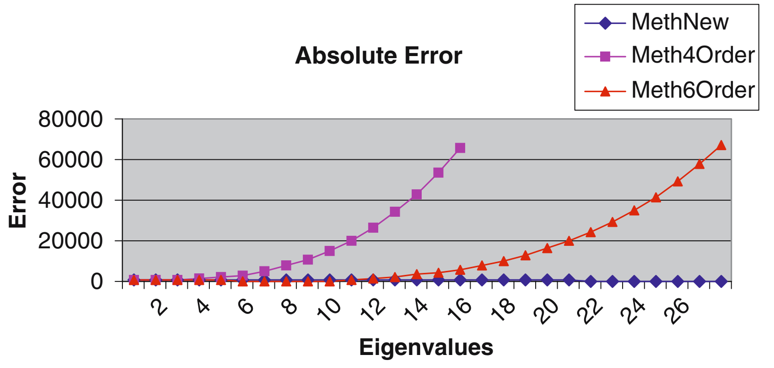

Figure 1. Absolute error ($\times 10^{-6}$) up to 28th eigenvalues for the harmonic oscillator.

Table 2
Errors ($\times 10^{-4}$) for the doubly anharmonic oscillator.

	Exact	*Meth4*	*Meth6*	*MethNew*
E_0	0.8074	2	2	2
E_2	5.5537	5	5	5
E_4	12.5343	12	10	10
E_6	21.1184	25	14	14
E_8	31.0309	55	18	19
E_{10}	42.1044	115	22	23
E_{12}	54.2225	225	22	27
E_{14}	67.2981	413	20	30
E_{16}	81.2629	714	12	35
E_{18}	96.0615	1170	5	40
E_{20}	111.6478	1832	39	44
E_{22}	127.9825	–	98	47
E_{24}	145.0317	–	192	52
E_{26}	162.7656	–	335	55
E_{28}	181.1582	–	547	58
E_{30}	200.1857	–	852	60
E_{32}	219.8273	–	1280	61
E_{34}	240.0637	–	1533	61

In this calculation, we use $b = -a = 4$, $\lambda_1 = \lambda_2 = 1/2$ and step $h = 1/40$. In table 2, we present the even state eigenvalues up to the 34th. The fourth-order method fails to compute even one correct decimal digit from the 16th eigenvalue. The sixth-order method has similar performance with our new modified fourth order method up to the 22nd eigenvalue, but the error increases rapidly from this eigenvalue. While, with our new method the error remains almost constant.

Overall, the new modified fourth-order method is very efficient method with only four stages and is superior to the sixth-order method which is a 10 stages method. In terms of computation time is similar to original fourth-order method.

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