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New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation

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The solution of the one-dimensional time-independent Schrödinger equation is considered by trigonometrically and 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, doubly anharmonic oscillator and the exponential potential.

KEY WORDS: Exponential fitting, trigonometric fitting, symplectic Integrators, Schrödinger equation, Hamiltonian canonical equation

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 or coupled differential equations of the Schrödinger type ([1–12]). Trigonometrically and exponentially fitted methods have been very widely used for the numerical integration of the Schrödinger equation ([13–16]) or related problems ([17]). Recently symplectic methods ([18–20]) have been applied to the numerical solution of the Schrödinger equation ([21]). The use of the symplectic methods for the numerical solution of the Schrödinger equation is based on their property of the energy preservation, which is an important property in quantum mechanics. In this work, we develop symplectic integrators with the trigonometrically and exponentially fitted property. Our new methods are tested on the computation of the eigenvalues of the one-dimensional harmonic oscillator, doubly anharmonic oscillator and the

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exponential potential. We note here that the calculation of the eigenvalues for the Schrödinger equation is an on going reserch problem (see [22] and references therein). In section 2, we present the Schrödinger equation, in section 3, we describe the second-order Yoshida type method of McLachlan [23] and we construct our new trigonometrically and exponentially fitted methods. Finally, in section 4, we give numerical results and conclusions.

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

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

Yoshida type [18] second-order, two stages method can be presented with the form

$$\begin{aligned} p_1 &= b_1\ \phi_n - c_1 h B \psi_n, \\ q_1 &= a_1\ \psi_n + d_1 h p_1, \\ \phi_{n+1} &= b_2\ \ p_1 - c_2 h B q_1, \\ \psi_{n+1} &= a_2\ \ q_1 + d_2 h \phi_{n+1}, \end{aligned}$$

where

$$b_i = a_i = 1 \quad \text{for} \quad i = 1, 2.$$

Yoshida in [18] suggested a second-order method with coefficients

$$c_1 = 0, \quad c_2 = 1, \quad d_1 = \frac{1}{2}, \quad d_2 = \frac{1}{2}, \tag{3}$$

while McLachlan and Atela [23] suggested a second-order method with coefficients

$$c_1 = \frac{2-\sqrt{2}}{2}, \quad c_2 = \frac{\sqrt{2}}{2}, \quad d_1 = \frac{\sqrt{2}}{2}, \quad d_2 = \frac{2-\sqrt{2}}{2}. \tag{4}$$

3.2. *Exponentially fitted methods*

In order a method to be exponentially fitted, we want to integrate exactly the functions $\psi(x) = e^{\pm w x}$. Based on the above requirement, we obtain the following conditions:

$$\begin{aligned} -b_1 b_2 + \mathrm{e}^v - (b_2 c_1 + a_1 c_2) v - b_1 c_2 d_1 v^2 - c_1 c_2 d_1 v^3 &= 0, \\ -a_1 a_2 + \mathrm{e}^v - (a_2 b_1 d_1 + d_2 \mathrm{e}^v) v - a_2 c_1 d_1 v^2 &= 0, \\ b_1 b_2 - e^{-v} - (b_2 c_1 + a_1 c_2) v + b_1 c_2 d_1 v^2 - c_1 c_2 d_1 v^3 &= 0, \\ a_1 a_2 - e^{-v} - (a_2 b_1 d_1 + d_2 e^{-v}) v + a_2 c_1 d_1 v^2 &= 0, \end{aligned} \tag{5}$$

where $v = wh$.

In order to preserve symplecticness we want

$$a_1 a_2 b_1 b_2 = 1.$$

3.2.1. *New exponentially fitted method*

We solve the system of equation (5) using the coefficients c_i and d_i given by (3). The following values for the coefficients a_i and b_i are obtained:

$$\begin{aligned} a_1 &= \frac{-(\mathrm{e}^{-v} - \mathrm{e}^v)}{2\,v}, \\ a_2 &= \frac{-((-2 + \mathrm{e}^{2\,v}\,(-2 + v) - v)\,v)}{2\,(-1 + \mathrm{e}^{2\,v})}, \\ b_1 &= \frac{(-1 + \mathrm{e}^{2\,v})\,(2 + \mathrm{e}^{2\,v}\,(-2 + v) + v)}{\mathrm{e}^v\,(-2 + \mathrm{e}^{2\,v}\,(-2 + v) - v)\,v^2}, \\ b_2 &= \frac{-4\,\mathrm{e}^{2\,v}\,v^2}{(-1 + \mathrm{e}^{2\,v})\,(2 + \mathrm{e}^{2\,v}\,(-2 + v) + v)}. \end{aligned}$$

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

$$
\begin{aligned}
a_1 &= 1 + \frac{v^2}{6} + \frac{v^4}{120} + \frac{v^6}{5040} + \frac{v^8}{362880} + O(v)^{10},\\
a_2 &= 1 - \frac{v^2}{6} - \frac{v^4}{45} + \frac{2\,v^6}{945} - \frac{v^8}{4725} + O(v)^{10},\\
b_1 &= 1 - \frac{v^4}{360} - \frac{v^6}{280} - \frac{281\,v^8}{604800} + O(v)^{10},\\
b_2 &= 1 + \frac{2\,v^4}{45} + \frac{2\,v^6}{315} + \frac{34\,v^8}{14175} + O(v)^{10}.
\end{aligned}
$$

3.2.2. Another new exponentially fitted method

We solve the system of equation (5) using the coefficients c_i and d_i given by (4). The following values for the coefficients a_i and b_i are obtained:

$$
\begin{aligned}
a_1 &= \frac{4T_3(-1+\mathrm{e}^{2v}) + (-2+\sqrt{2})(T_1 - T_2 + \sqrt{z_1+z_2})}{4T_3\sqrt{2}v\mathrm{e}^{v}},\\
a_2 &= \frac{\left(T_1 - T_2 + \sqrt{z_1+z_2}\right)\, T_3\, \left(2 + \left(-2+\sqrt{2}\right)\, v\right)}{\mathrm{e}^{v}\, T_4},
\end{aligned}
$$

$$
\begin{aligned}
b_1 &= \frac{2\,\left(1+\mathrm{e}^{2\,v}\right)\, T_3\, v}{T_1 - T_2 + \sqrt{z_1+z_2}},\\
b_2 &= \frac{T_1 + T_2 + \sqrt{z_1+z_2}}{4\,\mathrm{e}^{v}\, T_3\, v},
\end{aligned}
$$

where

$$
\begin{aligned}
T_1 &= -2\sqrt{2} + 4\sqrt{2}\,\mathrm{e}^{2\,v} - 2\sqrt{2}\,\mathrm{e}^{4\,v} + 2\,v - 2\sqrt{2}\,v - 2\,\mathrm{e}^{4\,v}\,v + 2\sqrt{2}\,\mathrm{e}^{4\,v}\,v,\\
T_2 &= -(\mathrm{e}^{v}\,v^3\,k_1 + \mathrm{e}^{2\,v}\,k_2 v))),\\
z_1 &= 32\sqrt{2}\,\mathrm{e}^{3\,v}\,v^3\,k_1 + \mathrm{e}^{2\,v}\,(2 - 2\sqrt{2} + (-4+3\sqrt{2})v)),\\
z_2 &= (-4\sqrt{2}\,\mathrm{e}^{2\,v} + 2\,\mathrm{e}^{4\,v}\,(\sqrt{2} + v - \sqrt{2}\,v) + \mathrm{e}^{v}\,v^3\,k_1 + 2\,(\sqrt{2} + (-1+\sqrt{2})v)\\
&\quad + \mathrm{e}^{3\,v}\,v^3\,k_2)^2,\\
T_3 &= -2 + 2\sqrt{2} - 4\,v + 3\sqrt{2}\,v + \ \mathrm{e}^{2\,v}\,k_2,\\
T_4 &= 8(1+\mathrm{e}^{2\,v})\,v^2\,(8 - 6\sqrt{2} + (-24+17\sqrt{2})\,v^2 + \mathrm{e}^{2\,v}\,k_3),
\end{aligned}
$$

and

$$
\begin{aligned}
k_1 &= -2 + 2\sqrt{2} - 4\,v + 3\sqrt{2}\,v,\\
k_2 &= 2 - 2\sqrt{2} + (-4+3\sqrt{2})\,v,\\
k_3 &= -8 + 6\sqrt{2} - 4\,(-7+5\sqrt{2})\,v + (-24+17\sqrt{2})\,v^2.
\end{aligned}
$$

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

$$
\begin{aligned}
a_1 &= 1 + 0.0690356v^2 + 0.0109038v^4 - 0.000140361v^6 + 0.0000586133v^8 \\
&\quad + O(v^{10}), \\
a_2 &= 1 - 0.0690356v^2 + 0.001011v^4 - 0.000437959v^6 + O(v^{10}), \\
b_1 &= 1 + 0.0976311v^2 + 0.000255231v^4 + 0.0000621746v^6 + 0.0000321169v^8 \\
&\quad + O(v^{10}), \\
b_2 &= 1 - 0.0976311v^2 + 0.00212773v^4 + 0.00101629v^6 - 0.000132096v^8 + O(v^{10}).
\end{aligned}
$$

3.3. *Trigonometrically fitted method*

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

$$
\begin{aligned}
-b_1 b_2 + b_1 c_2 d_1 v^2 + \cos(v) &= 0, \\
-(b_2 c_1 + a_1 c_2)v + c_1 c_2 d_1 v^3 + \sin(v) &= 0, \\
-a_1 a_2 + a_2 c_1 d_1 v^2 + \cos(v) + d_2 v \sin(v) &= 0, \\
-a_2 b_1 d_1 v - d_2 v \cos(v) + \sin(v) &= 0.
\end{aligned}
\tag{6}
$$

In order to preserve symplecticness we require the following condition:

$$a_1 a_2 b_1 b_2 = 1.$$

3.3.1. *New trigonometrically fitted method*

Using the coefficient c_i and d_i given by (3) and solving the system of equation (6) the following values for the coefficients a_i and b_i are obtained:

$$
\begin{aligned}
a_1 &= \frac{\sin(v)}{v}, \\
a_2 &= \frac{v\,(v + 2\,\cot(v))}{2}, \\
b_1 &= \frac{-2\,(v\,\cos(v) - 2\,\sin(v))\,\sin(v)}{v^2\,(2\,\cos(v) + v\,\sin(v))}, \\
b_2 &= \frac{v^2\,\csc(v)}{-(v\,\cos(v)) + 2\,\sin(v)}.
\end{aligned}
$$

The Taylor expansions of the coefficients are given by:

$$a_1 = 1 - \frac{v^2}{6} + \frac{v^4}{120} - \frac{v^6}{5040} + \frac{v^8}{362880} + O(v)^{10},$$
$$a_2 = 1 + \frac{v^2}{6} - \frac{v^4}{45} - \frac{2\,v^6}{945} - \frac{v^8}{4725} + O(v)^{10},$$
$$b_1 = 1 - \frac{v^4}{360} + \frac{v^6}{280} - \frac{281\,v^8}{604800} + O(v)^{10},$$
$$b_2 = 1 + \frac{2\,v^4}{45} - \frac{2\,v^6}{315} + \frac{34\,v^8}{14175} + O(v)^{10}.$$

3.3.2. Another new trigonometrically fitted method

Using the coefficients c_i and d_i given by (4) and solving the system of equation (6), the following values for the coefficients a_i and b_i are obtained:

$$a_1 = \frac{\csc(v)(\sin(v)q_1 + \sqrt{T})}{4vq_2},$$
$$a_2 = \frac{-2\,q_2\,v\,((-2+\sqrt{2})\,v - 2\,\cot(v))\,\sin(v)}{w_1 + \sqrt{T}\,\csc(v) - (-2+\sqrt{2})\,v\,\sin(2\,v)},$$
$$b_1 = \frac{q_3 + q_7 + \sqrt{T}\,(-4\,(-2+\sqrt{2})\,v\,\cos(v) - 8\,\sin(v))}{2\,v^2\,(q_6 - \sqrt{T}\,(2\,v - \sqrt{2}\,v + 2\,\cot(v)) - 5\,v^5\,\sin(2\,v))},$$
$$b_2 = \frac{4\,v^2\,(q_4 + \sqrt{T}\,\csc(v))}{q_5 - \sqrt{T}\,(-4\,(-2+\sqrt{2})\,v\,\cos(v) - 8\,\sin(v))},$$

where

$$T = \sin(v)^2\,(16\,(-1+\sqrt{2})\,v^3\,q_2 + q_1{}^2),$$
$$q_1 = (((-2+\sqrt{2})\,v^3 - 4\,\sin(v))\,\sin(v) + \cos(v)\,((3-2\sqrt{2})\,v^4 - 2\,(-2+\sqrt{2})\,v\,\sin(v))),$$
$$q_2 = (-1+\sqrt{2})\,v\,\cos(v) - \sqrt{2}\,\sin(v),$$
$$q_3 = v\,(8\,(-2+\sqrt{2})\,\sin(2\,v) - v^2\,(4 - 2\sqrt{2} + (-10+7\sqrt{2})\,v^2)\,\sin(3\,v) - 4\,(-2+\sqrt{2})\,\sin(4\,v)),$$
$$q_4 = (-3+2\sqrt{2})\,v^4\,\cos(v) - \sin(v)\,((-2+\sqrt{2})\,v^3 + 2\,(-2+\sqrt{2})\,v\,\cos(v) + 4\,\sin(v)),$$
$$q_5 = -q_3 - q_7,$$
$$q_6 = w_3 + w_4,$$
$$q_7 = w_1 + w_2,$$
$$w_1 = 2\,(6 + 3\,v^2 - 2\sqrt{2}\,v^2 - 6\,(-3+2\sqrt{2})\,v^4\,\cos(v) - 8\,\cos(2\,v) + 6\,v^4\,\cos(3\,v) - 4\sqrt{2}\,v^4\,\cos(3\,v)),$$
$$w_2 = (4 + (-6+4\sqrt{2})\,v^2)\,\cos(4\,v) + v^3\,(10\,(-2+\sqrt{2}) + (10-7\sqrt{2})\,v^2)\,\sin(v),$$
$$w_3 = 2\,(-3+2\sqrt{2})\,v^4\,\cos(2\,v) + (-2 + (3-2\sqrt{2})\,v^2)\,\cos(3\,v) - 2\,(-2+\sqrt{2})\,v\,\sin(v), \text{ and}$$
$$w_4 = \cos(v)\,(2 + (-3+2\sqrt{2})\,v^2 + 7\sqrt{2}\,v^5\,\sin(v)) - (-2+\sqrt{2})\,v\,(v^2\,\sin(2\,v) - 2\,\sin(3\,v)).$$

The Taylor expansions of the coefficients are

$$\begin{aligned} a_1 &= 1 - 0.0690356v^2 + 0.0109038v^4 + 0.000140361v^6 + 0.0000586133v^8 \\ &\quad + O(v^{10}), \\ a_2 &= 1 + 0.0690356v^2 + 0.001011v^4 + 0.000437959v^6 + O(v^{10}), \\ b_1 &= 1 - 0.0976311v^2 + 0.000255231v^4 - 0.0000621746v^6 + 0.0000321169v^8 \\ &\quad + O(v^{10}), \\ b_2 &= 1 + 0.0976311v^2 + 0.00212773v^4 - 0.00101629v^6 - 0.000132096v^8 + O(v^{10}). \end{aligned}$$

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 transformed into an initial value $y'(a)$. The results are independent of $y'(a)$ if $y'(a) \neq 0$. The eigenvalue E is a parameter in the computation. The value of E that makes $y(b) = 0$ is the eigenvalue computed.

We compare the numerical results produced by our new methods developed in sections 3.2.1–3.2.2 and 3.3.1–3.3.2 with Yoshida's [18] second, fourth and sixth-order methods (which are indicated as *Meth2*, *Meth4* and *Meth6*, respectively), McLachlan's [23] second-order method (which is indicated as *Meth2a*) and finally the well known Numerov's method.

4.1. The harmonic oscillator

The potential of the one-dimensional harmonic oscillator is given by:

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

We consider the case: $k = 1$. The exact eigenvalues are:

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

In table 1, we present several eigenvalues from E_0 to E_{50} computed by all methods tested.

Table 1
Errors ($\times 10^{-6}$) for the harmonic oscillator ($h = 0.1$).

	Meth2	*Meth2a*	*Meth4*	*Meth6*	*Numerov*	*New2*	*New2a*	*Exact*	*R*
E_0	315	365	417	416	0	416	416	0.5	5.5
E_3	7831	3287	1122	400	25	415	415	3.5	5.5
E_6	26673	12449	5036	229	148	414	414	6.5	6.5
E_{10}	69522	33307	20263	894	611	417	417	10.5	6.5
E_{13}	–	55498	43190	3259	1303	414	413	13.5	7.5
E_{17}	–	–	–	10243	2815	440	414	17.5	7.5
E_{20}	–	–	–	19972	4567	426	415	20.5	8.5
E_{23}	–	–	–	35191	6884	451	426	23.5	8.5
E_{27}	–	–	–	66939	10264	497	430	27.5	8.5
E_{30}	–	–	–	–	15127	573	445	30.5	9.5
E_{35}	–	–	–	–	23937	809	482	35.5	10.5
E_{40}	–	–	–	–	35665	1283	557	40.5	10.5
E_{50}	–	–	–	–	–	3639	842	50.5	11.5

4.2. *Doubly anharmonic oscillator*

The doubly anharmonic oscillator potential is given by:

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

with interval of integration $[a, b]$, and boundary conditions $y(a) = 0$ and $y(b) = 0$. In our experiments, 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 32th.

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

	Meth2	*Meth2a*	*Meth4*	*Meth6*	*Numerov*	*New2*	*New2a*	Exact
E_0	0	2	2	2	0	2	2	0.8074
E_2	21	3	5	5	0	5	5	5.5537
E_4	104	38	12	10	0	10	10	12.5343
E_6	297	127	25	14	1	14	14	21.1184
E_8	643	290	55	18	1	19	19	31.0309
E_{10}	1190	550	115	22	2	23	23	42.1044
E_{12}	1988	930	225	22	6	27	27	54.2225
E_{14}	3062	1451	413	20	13	30	30	67.2981
E_{16}	4475	2135	714	12	22	35	35	81.2629
E_{18}	6267	3003	1170	5	35	40	40	96.0615
E_{20}	8482	4079	1832	39	55	44	44	111.6478
E_{22}	–	5385	2762	98	84	48	48	127.9825
E_{24}	–	6942	4031	192	123	51	51	145.0317
E_{26}	–	8773	5726	335	173	56	56	162.7656
E_{28}	–	–	–	547	240	59	59	181.1582
E_{30}	–	–	–	852	323	64	64	200.1857
E_{32}	–	–	–	1280	429	68	68	219.8273

4.3. *Exponential potential*

The exponential potential is given by:

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

with interval of integration $[0, \pi]$, and boundary conditions $y(0) = 0$ and $y(\pi) = 0$. Again here we have computed the first 16 eigenvalues. In table 3 we give the exact eigenvalues and the absolute errors with all methods. We have used 50 points in the interval of integration $[0, \pi]$.

Table 3
Errors ($\times 10^{-4}$) for the exponential potential.

	Meth2	*Meth2a*	*Meth4*	*Meth6*	*Numerov*	*New2*	*New2a*	*Exact*
E_0	18	3	5	5	0	6	6	4.896689
E_1	110	45	13	8	0	8	11	10.045190
E_2	349	161	39	11	1	2	14	16.019267
E_3	919	442	123	9	2	12	12	23.266271
E_4	1473	1035	382	2	12	12	13	32.263707
E_5	2996	2116	1066	43	33	12	12	43.220020
E_6	–	–	2642	175	80	12	12	56.181594
E_7	–	–	–	532	176	13	12	71.152998
E_8	–	–	–	1396	355	13	13	88.132119
E_9	–	–	–	–	667	15	13	107.11668
E_{10}	–	–	–	–	1180	22	15	128.10502
E_{11}	–	–	–	–	1992	38	18	151.09604
E_{12}	–	–	–	–	–	77	25	176.08900
E_{13}	–	–	–	–	–	166	38	203.08337
E_{14}	–	–	–	–	–	357	62	232.07881
E_{15}	–	–	–	–	–	745	104	263.07507
E_{16}	–	–	–	–	–	1504	178	296.07196

5. Conclusions

- For all the potentials presented above the new developed methods are much more efficient compared with the well-known symplectic integrators mentioned above.
- The comparison with the higher algebraic order Numerov's method has the following conclusion: for the first few eigenvalues the Numerov's method presents more accurate results. For all the other eigenvalues and especially for high-state eigenvalues the new developed methods are much more accurate while in some cases Numerov's method divergences.

Based on the above, we conclude that the new developed methods can be used for the computation of high-state eigenvalues very effectively. We have seen that during the computation of the high-state eigenvalues, the absolute error remains almost constant for a wide range of eigenvalues.

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