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Symplectic methods of fifth order for the numerical solution of the radial Shrödinger equation

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In this paper the numerical solution of the radial Shrödinger equation via new proposed symplectic-schemes is investigated. In particular, the radial Schödinger equation is transformed into Hamiltonian canonical form and is solved via symplectic integrators. Based on this approach, fifth-order methods are proposed. We compare these methods with well-known existing symplectic methods. The numerical results show the efficiency of the proposed method.

KEY WORDS: radial Shrödinger equation, symplectic schemes, fifth order

1. Introduction

The approximate integration of Hamiltonian systems is of considerable importance to areas such as molecular dynamics, mechanics, astro-physics and others. By long-time integration of large systems it is possible to obtain better understanding of physical properties of the systems. It is well known that geometric integrators, such as symplectic and reversible integrators, are superior compared with non-symplectic methods for the integration of Hamiltonian systems [1]. The main characteristics of geometric integrators (which give them superiority in comparison with non-symplectic integrators) are: (1) preservation of the energy integral, (2) linear error growth and (3) correct qualitative behavior.

The radial time-independent Schrödinger equation has the form

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

where E is the energy eigenvalue, $V(x)$ is the potential and q is the wavefunction.

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In [2] Liu et al. has transformed (1) into Hamiltonian canonical equations using Legendre transformation. The Hamiltonian canonical equations are given below:

$$\begin{cases} \dot{p} = -\dfrac{\partial H}{\partial q} = -B(x)q, \\ \dot{q} = \dfrac{\partial H}{\partial p} = p, \end{cases} \tag{2}$$

where $B(x) = 2[E - V(x)]$, E is the energy eigenvalue, $V(x)$ is the potential, q is the wavefunction and H the Hamiltonian function

$$H(q, p, x) = \frac{1}{2}p^2 + \frac{1}{2}B(x)q^2. \tag{3}$$

Last decade some symplectic integrators have been developed. Ruth [3] first published symplectic methods for problems of the form (3). Integrators of order three were constructed by Ruth [3], integrators of order four were obtained by Candy and Rozmus [4] and Forest and Ruth [5]. Yoshida [6] has constructed reversible symplectic integrators of sixth and eighth order. Recently Tselios and Simos [7] have introduced low order symplectic integrators for the numerical solution of (2). In this paper new symplectic integrators of fifth order have been constructed. The new methods have been compared with well-known symplectic integrators (see [2,6]). The paper is constructed as follows. In section 2 basic theory on symplectic integrators is presented. The construction of symplectic integrators is presented in section 3. The new proposed fifth order method is developed in section 4. Finally, in section 5 numerical illustration of the new developed method is presented.

2. Symplectic integrators

From [1] it is known that the characterization of a canonical transformation is done by using matrix algebra or by using differential forms (2-form).

Definition 1 [1]. A mapping is symplectic if

$$L^T J L = J, \tag{4}$$

where L is the $2d$-dimensional Jacobian matrix of the mapping and

$$J = \begin{pmatrix} 0_d & I_d \\ -I_d & 0_d \end{pmatrix},$$

with I_d and 0_d denoting the unit and zero d-dimensional matrix.

Proposition 1 [1]. A transformation

$$\begin{pmatrix} q \\ p \end{pmatrix} \quad \to \quad \begin{pmatrix} q^* \\ p^* \end{pmatrix}$$

is symplectic (2-form) if and only if

$$\sum_{i=1}^{d} \mathrm{d}q_i^* \wedge \mathrm{d}p_i^* = \sum_{i=1}^{d} \mathrm{d}q_i \wedge \mathrm{d}p_i,$$

rewriting as $\mathrm{d}q^* \wedge \mathrm{d}p^* = \mathrm{d}q \wedge \mathrm{d}p$.

Our investigation on the construction of symplectic integrators is based on the procedure developed by Forest and Ruth [5], Yoshida [6], Liu et al. [2]:

$$\begin{cases} P_i = P_{i-1} - c_i h B^{n+1/2} Q_{i-1}, \\ Q_i = Q_{i-1} + d_i h P_i, \end{cases} \qquad i = 1, \dots, k, \tag{5}$$

where $Q_0 = q^n$, $P_0 = p^n$, $B^{n+1/2} = B(x_n + h/2)$, c_i and d_i are free parameters and k is the number of stages.

At the point x_{n+1} the solution is:

$$Q_k = q^{n+1}, \qquad P_k = p^{n+1}.$$

The parameters c_i and d_i have been obtained by Yoshida [6]:

$$\exp\bigl[h(A+B)\bigr] = \prod_{i=1}^{k} \exp(c_i hA)\exp(d_i hB) + O\bigl(h^{n+1}\bigr), \tag{6}$$

where k and n, are the number of stages and the order of method, respectively.

3. Construction of symplectic integrators

The determination of the coefficients c_i, d_i is based on the expansion of the left-hand side of (6) in powers of h,

$$S(h) = \mathrm{e}^{h(A+B)} = 1 + h(A+B) + \frac{1}{2}h^2\bigl(A^2 + AB + BA + B^2\bigr) + \cdots.$$

Expanding the right-hand side of (6) it follows:

$$\begin{aligned} \tilde{S}(h) &= \prod_{i=1}^{k} \exp(c_i hA)\exp(d_i hB) \\ &= 1 + h\left(\sum_{i=1}^{k} c_i A + \sum_{i=1}^{k} d_i B\right) \\ &\quad + \frac{1}{2}h^2\Biggl[\left(\sum_{i=1}^{k} c_i\right)^2 A^2 + 2\sum_{i=1}^{k} d_i \sum_{j=1}^{i} c_j AB + 2\sum_{i=1}^{k} d_i \sum_{j=i+1}^{k} c_j BA \end{aligned}$$

$$+\left(\sum_{i=1}^{k} d_i\right)^2 B\Bigg] + \cdots.$$

We want the two expressions to agree up to h^n. The resulting equations for the coefficients c_i, d_i are depended linearly and for fifth-order we have obtained 62 equations (see for more details in [8]). Finally, the number of linearly independent equations is 14 (see below).

The transformation into a linearly independent system of equations, leads to the following number of equations and the number of order conditions:

Order	1	2	3	4	5
Equations	2	3	5	8	14

4. Construction of the new fifth-order method

In this section we describe the development of the new proposed fifth-order method. Based on the above mentioned theory the new method is going to be a seven-stage method, of the form (5), i.e.,

$$\begin{cases}
P_1 = p^n - c_1 h B\left(x_n + \dfrac{h}{2}\right) q^n, \\
Q_1 = q^n + d_1 h P_1, \\
P_2 = P_1 - c_2 h B\left(x_n + \dfrac{h}{2}\right) Q_1, \\
Q_2 = Q_1 + d_2 h P_2, \\
P_3 = P_2 - c_3 h B\left(x_n + \dfrac{h}{2}\right) Q_2, \\
Q_3 = Q_2 + d_3 h P_3, \\
P_4 = P_3 - c_4 h B\left(x_n + \dfrac{h}{2}\right) Q_3, \\
Q_4 = Q_3 + d_4 h P_4, \\
P_5 = P_4 - c_5 h B\left(x_n + \dfrac{h}{2}\right) Q_4, \\
Q_5 = Q_4 + d_5 h P_5, \\
P_6 = P_5 - c_6 h B\left(x_n + \dfrac{h}{2}\right) Q_5, \\
Q_6 = Q_5 + d_6 h P_6, \\
p^{n+1} = P_6 - c_7 h B\left(x_n + \dfrac{h}{2}\right) Q_6, \\
q^{n+1} = Q_6 + d_7 h p^{n+1}.
\end{cases}$$

The linearly independent systems of fifth-order equations are:
Order 1.

$$\begin{cases} D_{1,1} = \sum_{i=1}^{k} c_i - 1, \\ D_{1,2} = \sum_{i=1}^{k} d_i - 1. \end{cases} \tag{7}$$

Order 2.

$$D_{2,1} = \sum_{i=1}^{k} d_i \sum_{j=1}^{i} c_j - \frac{1}{2}. \tag{8}$$

Order 3.

$$\begin{cases} D_{3,1} = \sum_{i=1}^{k} c_i \sum_{j=1}^{k} d_j \sum_{l=j+1}^{k} c_l - \frac{1}{6}, \\ D_{3,2} = \sum_{i=2}^{k} d_i \sum_{j=2}^{i} c_j \sum_{l=1}^{j-1} d_l - \frac{1}{6}. \end{cases} \tag{9}$$

Order 4.

$$\begin{cases} D_{4,1} = \frac{1}{6} \sum_{i=1}^{k} d_i \left(\sum_{j=i+1}^{k} c_j \right)^3 - \frac{1}{24}, \\ D_{4,2} = \frac{1}{6} \sum_{i=2}^{k} c_i \left(\sum_{j=1}^{i-1} d_j \right)^3 - \frac{1}{24}, \\ D_{4,3} = \sum_{i=1}^{k-2} d_i \sum_{j=i+1}^{k-1} c_j \sum_{m=j}^{k-1} d_m \sum_{t=m+1}^{k} c_t - \frac{1}{24}. \end{cases} \tag{10}$$

Order 5.

$$
\begin{cases}
D_{5,1} = \dfrac{1}{24}\displaystyle\sum_{i=1}^{k} d_i \left(\sum_{j=i+1}^{k} c_j\right)^4 - \dfrac{1}{120},\\[2ex]
D_{5,2} = \dfrac{1}{24}\displaystyle\sum_{i=2}^{k} c_i \left(\sum_{j=1}^{i-1} d_j\right)^4 - \dfrac{1}{120},\\[2ex]
D_{5,3} = \dfrac{1}{12}\displaystyle\sum_{i=1}^{k} d_i \sum_{j=i}^{k} d_j \left(\sum_{m=1}^{i} c_m\right)^3 + \dfrac{1}{12}\sum_{i=1}^{k} d_i \sum_{j=i+1}^{k} d_j \left(\sum_{m=1}^{i} c_m\right)^3 - \dfrac{1}{120},\\[2ex]
D_{5,4} = \dfrac{1}{12}\displaystyle\sum_{i=1}^{k} c_i \sum_{j=i}^{k} c_j \left(\sum_{m=j}^{k} d_j\right)^3 + \dfrac{1}{12}\sum_{i=1}^{k} c_i \sum_{j=i+1}^{k} c_j \left(\sum_{m=j}^{k} d_j\right)^3 - \dfrac{1}{120},\\[2ex]
D_{5,5} = \displaystyle\sum_{i=1}^{k-1} c_i \sum_{j=i}^{k-1} d_j \sum_{m=j+1}^{k} c_m \sum_{n=m}^{k-1} d_n \sum_{t=n+1}^{k} c_t - \dfrac{1}{120},\\[2ex]
D_{5,6} = \displaystyle\sum_{i=1}^{k-1} d_i \sum_{j=i+1}^{k-1} c_j \sum_{m=j}^{k} d_m \sum_{n=m+1}^{k} c_n \sum_{t=n}^{k} d_t - \dfrac{1}{120}.
\end{cases}
\tag{11}
$$

For fifth-order equations (7)–(11) should be zeroed, and for $k = 7$ (number of stages) we have fourteen equations and fourteen parameters. This set of equations can be solved numerically. Using the Newton method 46 solutions for fifth-order integrator have been obtained (see for more details [8]).

Minimizing the sum of squares of the fourteen functions (7)–(11), using the Levenberg–Marquardt method, the same solutions have been obtained.

For internal computations 40-digits of precision are used.

After check of all the 46 produced solutions we have found that the most efficient one (i.e., the solution which gives the most accurate results), is the following:

$$
\begin{aligned}
c_1 &= 0.4515650720436605661536769078444025927 72,\\
c_2 &= -0.0026255177260405503212166318348852182 46,\\
c_3 &= -0.2887462490910128204969177168706319164 95,\\
c_4 &= 0.4703720043422901320446596003861052932 32,\\
c_5 &= 0.3704466763359327321311653913528419374 09,\\
c_6 &= 0.1934796732533845648578957608942231680 79,\\
c_7 &= -0.1944916591582146243692633117720558567 51,\\
d_1 &= 1.9042327805084463874533312275884597491 90,\\
d_2 &= -1.9395863664419246052720045464619766543 74,\\
d_3 &= 0.3960766510231830289112974915012668544 24,
\end{aligned}
$$

$$d_4 = 0.5133868104090695626740381054834970276\,76,$$
$$d_5 = -2.9677394606045473652638582641642989867\,68,$$
$$d_6 = 0.0041774095286693157391416751180472532\,00,$$
$$d_7 = 3.0894521755771036757580543109350047566\,51.$$

5. Numerical examples

The implementation of the new developed method is based on the shooting technique. The comparison of the new method with existing ones has taken place for two potentials: (1) the harmonic oscillator and (2) the hydrogen atom.

5.1. *The harmonic oscillator*

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

$$V(x) = \frac{1}{2}x^2 \quad (-\infty < x < +\infty). \tag{12}$$

For this potential the exact eigenvalues are given by the formula

$$E_n = n + \frac{1}{2} \quad (n = 0, 1, 2, \ldots). \tag{13}$$

In order to compute the eigenvalues, we take as boundary conditions

$$y(x_{\min}) = 0, \qquad y(x_{\max}) = 0, \tag{14}$$

where $x_{\min}$ and $x_{\max}$ are respectively the left and right boundaries. We define N as a positive integer and then the space $x_{\max} - x_{\min}$ is divided into N equal intervals. The length of each interval is equal to $h = (x_{\max} - x_{\min})/N$ and this denote that $x_n = x_{\min} + nh$ $(n = 1, 2, \ldots, N-1)$. Then in order to calculate the eigenvalues, we use a symplectic scheme and the shooting method.

The new seven-stages fifth-order symplectic integrators have been compared with (i) the four-stages fourth-order and the eight-stages sixth-order symplectic methods obtained by Yoshida [6],[1] and (ii) the three-stages third-order symplectic methods [7].

In figure 1 we present the error graph for the 200, 210, 220, 230, 240, 250 states of eigenvalues, and the calculations are obtained in the intervals $[-26.5, 26.5]$, $[-27.5, 27.5]$, $[-28.5, 28.5]$, $[-29.5, 29.5]$, $[-30.5, 30.5]$, $[-31.5, 31.5]$, respectively, for $h = 0.02$.

[1] From the eight-stages sixth-order of Yoshida's methods we have selected for this comparison the one that gives the better results. For this method we have extended the precision of the given digits for its coefficients from 16 digits precision (that were proposed by Yoshida [6]) to 40 digits precision.

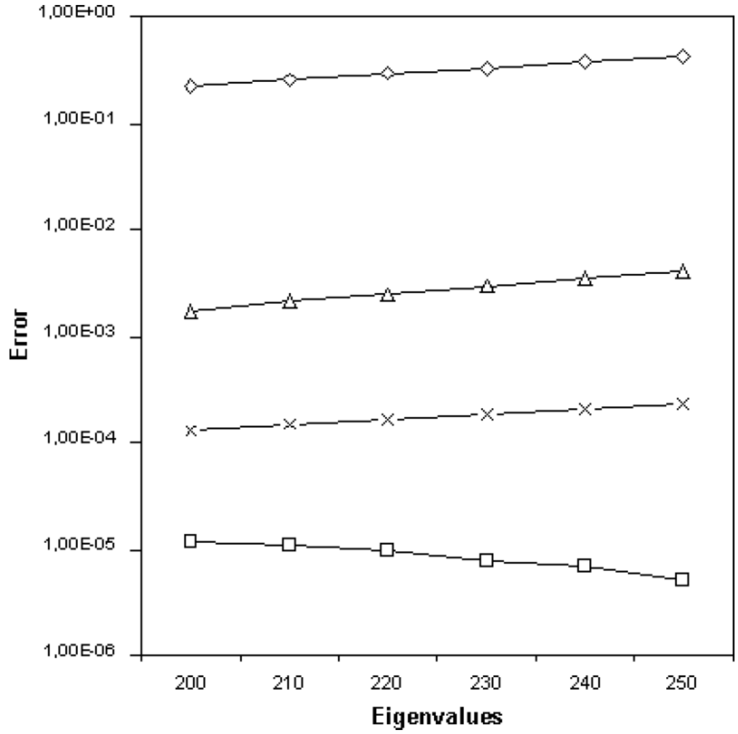

Figure 1. Values of $Err = -\log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ for the eigenvalues E_{200}, E_{210}, E_{220}, E_{230}, E_{240}, E_{250} of the harmonic oscillator. Methods used: (i) –◇–: Yoshida [6] symplectic-scheme method of four stage-fourth order, (ii) –△–: Yoshida [6] symplectic-scheme method of eight stage–six order, (iii) –×–: symplectic-scheme of three stage-third order [7], (iv) –□–: new method with symplectic-scheme of seven stage-fifth order.

5.2. The hydrogen atom

The radial wave function is determined by one-dimensional Shrödinger equation of the form

$$\ddot{y}(r) + \left(2E + \frac{2}{r} - \frac{l(l+1)}{r^2}\right)y(r) = 0, \quad 0 \leqslant r < +\infty, \tag{15}$$

where $l = 0, 1, 2, \ldots$. In this paper we solve the eigenvalue problem for $l = 0$. The boundary conditions are $y(0) = 0$ and $y(+\infty) = 0$, and the exact eigenvalues are calculated by the formula

$$E_n = -\frac{1}{2n^2} \quad (n = 1, 2, 3, \ldots). \tag{16}$$

The new seven-stages fifth-order symplectic integrators have been compared with the same methods mentioned in the previous example.

In figure 2 we present the error graph for the 10, 20, 30, 40, 50, 60, 70, 80 states of eigenvalues, and the calculations are obtained in the intervals $[0, 300]$, $[0, 1100]$,

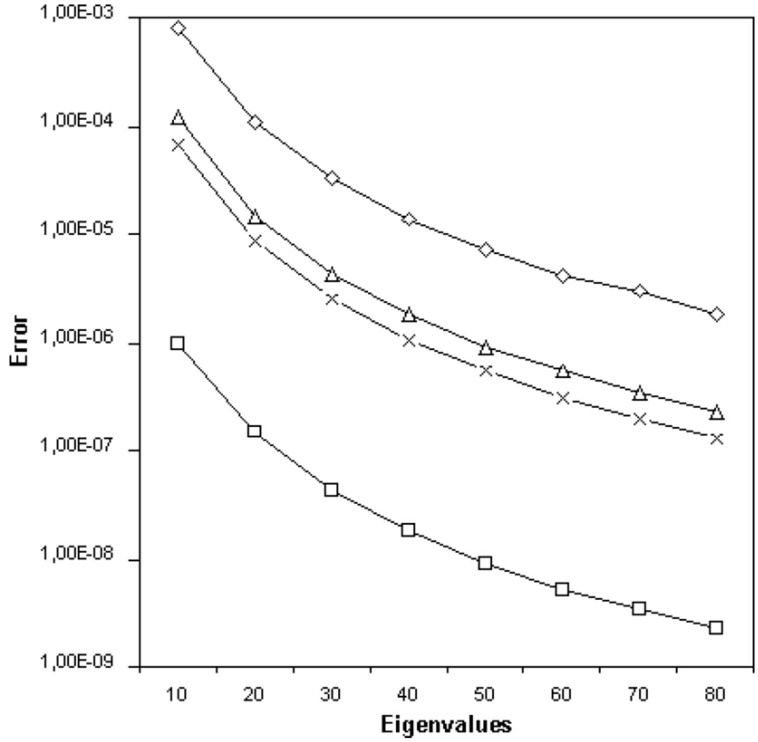

Figure 2. Values of $Err = -\log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ for the eigenvalues $E_{10}, E_{20}, \ldots, E_{80}$ of the hydrogen atom. Methods used: (i) –◇–: Yoshida [6] symplectic-scheme method of four stage-fourth order, (ii) –△–: Yoshida [6] symplectic-scheme method of eight stage-six order, (iii) –×–: symplectic-scheme of three stage-third order [7], (iv) –□–: new method with symplectic-scheme of seven stage-fifth order.

$[0, 300]$, $[0, 1100]$, $[0, 2200]$, $[0, 3800]$, $[0, 5800]$, $[0, 8000]$, $[0, 11500]$, $[0, 15000]$, respectively, for $h = 1$.

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