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# Symplectic methods for the numerical solution of the radial Shrödinger equation

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In this paper new symplectic-schemes for the numerical solution of the radial Shrödinger equation are proposed. In particular, symplectic integrators for Hamiltonian systems have been developed. Based on this approach, second- and third-order methods are proposed. These methods are more accurate than the existing ones. We compare these methods not only with the existing symplectic methods, but also with a classical Runge–Kutta–Nyström method.

**KEY WORDS:** radial Shrödinger equation, symplectic schemes

## 1. Introduction

The one-dimensional 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.

Many problems in molecular spectroscopy and quantum chemistry, theoretical physics, materials science and computational mechanics can be expressed as systems of equations of the form (1). Consequently there is a real need for reliable and efficient solution of (1) using numerical methods.

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

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

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where $B(x) = 2[E - V(x)]$ and $H$ is the Hamiltonian function

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

The symplectic integration of Hamiltonian dynamical systems is a recent research field. Third-order integrators were constructed by Ruth [2], fourth-order integrators were obtained by Candy and Rozmus [3] and Forest and Ruth [4]. Yoshida [5] has constructed symplectic integrators of sixth and eighth order.

In this paper new symplectic integrators of second and third order have been constructed. The new methods have been compared with well-known symplectic integrators (see [2–5]).

## 2. Symplectic integrators – basic theory

The characterization of a canonical transformation is done by using matrix algebra or by using differential forms (2-form).

**Definition 1** [6]. 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** [6]. A transformation $\binom{q}{p} \to \binom{q^*}{p^*}$ 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 $\mathrm{d}q^* \wedge \mathrm{d}p^* = \mathrm{d}q \wedge \mathrm{d}p$.

In this paper we will study symplectic integrators as proposed by Forest and Ruth [4], Yoshida [5]:

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

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.

The solution at the point $x_{n+1}$ is given by:

$$Q_k = q^{n+1}, \qquad P_k = p^{n+1}. \tag{6}$$

The parameters $c_i$ and $d_i$ are determined by Yoshida [5]

$$\exp\bigl[h(A+B)\bigr] = \prod_{i=1}^{k} \exp(c_i hA)\exp(d_i hB) + O\bigl(h^{n+1}\bigr), \tag{7}$$

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

## 3. Construction of symplectic integrators

In order to determine the coefficients $c_i$, $d_i$, we expand the left-hand side of (7) in powers of $h$,

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

Expanding the right-hand side of (7)

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

we want the two expressions to agree up to $h^n$. The resulting equations for the coefficients $c_i$, $d_i$ are:

*Order 1.*

$$\begin{aligned}
A\colon \quad D_{1,1} &= \sum_{i=1}^{k} c_i - 1, \\
B\colon \quad D_{1,2} &= \sum_{i=1}^{k} d_i - 1.
\end{aligned} \tag{8}$$

*Order 2.*

$$\begin{aligned}
AB\colon \quad D_{2,1} &= \sum_{i=1}^{k} d_i \sum_{j=1}^{i} c_j - \frac{1}{2}, \\
BA\colon \quad D_{2,2} &= \sum_{i=1}^{k-1} d_i \sum_{j=i+1}^{k} c_j - \frac{1}{2}.
\end{aligned} \tag{9}$$

*Order 3.*

$$
\begin{aligned}
A^2B:&\quad D_{3,1} = \frac{1}{2}\sum_{i=1}^{k} d_i \left(\sum_{j=1}^{i} c_j\right)^2 - \frac{1}{6},\\
AB^2:&\quad D_{3,2} = \frac{1}{2}\sum_{i=1}^{k} c_i \left(\sum_{j=i}^{k} d_j\right)^2 - \frac{1}{6},\\
BA^2:&\quad D_{3,3} = \frac{1}{2}\sum_{i=1}^{k} d_i \left(\sum_{j=i+1}^{k} c_j\right)^2 - \frac{1}{6},\\
B^2A:&\quad D_{3,4} = \frac{1}{2}\sum_{i=2}^{k} c_i \left(\sum_{j=1}^{i-1} d_j\right)^2 - \frac{1}{6},\\
ABA:&\quad D_{3,5} = \sum_{i=1}^{k} c_i \sum_{j=1}^{k} d_j \sum_{l=j+1}^{k} c_l - \frac{1}{6},\\
BAB:&\quad D_{3,6} = \sum_{i=2}^{k} d_i \sum_{j=2}^{i} c_j \sum_{l=1}^{j-1} d_l - \frac{1}{6}.
\end{aligned}
\tag{10}
$$

*Order 4.*

$$
\begin{array}{llllllll}
A^3B: & D_{4,1}, & AB^3: & D_{4,2}, & BA^3: & D_{4,3}, & B^3A: & D_{4,4},\\
A^2B^2: & D_{4,5}, & B^2A^2: & D_{4,6}, & A^2BA: & D_{4,7}, & AB^2A: & D_{4,8},\\
ABA^2: & D_{4,9}, & B^2AB: & D_{4,10}. & BA^2B: & D_{4,11}, & BAB^2: & D_{4,12},\\
ABAB: & D_{4,13}, & BABA: & D_{4,14}, & & & &
\end{array}
\tag{11}
$$

The functions of order four are presented analytically in section 4.2. The equations for higher orders can be found in a similar way.

The above equations are depended linearly. The transformation into a linearly independent system of equations, leads to the following number of equations.

The number of order condition is

| Order | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| Equations | 2 | 3 | 5 | 8 |

therefore a second-order method needs at least two stages while a third-order method needs at least three stages.

## 4. Development of the new methods

### 4.1. The second-order method

We are going to construct the second-order method. From the previous discussions this is going to be a two-stage method, of the form (5), i.e.,

$$\begin{cases} P_1 = p^n - c_1 h B\left(x_n + \dfrac{h}{2}\right) q^n, \\ Q_1 = q^n + d_1 h P_1, \\ p^{n+1} = P_1 - c_2 h B\left(x_n + \dfrac{h}{2}\right) Q_1, \\ q^{n+1} = Q_1 + d_2 h p^{n+1}. \end{cases}$$

Following approach described in section 3, equations (8), (9) are written as

$$\begin{cases} c_1 + c_2 = 1, & \text{(12a)} \\ d_1 + d_2 = 1, & \text{(12b)} \\ c_1 d_1 + (c_1 + c_2) d_2 = \dfrac{1}{2}, & \text{(12c)} \\ d_1 c_2 = \dfrac{1}{2}. & \text{(12d)} \end{cases}$$

For second-order equations 12(a)–(c) should be satisfied, while 12(d) follows from the first three equations.

Yoshida [5] derived his second-order method by letting $d_2 = 0$, then

$$c_1 = \frac{1}{2}, \quad c_2 = \frac{1}{2}, \quad d_1 = 1, \quad d_2 = 0. \tag{13}$$

Since we have three equations, we let $d_1$ be a free parameter, then

$$c_1 = 1 - \frac{1}{2d_1}, \quad c_2 = \frac{1}{2d_1}, \quad d_2 = 1 - d_1. \tag{14}$$

We minimize the error-function and we find the coefficients. The error-function is:

$$\mathit{error}(c_1, c_2, d_1, d_2) = \sqrt{D_{3,1}^2 + D_{3,2}^2 + D_{3,3}^2 + D_{3,4}^2 + D_{3,5}^2 + D_{3,6}^2}, \tag{15}$$

where $D_{3,1}, \ldots, D_{3,6}$ for two-stage method are:

$$D_{3,1} = -\frac{1}{6} + \frac{1}{2}\left(c_1^2 d_1 + (c_1 + c_2)^2 d_2\right),$$

$$
\begin{aligned}
D_{3,2} &= -\frac{1}{6} + \frac{1}{2}\big(c_2 d_2^2 + (d_1 + d_2)^2 c_1\big),\\
D_{3,3} &= -\frac{1}{6} + \frac{1}{2} c_2^2 d_1,\\
D_{3,4} &= -\frac{1}{6} + \frac{1}{2} c_2 d_1^2,\\
D_{3,5} &= -\frac{1}{6} + c_1 c_2 d_1,\\
D_{3,6} &= -\frac{1}{6} + c_2 d_1 d_2.
\end{aligned}
$$

From (14) the error-function becomes:

$$
error(d_1) = \frac{\sqrt{6}}{12}\sqrt{\left(\frac{-3+4d_1}{2d_1}\right)^2 + (-2+3d_1)^2}. \tag{16}
$$

Minimization of the error-function gives $d_1 = \sqrt{2}/2$ ($error(d_1) = 0.0350$), then

$$
c_1 = 1 - \frac{\sqrt{2}}{2}, \quad c_2 = \frac{\sqrt{2}}{2}, \quad d_1 = \frac{\sqrt{2}}{2}, \quad d_2 = 1 - \frac{\sqrt{2}}{2}. \tag{17}
$$

It is important to be noticed the symmetries, $c_1 = d_2$ and $c_2 = d_1$.

### 4.2. *The third-order method*

We are going to construct the third-order method. From the previous discussions this is going to be a three-stage method, of the form (5), i.e.,

$$
\begin{cases}
P_1 = p^n - c_1 h B\left(x_n + \dfrac{h}{2}\right) q^n,\\
Q_1 = q^n + d_1 h P_1,\\
P_2 = P_1 - c_2 h B\left(x_n + \dfrac{h}{2}\right) Q_1,\\
Q_2 = Q_1 + d_2 h P_2,\\
p^{n+1} = P_2 - c_3 h B\left(x_n + \dfrac{h}{2}\right) Q_2,\\
q^{n+1} = Q_2 + d_3 h p^{n+1}.
\end{cases}
$$

Following approach described in section 3, independent equations (8)–(10) are written as:

$$\begin{cases} c_1 + c_2 + c_3 = 1, & \text{(18a)} \\ d_1 + d_2 + d_3 = 1, & \text{(18b)} \\ c_1 d_1 + (c_1 + c_2) d_2 + (c_1 + c_2 + c_3) d_3 = \dfrac{1}{2}, & \text{(18c)} \\ c_2 c_3 d_2 + c_1\big((c_2 + c_3) d_1 + c_3 d_2\big) = \dfrac{1}{6}, & \text{(18d)} \\ c_2 d_1 d_2 + d_3\big((d_1 + d_2) c_3 + c_2 d_1\big) = \dfrac{1}{6}. & \text{(18e)} \end{cases}$$

For third-order method equations 18(a)–(e) should be satisfied.

Ruth [2] derived his third-order method ($error = 0.0495164$), which is given by:

$$c_1 = 1, \quad c_2 = -\frac{2}{3}, \quad c_3 = \frac{2}{3}, \quad d_1 = -\frac{1}{24}, \quad d_2 = \frac{3}{4}, \quad d_3 = \frac{7}{24}. \tag{19}$$

Since we have five equations (and six parameters), we let $d_2$ be a free parameter. We minimize the error-function and we find the coefficients. The error-function becomes:

$$error(c_1, c_2, c_3, d_1, d_2, d_3) = \sqrt{D_{4,1}^2 + D_{4,2}^2 + \cdots + D_{4,14}^2}, \tag{20}$$

where $D_{4,1}, D_{4,2}, \ldots, D_{4,14}$ for three-stage method are:

$$\begin{aligned}
D_{4,1} &= -\frac{1}{24} + \frac{1}{6}\big(c_1^3 d_1 + (c_1 + c_2)^3 d_2 + (c_1 + c_2 + c_3)^3 d_3\big), \\
D_{4,2} &= -\frac{1}{24} + \frac{1}{6}\big(c_3 d_3^3 + c_2 (d_2 + d_3)^3 + c_1 (d_1 + d_2 + d_3)^3\big), \\
D_{4,3} &= -\frac{1}{24} + \frac{1}{6}\big((c_2 + c_3)^3 d_1 + c_3^3 d_2\big), \\
D_{4,4} &= -\frac{1}{24} + \frac{1}{6}\big(c_2 d_1^3 + c_3 (d_1 + d_2)^3\big), \\
D_{4,5} &= \frac{1}{24}\big(-1 + 12 c_2 c_3 d_3^2 + 6 c_3^2 d_3^2 + 6 c_2^2 (d_2 + d_3)^2 + 6 c_1 (d_1 + d_2 + d_3)^2\big) \\
&\quad + \frac{1}{2}\big(c_1 c_3 d_3^2 + c_2 (d_2 + d_3)^2\big), \\
D_{4,6} &= -\frac{1}{24} + \frac{1}{4}\big(c_2^2 d_1^2 + 2 c_2 c_3 d_1^2 + c_3^2 d_1^2 + 2 c_3^2 d_1 d_2 + c_3^2 d_2^2\big),
\end{aligned}$$

$$D_{4,7} = -\frac{1}{24} + \frac{1}{2}c_1c_2c_3d_2 + \frac{1}{2}\big(c_2^2c_3d_2 + c_1\big(c_2c_3d_2 + c_1\big((c_2+c_3)d_1 + c_3d_2\big)\big)\big),$$
$$D_{4,8} = -\frac{1}{24} + \frac{1}{2}c_1c_3d_1d_2 + \frac{1}{2}\big(c_2c_3d_2^2 + c_1\big(c_3d_2^2 + d_1\big((c_2+c_3)d_1 + c_3d_2\big)\big)\big),$$
$$D_{4,9} = -\frac{1}{24} + \frac{1}{2}\big(c_2c_3^2d_2 + c_1\big((c_2+c_3)^2d_1 + c_3^2d_2\big)\big),$$
$$D_{4,10} = -\frac{1}{24} + \frac{1}{2}\big(c_2d_1^2d_2 + \big(c_2d_1^2 + c_3(d_1+d_2)^2\big)d_3\big),$$
$$D_{4,11} = -\frac{1}{24} + \frac{1}{2}c_2c_3d_1d_3 + \frac{1}{2}\big(c_3^2d_2d_3 + d_1\big(c_3^2d_3 + c_2\big(c_3d_3 + c_2(d_2+d_3)\big)\big)\big),$$
$$D_{4,12} = -\frac{1}{24} + \frac{1}{2}\big(c_3d_2d_3^2 + d_1\big(c_3d_3^2 + c_2\big(d_2+d_3\big)^2\big)\big),$$
$$D_{4,13} = -\frac{1}{24} + c_2c_3d_2d_3 + c_1\big(c_3d_2d_3 + d_1\big(c_3d_3 + c_2\big(d_2+d_3\big)\big)\big),$$
$$D_{4,14} = -\frac{1}{24} + c_2c_3d_1d_2.$$

Minimization of the error function gives

$$d_2 = -\tfrac{58623767696137}{811561628596785} \quad \text{or} \quad d_2 = \tfrac{5200281507982433}{4399167664813427} \quad (error(d_2) = 0.0374228),$$

then

$$c_1 = \tfrac{479561939695517}{1857710613287345}, \quad c_2 = \tfrac{5200281507982433}{4399167664813427}, \quad c_3 = -\tfrac{4618293127047827}{10490100451822575},$$
$$d_1 = \tfrac{108606835852797}{172086020422633}, \quad d_2 = -\tfrac{58623767696137}{811561628596785}, \quad d_3 = \tfrac{810034846678267}{1836329443349088},$$

or

$$c_1 = \tfrac{810034846678267}{1836329443349088}, \quad c_2 = -\tfrac{58623767696137}{811561628596785}, \quad c_3 = \tfrac{108606835852797}{172086020422633},$$
$$d_1 = -\tfrac{4618293127047827}{10490100451822575}, \quad d_2 = \tfrac{5200281507982433}{4399167664813427}, \quad d_3 = \tfrac{479561939695517}{1857710613287345}.$$

## 5. Numerical examples

The shooting technique has been used in order to implement the new methods. Comparison with existing methods for two potentials, the harmonic oscillator and the hydrogen atom is given.

### 5.1. *The harmonic oscillator*

Let the potential of the one-dimensional harmonic oscillator

$$V(x) = \frac{1}{2}x^2 \quad (-\infty < x < +\infty). \tag{21}$$

For this potential the exact eigenvalues are given by the formula

$$E_n = n + \frac{1}{2} \quad (n = 0, 1, 2, \ldots). \tag{22}$$

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

$$y(x_{\min}) = 0, \qquad y(x_{\max}) = 0, \tag{23}$$

where $x_{\min}$ and $x_{\max}$ are, respectively, the left and right boundaries. We define $N$ as a positive integer and then the space $[x_{\min}, x_{\max}]$ 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.

We have the following computations:

(1) The new two-stage second-order and the new three-stage third-order symplectic integrators have been compared with the two-stage second-order and the four-stage fourth-order methods obtained by Yoshida [5]. For comparison purposes we also use the method Runge–Kutta–Nyström 6(4)6FD developed in [7].

In figure 1 we present the error graph for the 20, 30, 40, 50, 60, 70, 80 states of eigenvalues, and the calculations are obtained in the intervals $[-8.5, 8.5]$, $[-9.5, 9.5]$, $[-10.5, 10.5]$, $[-11.5, 11.5]$, $[-12.5, 12.5]$, $[-13.5, 13.5]$, $[-14.5, 14.5]$, respectively, for $h = 0.02$.

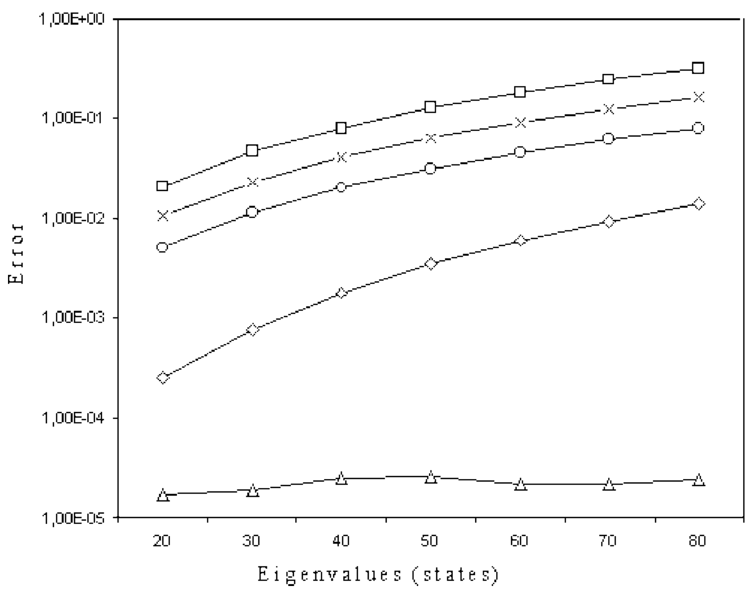


Figure 1. Values of $Err = -\log_{10} |E_{\text{calculated}} - E_{\text{analytical}}|$ for the eigenvalues $E_{20}$, $E_{30}$, $E_{40}$, $E_{50}$, $E_{60}$, $E_{70}$, $E_{80}$ of the Harmonic Oscillator. Methods used: (i) –□–: RKNystrom [7] method of six-order, (ii) –×–: Yoshida [5] method with symplectic-scheme of two-stage second order, (iii) –○–: new method with symplectic-scheme of two-stage second order, (iv) –◇–: Yoshida [5] method with symplectic-scheme of four-stage fourth order, (v) –△–: new method with symplectic-scheme of three-stage third order.

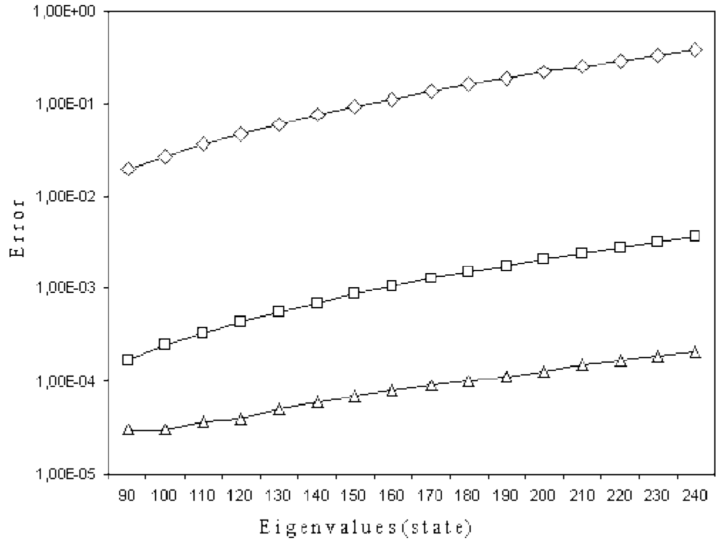


Figure 2. Values of $Err = -\log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ for the eigenvalues $E_{90}, E_{100}, \ldots, E_{240}$ of the Harmonic Oscillator. Methods used: (i) –◇–: Yoshida [5] symplectic-scheme method of four-stage fourth order, (ii) –□–: Ruth [2] method with symplectic-scheme of three-stage third order, (iii) –△–: new method with symplectic-scheme of three-stage third order.

(2) The new three-stage third-order symplectic integrators have been compared with the four-stage fourth-order methods obtained by Yoshida [5] and with the three-stage third-order methods obtained by Ruth [2].

In figure 2 we present the error graph for the 90, 100, 110, 120, 130, 140, 150, 160, 170, 180, 190, 200, 210, 220, 230, 240 states of eigenvalues, and the calculations are obtained in the intervals $[-15.5, 15.5]$, $[-16.5, 16.5]$, $[-17.5, 17.5]$, $[-18.5, 18.5]$, $[-19.5, 19.5]$, $[-20.5, 20.5]$, $[-21.5, 21.5]$, $[-22.5, 22.5]$, $[-23.5, 23.5]$, $[-24.5, 24.5]$, $[-25.5, 25.5]$, $[-26.5, 26.5]$, $[-27.5, 27.5]$, $[-28.5, 28.5]$, $[-29.5, 29.5]$, $[-30.5, 30.5]$, respectively, for $h = 0.02$.

### 5.2. *The hydrogen atom*

For the hydrogen atom the radial wave function is determined by one-dimensional Shrödinger equation of the form:

$$\ddot{y}(r) + \left(2E + \frac{2}{r} - \frac{l(l+1)}{r^2}\right)y(r) = 0, \quad 0 \leqslant r < +\infty, \tag{24}$$

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

$$E_n = -\frac{1}{2n^2} \quad (n = 1, 2, 3, \ldots). \tag{25}$$

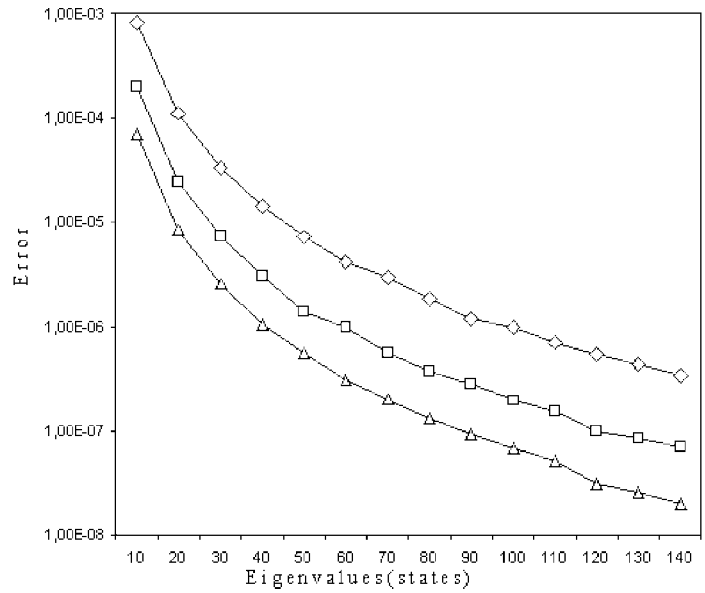


Figure 3. Values of $Err = -\log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ for the eigenvalues $E_{10}, E_{20}, \ldots, E_{140}$ of the Hydrogen Atom. Methods used: (i) –◇–: Yoshida [5] symplectic-scheme method of four-stage fourth order, (ii) –□–: Ruth [2] method with symplectic-scheme of three-stage third order, (iii) –△–: new method with symplectic-scheme of three-stage third order.

The new three-stage third-order symplectic integrators have been compared with the four-stage fourth-order methods obtained by Yoshida [5] and with the three-stage third-order methods obtained by Ruth [2].

In figure 3 we present the error graph for the 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140 states of eigenvalues, and the calculations are obtained in the intervals [0, 300], [0, 1100], [0, 2200], [0, 3800], [0, 5800], [0, 8200], [0, 11500], [0, 18500], [0, 22000], [0, 26000], [0, 30500], [0, 35500], [0, 41500], respectively, for $h = 1$.

## 6. Conclusions

In this paper new symplectic integrators for the approximate solution of the radial Shrödinger equation are proposed. Second- and third-order methods are proposed. From the numerical results presented above we conclude that the new proposed methods are more accurate than the existing ones.

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