Explicit symplectic adapted exponential integrators for charged-particle dynamics in a strong and constant magnetic field

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Abstract

This paper studies explicit symplectic adapted exponential integrators for solving charged-particle dynamics in a strong and constant magnetic field. We first formulate the scheme of adapted exponential integrators and then derive its symplecticity conditions. Based on the symplecticity conditions, we propose five practical explicit symplectic adapted exponential integrators. Two numerical experiments are carried out and the numerical results demonstrate the remarkable numerical behavior of the new methods.

Keywords: Charged particle dynamics; Exponential integrators; Symplectic methods

MSC (2000): 65P10, 65L05

1 Introduction

This paper is concerned with explicit symplectic adapted exponential integrators for the following charged-particle dynamics in a strong and constant magnetic field (see [8])

$$\ddot{x} = \frac{1}{2} \dot{x} \times B + F(x), \quad x(t_0) = x^0, \quad \dot{x}(t_0) = \dot{x}^0,$$

where $x(t) \in \mathbb{R}^3$ represents the position of a particle moving in an electro-magnetic field, $B = \nabla_x \times A(x)$ with the vector potential $A(x) = -\frac{1}{2} x \times B$ is a constant magnetic field, and $F(x)$ is the negative gradient of the scalar potential $U(x)$. We define $v = \dot{x}$ and then the energy of this dynamics is expressed by

$$H(x, v) = \frac{1}{2} |v|^2 + U(x).$$

It is known that this energy is conserved exactly by the exact solution of (1), i.e.

$$H(x(t), v(t)) \equiv H(x^0, \dot{x}^0)$$

for any $t$.

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In this paper, we denote the constant vector $B$ by $B = (B_1, B_2, B_3)^T$, where $B_i \in \mathbb{R}$ for $i = 1, 2, 3$. Then it follows from the definition of the cross product that $\dot{x} \times B = \tilde{B} \dot{x}$, where the skew symmetric matrix $\tilde{B}$ is given by

$$
\tilde{B} = \begin{pmatrix}
0 & B_3 & -B_2 \\
-B_3 & 0 & B_1 \\
B_2 & -B_1 & 0
\end{pmatrix}.
$$

According to the conjugate momenta $p = v + \frac{1}{\epsilon} A(x) = v - \frac{1}{2\epsilon} \tilde{B} x$, the charged-particle dynamics (1) can be converted into a Hamiltonian system with the non-separable Hamiltonian

$$
H(x, p) = \frac{1}{2} \left| p + \frac{1}{2\epsilon} \tilde{B} x \right|^2 + U(x).
$$

Charged-particle dynamics are of much importance and they have been studied for a long time (see, e.g. [1, 3, 5]). In order to solve the system effectively, various methods have been studied and developed. One popular integrator is Boris method [2] and more properties of this method were studied in [9, 18]. Another kind of methods developed for charged-particle dynamics is the volume-preserving integrators (see [15] for example). Recently, symmetric multistep methods were proposed for charged-particle dynamics in [10] and a variational integrator for charged-particle dynamics in a strong magnetic field was researched in [8]. On the other hand, it is well known that the symplecticity is a very important property for Hamiltonian system, which has been investigated by many researchers (see, e.g. [6, 7, 19, 29]). Sanz-Serna derived the symplecticity conditions for Runge-Kutta (RK) methods in [20] and Suris obtained the symplecticity conditions for Runge-Kutta-Nyström (RKN) methods in [22]. The authors in [16, 23, 30] constructed many symplectic integrators for the charged-particle dynamics. However, it seems that the symplectic exponential integrators for solving charged-particle dynamics have not been developed. As an efficient approach to solving first-order differential equations, exponential integrators have been widely investigated and developed and we refer to [17, 13, 14, 12, 24, 26, 27] for example. Therefore, this paper is devoted to symplectic exponential integrators for solving the charged-particle dynamics (1).

The main contributions of this paper are to present a novel kind of exponential integrators called as adapted exponential integrators for (1) and study its symplecticity. We will derive symplecticity conditions and based on them, explicit symplectic methods are constructed. This is different from normal exponential integrators since symplectic exponential integrators have to be implicit ([17]).

The rest of this paper is organised as follows. We first present the scheme of adapted exponential integrators in Section 2. In Section 3, we derive the symplecticity conditions for the adapted exponential integrators. Then some explicit symplectic adapted exponential integrators are constructed in Section 4. In Section 5, the obtained methods are compared with the corresponding symplectic RK methods by two numerical experiments. Section 6 is devoted to the conclusions of this paper.

## 2 Adapted exponential integrators

In order to solve the system (1) effectively, we formulate the following adapted exponential integrators.
Definition 2.1 An s-stage adapted exponential integrator (AEI) for solving \((1)\) is defined by:

\[
X_i = x_n + c_i h \varphi_1 (c_i \frac{h}{\tau} \tilde{B}) v_n + h^2 \sum_{j=1}^{s} \alpha_{ij} (c_i \frac{h}{\tau} \tilde{B}) F(X_j), \quad i = 1, 2, \ldots, s
\]

\[
x_{n+1} = x_n + h \varphi_1 (\frac{h}{\tau} \tilde{B}) v_n + h^2 \sum_{i=1}^{s} \beta_i (\frac{h}{\tau} \tilde{B}) F(X_i),
\]

\[
v_{n+1} = \varphi_0 (\frac{h}{\tau} \tilde{B}) v_n + h \sum_{i=1}^{s} \gamma_i (\frac{h}{\tau} \tilde{B}) F(X_i),
\]  

where \(h\) is a stepsize, \(c_i\) are real constants, \(\beta_i (\frac{h}{\tau} \tilde{B})\), \(\gamma_i (\frac{h}{\tau} \tilde{B})\) and \(\alpha_{ij} (\frac{h}{\tau} \tilde{B})\) are matrix-valued and bounded functions of \(\frac{h}{\tau} \tilde{B}\) for \(i, j = 1, 2, \ldots, s\). Here the \(\varphi\)-functions are defined by

\[
\varphi_0(z) = e^z, \quad \varphi_k(z) = \int_{0}^{1} e^{(1-\sigma)z} \frac{\sigma^{k-1}}{(k-1)!} d\sigma, \quad k = 1, 2, \ldots
\]

We denote this method by AEI.

The s-stage adapted exponential integrator can also be denoted by the following Butcher tableau

\[
c_1 \quad \alpha_{11} (\frac{h}{\tau} \tilde{B}) \quad \cdots \quad \alpha_{1s} (\frac{h}{\tau} \tilde{B}) \\
\vdots \quad \vdots \quad \ddots \quad \vdots \\
c_s \quad \alpha_{s1} (\frac{h}{\tau} \tilde{B}) \quad \cdots \quad \alpha_{ss} (\frac{h}{\tau} \tilde{B}) \\
\hline
\beta_1 (\frac{h}{\tau} \tilde{B}) \quad \cdots \quad \beta_s (\frac{h}{\tau} \tilde{B}) \\
\gamma_1 (\frac{h}{\tau} \tilde{B}) \quad \cdots \quad \gamma_s (\frac{h}{\tau} \tilde{B})
\]

It is explicit if \(\alpha_{ij} (\frac{h}{\tau} \tilde{B}) = 0\) for \(j \geq i\). Otherwise, it is implicit.

For the methods adapted to solving the Hamiltonian system \((3)\), we consider the s-stage adapted exponential integrator \((3)\) with an momenta calculation. This leads to the following definition.

Definition 2.2 An s-stage adapted exponential integrator for the Hamiltonian system \((3)\) is defined by:

\[
X_i = x_n + c_i h \varphi_1 (c_i \frac{h}{\tau} \tilde{B}) v_n + h^2 \sum_{j=1}^{s} \alpha_{ij} (c_i \frac{h}{\tau} \tilde{B}) F(X_j), \quad i = 1, 2, \ldots, s
\]

\[
x_{n+1} = x_n + h \varphi_1 (\frac{h}{\tau} \tilde{B}) v_n + h^2 \sum_{i=1}^{s} \beta_i (\frac{h}{\tau} \tilde{B}) F(X_i),
\]

\[
v_{n+1} = \varphi_0 (\frac{h}{\tau} \tilde{B}) v_n + h \sum_{i=1}^{s} \gamma_i (\frac{h}{\tau} \tilde{B}) F(X_i),
\]

\[
p_{n+1} = p_{n+1} - \frac{1}{\tau} \tilde{B} x_{n+1}.
\]

Remark 2.3 From the analysis given in \([17]\), it is known that symplectic exponential integrators have to be implicit. However, we will show in the following two sections that for the adapted exponential integrators \([5]\), explicit symplectic methods can be obtained.

3 Symplecticity conditions

Since \(\tilde{B}\) is a skew-symmetric matrix, \(\tilde{B}\) can be expressed as \(\tilde{B} = P \Lambda P^H\), where \(P\) is a unitary matrix, and \(\Lambda = \text{diag}(-|B|, 0, |B|)\). With the linear change of variable

\[
\tilde{x}(t) = P^H x(t), \quad \tilde{v}(t) = P^H v(t),
\]

3
the system [11] can be rewritten as

$$\frac{d}{dt} \begin{pmatrix} \tilde{x} \\ \tilde{v} \end{pmatrix} = \begin{pmatrix} 0 & I \\ 0 & \tilde{\Omega} \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{v} \end{pmatrix} + \begin{pmatrix} 0 \\ \tilde{F}(\tilde{x}) \end{pmatrix}, \quad \begin{pmatrix} \tilde{x}^0 \\ \tilde{v}^0 \end{pmatrix} = \begin{pmatrix} P^H x^0 \\ P^H p^0 \end{pmatrix}, \quad (7)$$

where $\tilde{\Omega} = \text{diag}(-\tilde{\omega}, 0, \tilde{\omega})$ with $\tilde{\omega} = \frac{|\tilde{\Omega}|}{e}$ and $\tilde{F}(\tilde{x}) = P^H F(P\tilde{x}) = -\nabla_{\tilde{x}} U(P\tilde{x})$.

It is noted that the vector $x$ is denoted by $x = (x_{-1}, x_0, x_1)^T$ and the same notation is used for all the vectors in $\mathbb{R}^3$ or $\mathbb{C}^3$ in this paper. According to (11) and the property of $P$, we observe that $\tilde{x}_{-1} = (\tilde{x}_1)$, $\tilde{v}_{-1} = (\tilde{v}_1)$, and $\tilde{x}_0$, $\tilde{v}_0 \in \mathbb{R}$. In the light of (11), the corresponding Hamiltonian system [10] becomes

$$\begin{aligned}
\tilde{x}' &= \nabla_p \tilde{H}(\tilde{x}, \tilde{p}) = \tilde{p} + \frac{1}{2} \tilde{\Omega} \tilde{x}, \\
\tilde{p}' &= -\nabla_{\tilde{x}} \tilde{H}(\tilde{x}, \tilde{p}) = -\frac{1}{2} (\tilde{\Omega})^H (\tilde{p} + \frac{1}{2} \tilde{\Omega} \tilde{x}) - \nabla_{\tilde{x}} \tilde{U}(P\tilde{x}), \\
\end{aligned} \quad (8)$$

with

$$\tilde{H}(\tilde{x}, \tilde{p}) = \frac{1}{2} \left| \tilde{p} + \frac{1}{2} \tilde{\Omega} \tilde{x} \right|^2 + \tilde{U}(P\tilde{x}).$$

For this transformed Hamiltonian system, our AEI method becomes

$$\begin{aligned}
\tilde{X}_i &= \tilde{x}_n + c_i \phi_1(c_i \tilde{\Omega} \tilde{x}) \tilde{v}_n + h^2 \sum_{j=1}^s \alpha_{ij}(h \tilde{\Omega}) \tilde{F}(\tilde{X}_j), \quad i = 1, 2, \ldots, s, \\
\tilde{x}_{n+1} &= \tilde{x}_n + h \phi_1(h \tilde{\Omega}) \tilde{v}_n + h^2 \sum_{i=1}^s \beta_i(h \tilde{\Omega}) \tilde{F}(\tilde{X}_i), \\
\tilde{v}_{n+1} &= \phi_0(h \tilde{\Omega}) \tilde{v}_n + h \sum_{i=1}^s \gamma_i(h \tilde{\Omega}) \tilde{F}(\tilde{X}_i), \\
\tilde{p}_{n+1} &= \tilde{p}_{n+1} - \frac{1}{2} \tilde{\Omega} \tilde{x}_{n+1}. \\
\end{aligned} \quad (9)$$

The following theorem gives the symplecticity conditions for the $s$-stage adapted exponential integrator [5].

**Theorem 3.1** For solving the Hamiltonian system [10], consider the $s$-stage adapted exponential integrator [5]. Then the map $(x_n, p_n) \rightarrow (x_{n+1}, p_{n+1})$ is symplectic if the following conditions are satisfied

$$\begin{aligned}
\gamma_j(K) - K \beta_j(K) &= d_j I, \quad d_j \in \mathbb{C}, \\
\gamma_j(K) [\tilde{\phi}_1(K) - c_j \tilde{\phi}_1(c_j K)] &= \beta_j(K) [c_j \tilde{\phi}_1(K) - c_j K \tilde{\phi}_1(c_j K)], \\
\beta_j(K) \gamma_j(K) - \frac{1}{2} K \beta_j(K) \beta_j(K) &= \beta_j(K) [\tilde{\gamma}_j(K) - K \beta_j(K)] \\
\beta_j(K) \gamma_j(K) - \frac{1}{2} K \beta_j(K) \beta_j(K) &= \beta_j(K) [\tilde{\gamma}_j(K) - K \beta_j(K)] \\
\gamma_j(K) - K \beta_j(K) &= d_j I, \quad d_j \in \mathbb{C}, \\
\gamma_j(K) [\tilde{\phi}_1(K) - c_j \tilde{\phi}_1(c_j K)] &= \beta_j(K) [c_j \tilde{\phi}_1(K) - c_j K \tilde{\phi}_1(c_j K)], \\
\beta_j(K) \gamma_j(K) - \frac{1}{2} K \beta_j(K) \beta_j(K) &= \beta_j(K) [\tilde{\gamma}_j(K) - K \beta_j(K)] \\
\beta_j(K) \gamma_j(K) - \frac{1}{2} K \beta_j(K) \beta_j(K) &= \beta_j(K) [\tilde{\gamma}_j(K) - K \beta_j(K)], \\
\end{aligned} \quad (10)$$

where $i, j = 1, 2, \ldots, s$, and $K = h \tilde{\Omega}$. Here $\tilde{\phi}_1$ denotes the conjugate of $\phi_1$ and the same notation is used for other functions.

**Proof** With the notation of differential 2-form, we need to prove that (see [11])

$$\sum_{j=1}^3 dx_{n+1}^j \wedge dp_n^j = \sum_{j=1}^3 dx_n^j \wedge dp_n^j.$$
We compute
\[ \sum_{j=1}^{3} dx_{n+1}^J \wedge dp_n^J = \sum_{j=1}^{3} d\tilde{x}_{n+1}^J \wedge dp_n^J = \sum_{j=1}^{3} (P\tilde{x}_{n+1})^J \wedge (P\tilde{p}_{n+1})^J \]
\[ = \sum_{j=1}^{3} \left( d \sum_{i=1}^{3} (\hat{P}_{ji}\tilde{x}_{n+1}^i) \right) \wedge \left( d \sum_{k=1}^{3} (P_{jk}\tilde{p}_{n+1}^k) \right) \]
\[ = \sum_{j=1}^{3} \left( \sum_{i=1}^{3} (\hat{P}_{ji}d\tilde{x}_{n+1}^i) \right) \wedge \left( \sum_{k=1}^{3} (P_{jk}d\tilde{p}_{n+1}^k) \right) \]
\[ = \sum_{j=1}^{3} \sum_{i=1}^{3} \sum_{k=1}^{3} \hat{P}_{ji}P_{jk}(d\tilde{x}_{n+1}^i \wedge d\tilde{p}_{n+1}^k) \]
\[ = \sum_{j=1}^{3} d\tilde{x}_{n+1}^J \wedge d\tilde{p}_{n+1}^J = \sum_{j=1}^{3} d\tilde{x}_{n+1}^J \wedge d\tilde{p}_{n+1}^J. \]

Similarly, one has \( \sum_{j=1}^{3} dx_n^J \wedge dp_n^J = \sum_{j=1}^{3} d\tilde{x}_n^J \wedge d\tilde{p}_n^J. \) Thus we only need to prove
\[ \sum_{j=1}^{3} d\tilde{x}_{n+1}^J \wedge d\tilde{p}_{n+1}^J = \sum_{j=1}^{3} d\tilde{x}_n^J \wedge d\tilde{p}_n^J, \]
i.e.
\[ \sum_{j=1}^{3} d\tilde{x}_{n+1}^J \wedge d\tilde{p}_{n+1}^J - \frac{1}{2} \sum_{j=1}^{3} d\tilde{x}_n^J \wedge d(\tilde{\Omega}^J i\tilde{x}_n^J) = \sum_{j=1}^{3} d\tilde{x}_n^J \wedge d\tilde{v}_n^J - \frac{1}{2} \sum_{j=1}^{3} d\tilde{x}_n^J \wedge d(\tilde{\Omega}^J i\tilde{x}_n^J). \]

It is noted that \( d\tilde{x}_n^J \wedge d\tilde{v}_n^J \) and \( d\tilde{x}_n^J \wedge d\tilde{p}_n^J \in i\mathbb{R}. \) Denote the method by
\[ \tilde{X}_n^i = \tilde{x}_n^i + c_i h\varphi_1(c_i h\tilde{\Omega}^i)\tilde{v}_n^i + h^2 \sum_{j=1}^{s} \alpha_{ij} (h\tilde{\Omega}^i)\tilde{F}_n^J, \]
\[ \tilde{x}_{n+1}^J = \tilde{x}_n^J + h\varphi_1(h\tilde{\Omega}^i)\tilde{v}_n^i + h^2 \sum_{j=1}^{s} \beta_{ij} (h\tilde{\Omega}^i)\tilde{F}_n^J, \]
\[ \tilde{v}_n^i = e^{h\tilde{\Omega}^i} \tilde{v}_n^i + h \sum_{i=1}^{s} \gamma_i (h\tilde{\Omega}^i)\tilde{F}_n^J. \] (11)

where the superscript index \( J \) denotes the \( J \)th entry of a vector or a matrix and \( \tilde{F}_n^J \) denotes the \( J \)th entry of \( \tilde{F}(\tilde{x}_i). \)
In the light of the scheme of the methods, it is obtained that

\[
\begin{align*}
&d\tilde{x}_{n+1}^J \land d\tilde{v}_{n+1}^J - \frac{1}{2} d\tilde{x}_{n}^J \land d(\tilde{\Omega}^J \tilde{x}_{n+1}^J) \\
&= (d\tilde{x}_{n}^J + h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J + h^2 \sum_{i=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{i}^J) \land (e^{h\tilde{\Omega}^J_1}d\tilde{v}_{n}^J + h \sum_{j=1}^{s} \gamma_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J) \\
&- \frac{1}{2}(d\tilde{x}_{n}^J + h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J + h^2 \sum_{i=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{i}^J) \land (d(\tilde{\Omega}^J_1 \tilde{x}_{n}^J_1) + \tilde{\Omega}^J_1h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J) \\
&+ h^3\tilde{\Omega}^J_1 \sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \\
&= e^{h\tilde{\Omega}^J_1}d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J + h \sum_{j=1}^{s} \gamma_j(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{F}_{j}^J + he^{h\tilde{\Omega}^J_1}\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J \\
&+ h^3 \sum_{i=1}^{s} \sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)\gamma_j(h\tilde{\Omega}^J_1)d\tilde{F}_{i}^J \land d\tilde{F}_{j}^J - \frac{1}{2} d\tilde{x}_{n}^J \land d(\tilde{\Omega}^J_1 \tilde{x}_{n}^J) \\
&- \frac{1}{2} h\tilde{\Omega}^J_1h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J - \frac{1}{2} h^2\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \\
&- \frac{1}{2} h^2\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{F}_{j}^J) \\
&- \frac{1}{2} h^3\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \land d\tilde{v}_{n}^J - \frac{1}{2} h^2\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \land d\tilde{F}_{j}^J) \\
&- \frac{1}{2} h^3\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \land d\tilde{v}_{n}^J - \frac{1}{2} h^2\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \land d\tilde{F}_{j}^J). \\
\end{align*}
\]

According to the fact that any exterior product \( \land \) appearing here is real, we obtain

\[
\begin{align*}
&- \frac{1}{2} h\tilde{\Omega}^J_1h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J = - \frac{1}{2} h\tilde{\Omega}^J_1h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J, \\
&- \frac{1}{2} h^2\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{F}_{j}^J = - \frac{1}{2} h^2\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{F}_{j}^J, \\
&- \frac{1}{2} h^3\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \land d\tilde{v}_{n}^J = - \frac{1}{2} h^3\tilde{\Omega}^J_1(\sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)d\tilde{F}_{j}^J \land d\tilde{F}_{j}^J, \\
&h^2 \sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)e^{h\tilde{\Omega}^J_1}d\tilde{F}_{j}^J \land d\tilde{v}_{n}^J = - h^2 \sum_{j=1}^{s} \beta_j(h\tilde{\Omega}^J_1)e^{h\tilde{\Omega}^J_1}d\tilde{v}_{n}^J \land d\tilde{F}_{j}^J. \\
\end{align*}
\]

Based on these important properties, one gets

\[
\begin{align*}
&d\tilde{x}_{n+1}^J \land d\tilde{v}_{n+1}^J - \frac{1}{2} d\tilde{x}_{n}^J \land d(\tilde{\Omega}^J_1 \tilde{x}_{n+1}^J) \\
&= [e^{h\tilde{\Omega}^J_1} - h\varphi_1(h\tilde{\Omega}^J_1)d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J - \frac{1}{2} d\tilde{x}_{n}^J \land d(\tilde{\Omega}^J_1 \tilde{x}_{n}^J)] \\
&+ h \sum_{j=1}^{s} \gamma_j(h\tilde{\Omega}^J_1) - h\tilde{\Omega}^J_1 \gamma_j(h\tilde{\Omega}^J_1)]d\tilde{v}_{n}^J \land d\tilde{F}_{j}^J \\
&+ [h e^{h\tilde{\Omega}^J_1} \varphi_1(h\tilde{\Omega}^J_1) - \frac{1}{2} h^2 \tilde{\Omega}^J_1 \varphi_1(h\tilde{\Omega}^J_1) \varphi_1(h\tilde{\Omega}^J_1)]d\tilde{v}_{n}^J \land d\tilde{v}_{n}^J \\
&+ h^2 \sum_{j=1}^{s} [\varphi_1(h\tilde{\Omega}^J_1) \gamma_j(h\tilde{\Omega}^J_1) - \beta_j(h\tilde{\Omega}^J_1)e^{-h\tilde{\Omega}^J_1} - h\tilde{\Omega}^J_1 \varphi_1(h\tilde{\Omega}^J_1) \beta_j(h\tilde{\Omega}^J_1)]d\tilde{F}_{j}^J \land d\tilde{v}_{n}^J \\
&+ h^3 \sum_{i,j=1}^{s} [\beta_i(h\tilde{\Omega}^J_1) \gamma_j(h\tilde{\Omega}^J_1) - \frac{1}{2} h\tilde{\Omega}^J_1 \beta_i(h\tilde{\Omega}^J_1) \beta_j(h\tilde{\Omega}^J_1)]d\tilde{F}_{i}^J \land d\tilde{F}_{j}^J. \\
\end{align*}
\]

According to the definition of \( \varphi \)-functions, we have \( \varphi_1(h\tilde{\Omega}^J_1) = \frac{1}{h\tilde{\Omega}^J_1}(e^{h\tilde{\Omega}^J_1} - I) \), which yields \( h\tilde{\Omega}^J_1 \varphi_1(h\tilde{\Omega}^J_1) = e^{h\tilde{\Omega}^J_1} - I \). Thus, we get \( e^{h\tilde{\Omega}^J_1} - h\tilde{\Omega}^J_1 \varphi_1(h\tilde{\Omega}^J_1) = I \).
On the other hand, from the first formula of (11), it follows that
\[
dx_n^d = d\tilde{X}_n^d - c_j \varphi_1(c_j \tilde{\Omega}^d_i) d\bar{v}_n^d - h^2 \sum_{j=1}^s \alpha_{ji}(\tilde{\Omega}^d_i) d\tilde{F}_i^d, \quad i = 1, 2, \ldots, s.
\]

Then
\[
d\tilde{x}_n^d \wedge d\tilde{F}_j^d = d\tilde{X}_n^d \wedge d\tilde{F}_j^d - c_j \varphi_1(c_j \tilde{\Omega}^d_i) d\bar{v}_n^d \wedge d\tilde{F}_j^d - h^2 \sum_{i=1}^s \tilde{\alpha}_{ji}(\tilde{\Omega}^d_i) d\tilde{F}_i^d \wedge d\tilde{F}_j^d, \quad j = 1, 2, \ldots, s.
\]

Thus (12) can be rewritten as
\[
dx_{n+1}^d \wedge dx_{n+1}^d - \frac{1}{3} d\bar{x}_n^d \wedge d(\tilde{\Omega}^d_i \tilde{x}_n^d) = \
\frac{1}{3} d\bar{x}_n^d \wedge d\tilde{v}_n^d - \frac{1}{3} d\tilde{x}_n^d \wedge d(\tilde{\Omega}^d_i \tilde{x}_n^d) \
+ h \sum_{j=1}^s [\gamma_j(\tilde{\Omega}^d_i) - \tilde{\Omega}^d_i \beta_j(\tilde{\Omega}^d_i)] d\tilde{X}_n^d \wedge d\tilde{F}_j^d \
+ [he^{\tilde{\Omega}^d_i} \varphi_1(\tilde{\Omega}^d_i) - \frac{1}{2} h^2 \tilde{\Omega}^d_i \varphi_1(\tilde{\Omega}^d_i) \varphi_1(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d \
+ h^2 \sum_{j=1}^s [\varphi_1(\tilde{\Omega}^d_i) \gamma_j(\tilde{\Omega}^d_i) - \beta_j(\tilde{\Omega}^d_i) e^{-\tilde{\Omega}^d_i}] \
- \tilde{\alpha}_{ji}(\tilde{\Omega}^d_i) \gamma_j(\tilde{\Omega}^d_i) - h \tilde{\Omega}^d_i \beta_j(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{F}_j^d \
+ h^3 \sum_{i,j=1}^s [\tilde{\beta}_i(\tilde{\Omega}^d_i) \gamma_j(\tilde{\Omega}^d_i) - \tilde{\beta}_j(\tilde{\Omega}^d_i) \gamma_i(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d.
\]

Summing over all \( J \) yields
\[
\sum_{j=1}^3 d\tilde{x}_{n+1}^d \wedge d\tilde{v}_{n+1}^d - \frac{1}{3} d\tilde{x}_n^d \wedge d(\tilde{\Omega}^d_i \tilde{x}_n^d) = \
\frac{1}{3} d\tilde{x}_n^d \wedge d\tilde{v}_n^d - \frac{1}{3} d\tilde{x}_n^d \wedge d(\tilde{\Omega}^d_i \tilde{x}_n^d) \
+ h \sum_{j=1}^s [\gamma_j(\tilde{\Omega}^d_i) - \tilde{\Omega}^d_i \beta_j(\tilde{\Omega}^d_i)] d\tilde{X}_n^d \wedge d\tilde{F}_j^d \
+ [he^{\tilde{\Omega}^d_i} \varphi_1(\tilde{\Omega}^d_i) - \frac{1}{2} h^2 \tilde{\Omega}^d_i \varphi_1(\tilde{\Omega}^d_i) \varphi_1(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d \
+ h^2 \sum_{j=1}^s [\varphi_1(\tilde{\Omega}^d_i) \gamma_j(\tilde{\Omega}^d_i) - \beta_j(\tilde{\Omega}^d_i) e^{-\tilde{\Omega}^d_i}] \
- \tilde{\alpha}_{ji}(\tilde{\Omega}^d_i) \gamma_j(\tilde{\Omega}^d_i) - h \tilde{\Omega}^d_i \beta_j(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{F}_j^d \
+ h^3 \sum_{i,j=1}^s [\tilde{\beta}_i(\tilde{\Omega}^d_i) \gamma_j(\tilde{\Omega}^d_i) - \tilde{\beta}_j(\tilde{\Omega}^d_i) \gamma_i(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d.
\]

Moreover, it can be checked that
\[
\sum_{j=1}^3 [he^{\tilde{\Omega}^d_i} \varphi_1(\tilde{\Omega}^d_i) - \frac{1}{2} h^2 \tilde{\Omega}^d_i \varphi_1(\tilde{\Omega}^d_i) \varphi_1(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d = \
[he^{\tilde{\Omega}^d_i} \varphi_1(\tilde{\Omega}^d_i) - \frac{1}{2} h^2 \tilde{\Omega}^d_i \varphi_1(\tilde{\Omega}^d_i) \varphi_1(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d \
+ [he^{\tilde{\Omega}^d_i} \varphi_1(\tilde{\Omega}^d_i) - \frac{1}{2} h^2 \tilde{\Omega}^d_i \varphi_1(\tilde{\Omega}^d_i) \varphi_1(\tilde{\Omega}^d_i)] d\tilde{v}_n^d \wedge d\tilde{v}_n^d.
According to the property of $\tilde{v}_n$, we have
\[ d\tilde{v}_n^1 \wedge d\tilde{v}_n^1 = -d\tilde{v}_n^3 \wedge d\tilde{v}_n^3, \quad d\tilde{v}_n^2 \wedge d\tilde{v}_n^2 = 0, \]
and
\[ he^{\tilde{\mathcal{H}}_n^i} \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^i) - \frac{1}{2} h^2 \tilde{\mathcal{H}}_n^i \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^i) \varphi_1(h\tilde{\mathcal{H}}_n^i) = he^{\tilde{\mathcal{H}}_n^i} \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^i) - \frac{1}{2} h^2 \tilde{\mathcal{H}}_n^i \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^i) \varphi_1(h\tilde{\mathcal{H}}_n^i). \]
Therefore, it is arrived that
\[ \sum_{j=1}^3 [he^{\tilde{\mathcal{H}}_n^j} \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^j) - \frac{1}{2} h^2 \tilde{\mathcal{H}}_n^j \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^j) \varphi_1(h\tilde{\mathcal{H}}_n^j)] d\tilde{v}_n^j \wedge d\tilde{v}_n^j = 0. \]
Based on the first condition of (10), $\tilde{F}(\dot{x}) = -\nabla_x U(P\dot{x})$ and (11), it can be checked that $d\tilde{X}_j^1 \wedge d\tilde{F}_j^1 = dX_j^1 \wedge dF_j^1$. Thus, one has
\[ \sum_{j=1}^3 [\gamma_j(h\tilde{\mathcal{H}}_n^j) - h\tilde{\mathcal{H}}_n^j \beta_j(h\tilde{\mathcal{H}}_n^j)] d\tilde{X}_j^1 \wedge d\tilde{F}_j^1 = d_j \sum_{j=1}^3 d\tilde{X}_j^1 \wedge dF_j^1 = -d_j \sum_{j=1}^3 dF_j^1 \wedge dX_j^1. \]
In the light of the second and third formulae of (10), the last two terms of (13) vanish. Therefore, we obtain
\[ \sum_{j=1}^3 d\tilde{v}_{n+1}^j \wedge d\tilde{v}_{n+1}^j - \frac{1}{2} \beta_i \sum_{j=1}^3 d\tilde{v}_{n+1}^j \wedge d((\tilde{\mathcal{H}}_n^i \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^i))) = \sum_{j=1}^3 d\tilde{v}_{n}^j \wedge d\tilde{v}_{n}^j - \frac{1}{2} \beta_i \sum_{j=1}^3 d\tilde{v}_{n}^j \wedge d(\tilde{\mathcal{H}}_n^i \dot{\varphi}_1(h\tilde{\mathcal{H}}_n^i)). \]
Thus the method with the coefficients satisfying (10) is symplectic. The proof is complete.

4 Explicit symplectic AEI methods

In this section, we are devoted to the construction of practical explicit symplectic AEI methods. To this end, we consider a kind of explicit AEI methods with the coefficients
\[ a_{ij} = a_{ij}(c_i - c_j) \varphi_1((c_i - c_j)\frac{B}{h}), \quad \beta_i = b_i(1 - c_i) \varphi_1((1 - c_i)\frac{B}{h}), \quad \gamma_i = b_i e^{(1-c_i)\frac{B}{h}}, \quad i = 1, \ldots, s, \quad j = 1, \ldots, i - 1, \]
(14)
where $c = (c_1, \ldots, c_s), \ b = (b_1, \ldots, b_s)$ and $A = (a_{i,j})_{s \times s}$ are coefficients of an $s$-stage diagonal implicit RK method.

In the light of the analysis of exponential integrators given in [17], the following result is obtained.

Theorem 4.1 (See [17].) If the $s$-stage diagonal implicit RK method is of order $p$, then the AEI method with the coefficients (14) is also of order $p$. 

\[ \text{8} \]
In what follows, we will construct five explicit symplectic AEI methods of up to order four following three steps. First we will present diagonal implicit symplectic RK method and verify its order. Then the coefficients of explicit AEI method are obtained by considering (14) and the order of the method is arrived in the light of Theorem 4.1. Finally, we will check the conditions given in Theorem 3.1 and show the symplecticity of our AEI methods.

The symplecticity and order conditions of RK methods will be used in this section and we represent them by the following results.

**Theorem 4.2** *(See [11].)* If the coefficients of a Runge-Kutta method satisfy

\[ b_1 a_{ij} + b_j a_{ji} = b_i b_j \]

for \( i, j = 1, \ldots, s, \)

then it is symplectic.

**Theorem 4.3** *(See [11].)* If \( B(p), C(\eta) \) and \( D(\zeta) \) are satisfied with \( p \leq 2 \eta + 2 \) and \( p \leq \zeta + \eta + 1 \), then the Runge-Kutta method is of order \( p \). The definitions of \( B(p), C(\eta), D(\zeta) \) are referred to [11].

### 4.1 One-stage explicit symplectic AEI methods

Denote the coefficients of one-stage diagonal implicit RK methods by a Butcher tableau:

\[
\begin{array}{c|cc}
  \frac{c_1}{b_1} & a_{11} \\
\end{array}
\]

In the light of the symplecticity conditions, it can be obtained that this method is symplectic if

\[ b_1 a_{11} + b_1 a_{11} = b_1^2. \] (16)

On the other hand, on the basis of the order conditions, an one-stage diagonal implicit RK method is be of order two if

\[ a_{11} = c_1, \quad b_1 = 1, \quad b_1 c_1 = \frac{1}{2}. \] (17)

By (16) and (17), we get \( b_1 = 1, a_{11} = \frac{1}{2}, c_1 = \frac{1}{2} \). This method is implicit midpoint rule which is denoted by RK1s2. Then the coefficients of AEI method are given by

\[ c_1 = \frac{1}{2}, \quad \beta_1 = b_1(1 - c_1) \varphi_1((1 - c_1) \frac{h}{\varepsilon} B), \quad \gamma_1 = b_1 e^{(1 - c_1) \frac{h}{\varepsilon} B}. \]

It can be checked easily that these coefficients satisfy the symplecticity conditions (10). Therefore, this is an explicit symplectic AEI method of order two and we denoted it by AEI1s2.

### 4.2 Two-stage explicit symplectic AEI methods

We use a Butcher tableau to show two-stage diagonal implicit RK methods:

\[
\begin{array}{c|ccc}
  c_1 & a_{11} & & \\
  c_2 & a_{21} & a_{22} & \\
  & b_1 & b_2 & \\
\end{array}
\]
The symplecticity conditions of this method are given by
\[ b_2a_{21} = b_1b_2, \quad b_1a_{11} + b_1a_{11} = b_1b_1, \quad b_2a_{22} + b_2a_{22} = b_2b_2. \] (18)

Its second-order conditions are
\[ a_{11} + a_{12} = c_1, \quad a_{21} + a_{22} = c_2, \quad b_1 + b_2 = 1, \quad b_1c_1 + b_2c_2 = \frac{1}{2}, \] (19)

and the three-order conditions read the above formulae as well as the following two conditions
\[ b_1c_1^2 + b_2c_2^2 = \frac{4}{3}, \quad b_1a_{21}c_1 + b_2a_{21}c_1 + b_2a_{22}c_2 = \frac{1}{6}. \] (20)

Without loss of generality we assume that \( b_k \neq 0 \) \( (i = 1, \ldots, s) \) since condition (15) shows that, if \( b_k = 0 \), then \( b_k a_{ik} = 0 \) \( (i = 1, \ldots, s) \) and so the method is equal to a method with fewer stages. From (18) and (19), we obtain
\[ b_2 = 1 - b_1, a_{11} = \frac{1}{2}b_1, a_{21} = b_1, a_{22} = \frac{1}{2}(1 - b_1), c_1 = \frac{1}{2}b_1, c_2 = \frac{1}{2}(1 + b_1), \] (21)

where \( b_1 \) is a parameter.

Inserting (21) into (20) yields \( 3b_1^2 - 3b_1 + 1 = 0 \), which can be verified that this equation does not have real roots. Thus there is no two-stage diagonal implicit symplectic RK method of order three. In what follows, we present two choices for implicit symplectic RK method of order two.

Case one. If we choose \( b_1 = \frac{1}{3} \) and then get \( b_2 = \frac{1}{3}, a_{11} = \frac{1}{3}, a_{21} = \frac{1}{3}, a_{22} = \frac{1}{3}, c_1 = \frac{1}{3}, c_2 = \frac{2}{3} \)

by (21) (denote this RK method by RK2s2). Then by considering (14), we obtain the coefficients of a two-stage explicit AEI (4)
\[ \alpha_{21} = a_{21}(c_2 - c_1)\varphi_1((c_2 - c_1)h\frac{B}{2}), \quad \beta_1 = b_1(1 - c_1)\varphi_1((1 - c_1)h\frac{B}{2}), \quad \gamma_1 = b_1c_1e^{(1-c_1)h\frac{B}{2}}, \quad \beta_2 = b_2(1 - c_2)\varphi_1((1 - c_2)h\frac{B}{2}), \quad \gamma_2 = b_2c_2e^{(1-c_2)h\frac{B}{2}}. \]

From Theorem 4.1, it follows that this method is of order two and we denote it by AEI2s2.

Case two. Considering \( b_1 = \frac{1}{3} \), (21) gives \( b_2 = \frac{2}{3}, a_{11} = \frac{1}{3}, a_{21} = \frac{1}{3}, a_{22} = \frac{1}{3}, c_1 = \frac{1}{6}, c_2 = \frac{2}{3} \).

The following coefficients of a two-stage AEI are obtained
\[ \alpha_{21} = a_{21}(c_2 - c_1)\varphi_1((c_2 - c_1)h\frac{B}{2}), \quad \beta_1 = b_1(1 - c_1)\varphi_1((1 - c_1)h\frac{B}{2}), \quad \gamma_1 = b_1c_1e^{(1-c_1)h\frac{B}{2}}, \quad \beta_2 = b_2(1 - c_2)\varphi_1((1 - c_2)h\frac{B}{2}), \quad \gamma_2 = b_2c_2e^{(1-c_2)h\frac{B}{2}}. \]

It is easily proved that these two AEI methods satisfy all the symplecticity conditions (10). Therefore, both of them are symplectic.

### 4.3 Three-stage explicit symplectic AEI methods

The following Butcher tableau is given to describe three-stage diagonal implicit RK methods:

| \( c_1 \) | \( a_{11} \) |
| --- | --- |
| \( c_2 \) | \( a_{21} \) | \( a_{22} \) |
| \( c_3 \) | \( a_{31} \) | \( a_{32} \) | \( a_{33} \) |
| \( b_1 \) | \( b_2 \) | \( b_3 \) |
This method is symplectic if the following conditions are true
\[ b_2a_{21} = b_1b_2, \quad b_3a_{31} = b_1b_3, \quad b_3a_{32} = b_2b_3, \]
\[ b_1a_{11} + b_1a_{11} = b_1^2, \quad b_2a_{22} + b_2a_{22} = b_2^2, \quad b_3a_{33} + b_3a_{33} = b_3^2. \] (22)

Meanwhile, this method is of order three if
\[ a_{11} = c_1, \quad a_{21} + a_{22} = c_2, \quad a_{31} + a_{32} + a_{33} = c_3, \]
\[ b_1 + b_2 + b_3 = 1, \quad b_1c_1 + b_2c_2 + b_3c_3 = \frac{1}{3}, \]
\[ b_1c_1^2 + b_2c_2^2 + b_3c_3^2 = \frac{1}{5}, \quad b_1a_{11}c_1 + b_2(a_{21}c_1 + a_{22}c_2) + b_3(a_{31}c_1 + a_{32}c_2 + a_{33}c_3) = \frac{1}{3}. \] (23)

The fourth-order conditions for this methods are given by
\[ a_{11} = c_1, \quad a_{21} + a_{22} = c_2, \quad a_{31} + a_{32} + a_{33} = c_3, \]
\[ b_1 + b_2 + b_3 = 1, \quad b_1c_1 + b_2c_2 + b_3c_3 = \frac{1}{3}, \]
\[ b_1c_1^2 + b_2c_2^2 + b_3c_3^2 = \frac{1}{5}, \quad b_1a_{11}c_1 + b_2(a_{21}c_1 + a_{22}c_2) + b_3(a_{31}c_1 + a_{32}c_2 + a_{33}c_3) = \frac{1}{15}, \]
\[ b_1a_{11}c_1 + b_2(a_{21}c_1 + a_{22}c_2) + b_3(a_{31}c_1 + a_{32}c_2 + a_{33}c_3) = \frac{1}{15}, \]
\[ b_1a_{11}c_1 + b_2(a_{21}c_1 + a_{22}c_2) + b_3(a_{31}c_1 + a_{32}c_2 + a_{33}c_3) = \frac{1}{15}, \]
\[ b_1a_{11}c_1 + b_2(a_{21}c_1 + a_{22}c_2) + b_3(a_{31}c_1 + a_{32}c_2 + a_{33}c_3) = \frac{1}{15}. \] (24)

From (22) and the first four formulae of (23), we get
\[ b_1 = 1 - b_1 - b_2, \quad a_{11} = \frac{1}{4}b_1, \quad a_{21} = b_1, \quad a_{22} = \frac{1}{2}b_2, \quad a_{31} = b_1, \quad a_{32} = b_2, \]
\[ a_{33} = \frac{1}{3}(1 - b_1 - b_2), \quad c_1 = \frac{1}{2}b_1, \quad c_2 = b_1 + \frac{1}{2}b_2, \quad c_3 = \frac{1}{3}(1 + b_1 + b_2), \] (25)

where \( b_1, b_2 \) are parameters.

**Case one.** Inserting (25) into the the condition \( \sum_{i=1}^{3} b_i c_i^2 = \frac{1}{5} \) appearing in (23) yields
\[ \frac{1}{4}b_1^2b_2 + \frac{1}{4}b_1b_2^2 + \frac{1}{4}b_1 + \frac{1}{4}b_2 - \frac{1}{4}b_1^2 - \frac{1}{2}b_1b_2 + \frac{1}{4} = \frac{1}{3}. \]

We assume that \( b_1 = b_2 \) and then the above condition becomes
\[ 6b_1^3 - 12b_1^2 + 6b_1 - 1 = 0, \] (26)

which has a real root \( b_1 = \sqrt[3]{\frac{8}{6}} \sqrt[3]{2} + \sqrt[3]{2} \). Then, by (25) we get other coefficients as follows
\[ b_2 = 4 + \sqrt[3]{2} + \sqrt[3]{2}, \quad b_1 = 1 - \sqrt[3]{2} - \sqrt[3]{2}, \quad c_1 = 4 + \sqrt[3]{2} + \sqrt[3]{2}, \quad c_2 = 4 + \sqrt[3]{2} + \sqrt[3]{2}, \]
\[ a_{31} = 4 + \sqrt[3]{2} + \sqrt[3]{2}, \quad a_{32} = 4 + \sqrt[3]{2} + \sqrt[3]{2}, \quad a_{33} = 4 - \sqrt[3]{2} - \sqrt[3]{2}. \]

It can be checked that these coefficients satisfy all the third-order conditions (23) and it is denoted by RK3s3 (it was presented in [4]). Then the coefficients of three-stage AEI (41) of order three are given by
\[ a_{21} = a_{21}(c_2 - c_1)φ_1((c_2 - c_1)h\frac{1}{2}B), \quad a_{31} = a_{31}(c_3 - c_1)φ_1((c_3 - c_1)h\frac{1}{2}B), \]
\[ a_{32} = a_{32}(c_3 - c_2)φ_1((c_3 - c_2)h\frac{1}{2}B), \quad a_{21} = a_{21}(c_2 - c_1)φ_1((c_2 - c_1)h\frac{1}{2}B), \]
\[ α_1 = b_1(e^{1-c_1})h\frac{1}{2}B, \quad γ_1 = b_1(e^{1-c_1})h\frac{1}{2}B, \quad γ_2 = b_2(e^{1-c_2})h\frac{1}{2}B, \]
\[ γ_3 = b_3(e^{1-c_3})h\frac{1}{2}B, \quad γ_4 = b_4(e^{1-c_4})h\frac{1}{2}B. \] (27)
We denote this method by AEI3s3.

**Case two.** Similarly, by [22] and [24], we obtain

\[ \frac{1}{4} b_1^2 b_3 + \frac{1}{4} b_1 b_3^2 + \frac{1}{4} b_1 + \frac{1}{4} b_3 - \frac{1}{4} b_1^2 - \frac{1}{2} b_1 b_3 + \frac{1}{4} = \frac{1}{3}, \]

where \( b_1 \) and \( b_3 \) are parameters. If \( b_1 = b_3 \) is considered, one has \( b_1 = b_3 = \frac{4 + 3 \sqrt{3} - \sqrt{7}}{6} \). Other coefficients are got from [25].

\[ b_2 = \frac{-1 - 3 \sqrt{7} - \sqrt{3}}{2}, \quad c_1 = \frac{4 + 3 \sqrt{7} + \sqrt{3}}{2}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{8 - 2 \sqrt{7} - \sqrt{3}}{2}, \]

\[ a_{11} = \frac{4 + 3 \sqrt{7} + \sqrt{3}}{6}, \quad a_{21} = \frac{4 + 3 \sqrt{7} + \sqrt{3}}{6}, \quad a_{22} = \frac{-1 - 3 \sqrt{7} - \sqrt{3}}{2}, \]

\[ a_{31} = \frac{4 + 3 \sqrt{7} + \sqrt{3}}{6}, \quad a_{32} = \frac{-1 - 3 \sqrt{7} - \sqrt{3}}{2}, \quad a_{33} = \frac{4 + 3 \sqrt{7} + \sqrt{3}}{6}. \]

This RK method can be checked to be of order four and it is denoted by RK3s4 (this RK method was given in [21]). Then the coefficients of AEI can be obtained as [27]. This method is of order four and we denote it by AEI3s4.

According to Theorem 3.1 it can be verified that both of these AEI methods are symplectic.

### 5 Numerical tests

In this section, we carry out two numerical experiments to show the efficiency of our AEI methods. The methods for comparison are chosen as follows:

- AEI1s2: the one-stage symplectic AEI of order two presented in this paper;
- AEI2s2: the two-stage symplectic AEI of order two presented in this paper;
- AEI3s3: the three-stage symplectic AEI of order three presented in this paper;
- AEI3s4: the three-stage symplectic AEI of order four presented in this paper;
- RK1s2: the one-stage symplectic RK of order two (implicit midpoint rule);
- RK2s2: the two-stage symplectic RK of order two presented in this paper;
- RK3s3: the three-stage symplectic RK of order three presented in [4];
- RK3s4: the three-stage symplectic RK of order four presented in [21].

**Problem 1.** For the charged-particle dynamics [1], we consider the scalar potential \( U(x) = \frac{1}{100 \sqrt{x_1^2 + x_2^2}} \) and the constant magnetic field \( B = (0, 0, 1)^T \). The initial values are chosen as \( x(0) = (0.7, 1, 0.1)^T, \ v(0) = (0.9, 0.5, 0.4)^T \). For \( \epsilon = 10^{-3} \), we solve the problem with \( t_{end} = 10 \) and \( h = \frac{1}{1000} \), where \( i = 1, 2, 3, 4 \). The global errors against \( \frac{t_{end}}{h} \) are shown in Figure 1(i). Then the results of energy conservation with a fixed step size \( h = \frac{1}{1000} \) in the interval \([0, t_{end}]\) with \( t_{end} = [1, 10, 100, 1000] \) are presented in Figure 1(ii). For \( \epsilon = 10^{-4} \), we solve the problem in \( t_{end} = 10 \) with \( h = [1/10, 1/100, 1/1000, 1/10000] \), and the efficiency curves are presented in Figure 1(iii). Then we integrate this problem with step size \( h = \frac{1}{10000} \) in the interval \([0, t_{end}]\) and \( t_{end} = [1, 10, 100, 1000] \). Figure 1(iv) shows the energy conservation for different methods. We also choose the methods...
AEI1s2, AEI3s4, RK1s2, RK3s4 and then solve this problem on the interval $[0, 300]$ with different stepsizes $h = 1/2, 1/20, 1/60, 1/100$. The numerical flows at the time points $\{\frac{i}{2}\}^6_{i=1}$ are shown in Figure 2. It can be seen clearly that our methods perform uniformly well for all the stepsizes while RK methods behave badly for large stepsizes.

Problem 2. We consider the charged-particle dynamics with another scalar potential $U(x) = x_1^3 - x_2^3 + \frac{1}{5}x_1^4 + x_2^4 + x_3^4$, and the constant magnetic field $B = \frac{1}{2}(0.9, 0.1, 1)^T$. We choose the initial values as $x(0) = (0.0, 1.0, 0.1)^T$ and $v(0) = (0.09, 0.55, 0.30)^T$. Firstly the problem is solved in $[0, 10]$ with $\epsilon = 10^{-3}$ and $h = \frac{1}{100 \times 2^i}$, where $i = 0, 1, 2, 3$. The numerical results are shown in Figure 3(i). Then we integrate this problem with $h = \frac{1}{1000}$ on the interval $[0, t_{end}]$ with $t_{end} =
Figure 2: Problem 1: the flow of different methods.
[1, 10, 100, 1000]. See Figure 3(ii) for the results. For $\epsilon = 10^{-4}$, we solve the problem in $[0, 10]$ with $h = [1/100, 1/1000, 1/10000, 1/100000]$, and present the global errors against $t_{\text{end}}/h$ in Figure 3(iii). Then the results of energy conservation with a fixed step size $h = \frac{1}{10000}$ in the interval $[0, t_{\text{end}}]$ with $t_{\text{end}} = [1, 10, 100, 1000]$ are presented in Figure 3(iv). Finally, we solve it on the interval $[0, 100]$ with $h = 1/20, 1/40, 1/80, 1/160$ and present the numerical flows at the time points $\{\frac{1}{10^i}\}_{i=1}^{1000}$ in Figure 4.

Figure 3: (i) (iii): The logarithm of the global error ($GE$) over the integration interval against the logarithm of $\log_{10}(t_{\text{end}}/h)$. (ii) (iv): The logarithm of the maximum global error of Hamiltonian (GEH) against $\log_{10}(t_{\text{end}})$.

It can be observed from the numerical experiments that the numerical behaviour of the AEI methods is much more better than that of the RK methods.
Figure 4: Problem 2: the flow of different methods.
6 Conclusions

In this paper, explicit symplectic adapted exponential integrators for solving charged-particle dynamics \( \Pi \) are presented and studied. We derive the symplecticity conditions for adapted exponential integrators, and based on those conditions, some explicit symplectic AEI methods up to order four are constructed for solving charged-particle dynamics in a strong and constant magnetic field. Furthermore, the numerical experiments show that our methods derived in this paper have remarkable efficiency in comparison with some symplectic RK methods in the scientific literature.

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