A two-step symmetric method for charged-particle dynamics in a normal or strong magnetic field

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Abstract
The study of the long time conservation for numerical methods poses interesting and challenging questions from the point of view of geometric integration. In this paper, we analyze the long time energy and magnetic moment conservations of two-step symmetric methods for charged-particle dynamics. A two-step symmetric method is proposed and its long time behaviour is shown not only in a normal magnetic field but also in a strong magnetic field. The approaches to dealing with these two cases are based on the backward error analysis and modulated Fourier expansion, respectively. It is obtained from the analysis that the method has better long time conservations than the variational method which was researched recently in the literature.

Keywords Charged-particle dynamics · Two-step symmetric methods · Backward error analysis · Modulated Fourier expansion

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1 Introduction

The numerical investigation for charged-particle dynamics has received much attention in the last few decades (see e.g. [1, 8, 9, 12, 13, 17]). In this paper, we analyze the long time conservations of two two-step symmetric methods for solving charged-particle dynamics of the form (see [10])

\[ \ddot{x} = \dot{x} \times \frac{1}{\epsilon} B(x) + F(x), \quad x(0) = x_0, \quad \dot{x}(0) = \dot{x}_0, \quad t \in [0, T], \]

where \( B(x) = \nabla \times A(x) \) is a magnetic field with the vector potential \( A(x) \in \mathbb{R}^3 \), the position of a particle moving in this field is denoted by \( x(t) \in \mathbb{R}^3 \), and \( F(x) = -\nabla U(x) \) is an electric field with the scalar potential \( U(x) \). The energy of this dynamics

\[ E(x, v) = \frac{1}{2} |v|^2 + U(x) \]

is preserved exactly along the solution \( x \) and the velocity \( v = \dot{x} \) of the particle. It is assumed that the initial values are bounded as

\[ x_0 = O(1), \quad v_0 := \dot{x}_0 = O(1). \]

In this work, we focus on the study of the following two regimes of \( \epsilon \):

- one regime is that \( \epsilon \) in (1) is assumed to be one which means that the magnetic field is “normal”;
- the other regime is that \( \epsilon \) in (1) is assumed to satisfy \( 0 < \epsilon \ll 1 \) which means that the magnetic field is “strong”.

For the normal magnetic field, if the scalar and vector potentials have the invariance properties

\[ U(e^{\tau S} x) = U(x), \quad e^{-\tau S} A(e^{\tau S} x) = A(x) \]

for all real \( \tau \) with a skew-symmetric matrix \( S \), then the momentum

\[ M(x, v) = (v + A(x))^T S x \]

is conserved along solutions of (1). This momentum is an invariance of the charged-particle dynamics which was given in [8, 9] and the conservation property can be shown by using Noether’s theorem.

For the strong magnetic field, it has been shown in [10] that the magnetic moment

\[ I(x, v) = \frac{1}{2} \frac{|v_\perp|^2}{|B(x)|} \]

is nearly conserved along the solution over long time scales, where \( v_\perp \) is orthogonal to \( B(x) \) and is given by \( v_\perp = \frac{\nabla \times B(x)}{|B(x)|} \).
In order to effectively solve charged-particle dynamics, many methods have been developed and studied in recent decades, such as the Boris method (see e.g. [1, 8, 16]), symplectic or K-symplectic algorithms (see e.g. [13, 14, 17, 19, 20]), symmetric multistep methods (see e.g. [9]), volume-preserving algorithms (see e.g. [12]), energy-preserving methods (see e.g. [14, 15]), variational integrators in a strong magnetic field (see e.g. [10]) and exponential integrators in a constant magnetic field (see e.g. [14]).

On the basis of these studies, this paper analyzes the long time conservations of a two-step symmetric method for charged-particle dynamics not only in a normal magnetic field but also in a strong magnetic field. We will show the energy and momentum conservations of the method in a normal magnetic field and derive the modified energy and modified magnetic moment preservations in a strong magnetic field. To this end, the backward error analysis is employed for the first case, and the modulated Fourier expansion is used for the strong magnetic field.

The main contribution of this paper is to show that the method has better long time conservations than the variational method which was researched recently in [10]. The paper is organized as follows. In Sect. 2, we formulate the scheme of the method. Section 3 gives the main results of this paper and carries out some illustrative numerical experiments. Then the results in a normal magnetic field are proved in Sect. 4, and the conservations in a strong magnetic field are shown in Sect. 5. The last section is concerned with the conclusions of this paper.

2 The scheme of the method

A variational integrator is constructed as follows. We first approximate $x(t)$ as the linear interpolant of $x_n$ and $x_{n+1}$ and then approximate the integral of the Lagrangian $L(x(t), \dot{x}(t))$ by the midpoint rule (see e.g. Example 6.3, Chap. VI of [11, 19]). This gives the following variational integrator.

**Definition 1** The method for solving the charged-particle dynamics (1) is defined by a two-step method

$$x_{n+1} - 2x_n + x_{n-1} = \frac{h}{2} A^T(x_{n+1/2}) (x_{n+1} - x_n) + \frac{h}{2} A^T(x_{n-1/2}) (x_n - x_{n-1})$$

$$- \frac{h}{e} (A(x_{n+1/2}) - A(x_{n-1/2})) + \frac{h^2}{2} (F(x_{n+1/2}) + F(x_{n-1/2})),$$

and $v_{n+1} = 2 \frac{x_{n+1} - x_n}{h} - v_n$, where $h$ is a stepsize and $x_{n+1/2} = \frac{x_n + x_{n+1}}{2}$. We denote this method by TSM.

**Remark 1** It is clear that this method is a symmetric method of order two. From the fact that the method (5) is a variational integrator, it follows that for TSM, with the momenta $p_n = v_n + A(x_n)$, the map $(x_n, p_n) \to (x_{n+1}, p_{n+1})$ is symplectic.
Remark 2 Another variational integrator for charged-particle dynamics was presented in [10] where the integrator is derived by replacing x(t) with the linear interpolant of the endpoint positions and then approximating the integral by the trapezoidal rule (see e.g. Example 6.2, Chap. VI of [11]). In comparison with this method, TSM takes advantage of the midpoint rule, which makes it have different modified energy and momentum conservations.

3 Main results and numerical experiment

3.1 Results in a normal magnetic field

The results of this subsection are given for the method applied to charged-particle dynamics in a normal magnetic field.

Theorem 1 (Energy conservation of TSM) Assume that the numerical solution (5) stays in a compact set that is independent of h, then the two-step symmetric method (5) has a long time energy conservation

\[ |E(x_{n+1/2}, v_{n+1/2}) - E(x_{1/2}, v_{1/2})| \leq C h^2 \quad \text{for} \quad nh \leq h^{-N}, \]

where \( N \geq 2 \) is an arbitrary truncation number and the constant \( C \) is independent of \( n \) and \( h \) as long as \( nh \leq h^{-N} \).

Remark 3 It is noted that the long term energy conservation of symplectic methods has been studied for different kinds of systems, such as for Hamiltonian systems in [3, 6], wave equations in [4, 5, 18], Schrödinger equations in [2], charged-particle dynamics in a strong magnetic field in [10]. Meanwhile, a kind of symmetric multi-step methods has been researched in [9] for charged-particle dynamics in a normal magnetic field. However, it seems that the long time energy conservation of symplectic methods for charged-particle dynamics in a normal magnetic field has not been considered, which motivates Theorem 1.

Theorem 2 (Momentum conservation of TSM) For the two-step symmetric integrator (5), it is assumed that the numerical solution (5) stays in a compact set which is independent of h. Then the momentum is nearly conserved along the numerical solution as follows

\[ |M(x_{n+1/2}, v_{n+1/2}) - M(x_{1/2}, v_{1/2})| \leq C h^2 \quad \text{for} \quad nh \leq h^{-N}, \]

where \( N \geq 2 \) is the truncation number and \( C \) is a constant independent of \( n \) and \( h \).

Remark 4 With these two results, it is confirmed that the method TSM has good long time conservations of energy and momentum for a normal magnetic field.
3.1.1 Experiment

In order to show the efficiency of the method, we choose the following two well-known methods for comparison.

- BORIS. The Boris method given in [1]:
  \[ x_{n+1} - 2x_n + x_{n-1} = \frac{h}{2} \left( x_{n+1} - x_{n-1} \right) \times \frac{1}{e} B(x_n) - h^2 \nabla U(x_n). \]

- VARM. The variational method given by Example 6.2, Chap. VI of [11] and also discussed in [9, 19]:
  \[ x_{n+1} - 2x_n + x_{n-1} = \frac{h}{2} A^t(x_n) \left( x_{n+1} - x_n \right) - \frac{h}{2} e (A(x_{n+1}) - A(x_n)) - h^2 \nabla U(x_n). \]

We consider the charged particle system (1) with (see [9])

\[ e = 1, \quad U(x) = \frac{1}{100} \sqrt{x_1^2 + x_2^2}, \quad B(x) = \left( 0, 0, \sqrt{x_1^2 + x_2^2} \right)^T. \]

The momentum of this problem is given by

\[ M(x, v) = \left( v_1 - \frac{x_2}{3} \sqrt{x_1^2 + x_2^2} \right) x_2 - \left( v_2 + \frac{x_1}{3} \sqrt{x_1^2 + x_2^2} \right) x_1. \]

We choose the initial values \( x(0) = (0, 1, 0.1)^T, \quad v(0) = (0.09, 0.05, 0.20)^T \) and solve it on \([0, 10,000]\) with \( h = 0.1, 0.05 \). The conservations of the energy and momentum for different methods are displayed in Figs. 1 and 2. It can be observed from Figs. 1 and 2 that the method TSM proposed in this paper shows remarkable long-time numerical behaviour.

![Energy conservation with h=0.1](image1)

![Energy conservation with h=0.05](image2)

Fig. 1 The errors of energy against \( t \)
3.2 Results in a strong field

When the magnetic field is strong, long time conservations can also be obtained for the method TSM. In this subsection, we present the results of the method TSM for charged-particle dynamics in a strong magnetic field.

3.2.1 Near-conservation of energy

We define

$$\xi(x) = 2 \arctan\left( \frac{h}{2e|B(x)|} \right)$$

and consider the modified energy

$$H_h(x, v) = H(x, v) + (\xi \csc(\xi) - 1)I(x, v)|B(x)|.$$ 

**Theorem 3** (Energy conservation of TSM) Suppose that for $0 < \epsilon \leq \epsilon_0$ and $0 < h \leq h_0$ with $\epsilon_0 > 0$ and $h_0 > 0$, the following holds. Let $N \geq 1$ be an arbitrary integer and the stepsize $h$ is chosen such that $\epsilon h|B(x_n)| \leq 2 \tan\left( \frac{\pi}{2(N+3)} \right)$ for some $N \geq 1$. It is assumed further that the numerical solution of the TSM stays in a compact set $K$. Then TSM has the following near conservation of modified energy

$$\left| H_h(x_{n+1/2}, v_{n+1/2}) - H_h(x_{1/2}, v_{1/2}) \right| \leq Ce \quad \text{for} \quad nh \leq \epsilon^{-N},$$

Fig. 2 The errors of momentum against $t$
where the constant $C$ is independent of $\epsilon$, $n$ and $h$ as long as $nh \leq h^{-N}$, but depends on $N$, the bounds of the $N+1$ derivatives of $B$ and $E$ on the compact set $K$, and the constants in (3).

**Remark 5** It is noted that when the magnetic field is strong ($0 < \epsilon \ll 1$), by using backward error analysis, the result of Theorem 1 is true only under the condition that $\frac{h}{\epsilon}$ is small. This brings a very strict requirement of the stepsize $h$. In other words, backward error analysis can only be successfully applied to numerical solutions of charged-particle dynamics in a normal magnetic field. For the dynamics in a strong magnetic field, the technique of modulated Fourier expansions will be used to derive the energy conservation of TSM. The result given in Theorem 3 does not rely on the smallness of $\frac{h}{\epsilon}$ and this is of major importance in the context of charged-particle dynamics in a strong magnetic field.

### 3.2.2 Near-conservation of the magnetic moment

We define the modified magnetic moment

$$I_h(x, v) = \sec^2(\frac{\xi(x)}{2})I(x, v) = (\tan^2(\frac{\xi(x)}{2}) + 1)I(x, v) = \left(\frac{h^2}{4\epsilon^2} |B(x)|^2 + 1\right)I(x, v).$$

**Theorem 4** (Magnetic moment conservation of TSM.) Under the conditions of Theorem 4, the modified magnetic moment is nearly conserved over long times

$$|I_h(x_{n+1/2}, v_{n+1/2}) - I_h(x_{1/2}, v_{1/2})| \leq C\epsilon \quad \text{for } nh \leq \epsilon^{-N}.$$

**Remark 6** We remark that the modified energy $H_h$ and modified magnetic moment $I_h$ are artificial such that the proof of Theorems 3 and 4 works. In other words, the scheme of numerical method determines its modulated Fourier expansion and two almost-invariants of the modulated functions, which imply the scheme of modified energy and modified magnetic moment. Different numerical methods may possess different modified energies and modified magnetic moments. For example, the method VARM researched recently in [10] was shown to have another modified energy and modified magnetic moment which are different from $H_h$ and $I_h$ given in this paper. It also should be noted that if a method does not have the almost-invariants of the modulated functions, long term conservations of modified energy and modified magnetic moment cannot be obtained.

**Remark 7** It is noted that the long term analysis of the method VARM was researched recently in [10] for charged-particle dynamics in a strong magnetic field. The conservations of a modified energy and a modified magnetic moment were proved there for VARM. It can be seen from Theorems 3 and 4 that TSM also has modified energy and modified magnetic moment conservations. Moreover, according to the analysis of [10] and the results of Theorems 3 and 4, for small $\xi$, the
modified energy and modified magnetic moment of VARM and TSM are given respectively as

| Method | Modified energy | Modified magnetic moment |
|--------|-----------------|--------------------------|
| VARM   | $H + \frac{5}{12} \varepsilon^2 |B|$ | $(1 + \frac{1}{5} \varepsilon^2)I$ |
| TSM    | $H + \frac{1}{6} \varepsilon^2 |B|$ | $(1 + \frac{1}{4} \varepsilon^2)I$ |

This shows that compared with VARM, the modified energy and modified magnetic moment that TSM nearly preserves are closer to the original energy $H$ and magnetic moment $I$.

### 3.2.3 Experiments

**Problem 1** We still consider the problem given in Sect. 3.1.1 but with $\varepsilon = 0.01$. We solve it on $[0, 10000]$ by the second method with $h = 0.01$ and $0.005$. The conservations of the modified energy and the modified magnetic moment are displayed in Fig. 3. Then we choose $h = \varepsilon$ and show the results in Fig. 4 for different $\varepsilon, \varepsilon/4, \varepsilon/16$ with $\varepsilon = 0.1$.

**Problem 2** We consider another magnetic field (see [10])

![Conservations with h=0.01](image1)

**Fig. 3** Results of Problem 1. The errors of modified energy (ME) and modified magnetic moment (MM) against $t$
and the initial values are taken as $x(0) = (0.0, 1.0, 0.1)^T$ and $v(0) = (0.09, 0.55, 0.30)^T$. We solve this problem on $[0, 10000]$ with $h = 0.01, 0.005$ and the conservations of the modified energy and the modified magnetic moment are displayed in Fig. 5. Figure 6 shows the results for $h = \epsilon$ and for different $\epsilon, \epsilon/4, \epsilon/16$ with $\epsilon = 0.05$. 

$B(x) = \nabla \times \left( \frac{1}{4} (x_3^2 - x_1^2, x_3^2 - x_2^2, x_2^2 - x_1^2) \right)$

and the initial values are taken as $x(0) = (0.0, 1.0, 0.1)^T$ and $v(0) = (0.09, 0.55, 0.30)^T$. We solve this problem on $[0, 10000]$ with $h = 0.01, 0.005$ and the conservations of the modified energy and the modified magnetic moment are displayed in Fig. 5. Figure 6 shows the results for $h = \epsilon$ and for different $\epsilon, \epsilon/4, \epsilon/16$ with $\epsilon = 0.05$. 

$B(x) = \nabla \times \left( \frac{1}{4} (x_3^2 - x_1^2, x_3^2 - x_2^2, x_2^2 - x_1^2) \right)$
4 Long term analysis in a normal magnetic field (Proof of Theorems 1–2)

In the analysis of this section, we will use backward error analysis (see Chap. IX of [11]).

4.1 Proof of Theorem 1

Following the idea of backward error analysis, we search for two modified differential equations (as a formal series in powers of $h$) such that their solutions $y(t)$ and $w(t)$ formally satisfy $y(nh) = x_n$ and $w(nh) = v_n$, where $x_n$ and $v_n$ represent the numerical solution obtained by the method (5). According to the scheme of the method, such functions have to satisfy

$$y(t + h) - 2y(t) + y(t - h) = \frac{h}{2}A(t)((y(t + h) + y(t))/2)(y(t + h) - y(t)) + \frac{h}{2}A(t)((y(t) + y(t - h))/2)(y(t) - y(t - h)) - h(A((y(t + h) + y(t))/2) - A((y(t) + y(t - h))/2)) + \frac{h^2}{2}(F((y(t + h) + y(t))/2) + F((y(t) + y(t - h))/2)).$$

By the operators

$$L_1(\zeta) = \zeta - 1, \quad L_2(\zeta) = \frac{\zeta + 1}{2},$$

and by letting $z(t) = L_2(e^{hD})y(t)$, these can be rewritten as

---

**Fig. 6** Results of Problem 2. The errors of modified energy and modified magnetic moment for different $\epsilon$.
\[
\frac{1}{h^2}L_1^2L_2^{-2}(e^{hD})z = \frac{1}{h}A'(z)(L_1L_2^{-1}(e^{hD})z) - \frac{1}{h}L_1L_2^{-1}(e^{hD})A(z) + F(z). \tag{6}
\]

Using the following properties
\[
L_1^2L_2^{-2}(e^{hD}) = h^2D^2 - \frac{1}{6}h^4D^4 + \frac{17}{720}h^6D^6 + \cdots,
\]
\[
L_1L_2^{-1}(e^{hD}) = hD - \frac{1}{12}h^3D^3 + \frac{1}{120}h^5D^5 + \cdots,
\]
we get the modified differential equation
\[
\ddot{z} = \dot{z} \times B(z) + F(z) + h^2G_2(z, \dot{z}) + h^4G_4(z, \dot{z}) + \cdots,
\]
where \( G_j(z, \dot{z}) \) for \( j = 1, \ldots \) are \( h \)-independent functions determined uniquely.

A multiplication of (6) with \( \dot{z}^\dagger \) yields
\[
\frac{1}{h^2}\ddot{z}^\dagger(L_1^2L_2^{-2}(e^{hD})z) = \frac{1}{h}\dot{z}^\dagger(A'(z)(L_1L_2^{-1}(e^{hD})z) - L_1L_2^{-1}(e^{hD})A(z))
- \frac{d}{dt}U(z) + \mathcal{O}(h^N). \tag{8}
\]

The left-hand side is the time derivative of an expression in which the appearing second and higher derivatives of \( z \) can be substituted as functions of \( (z, \dot{z}) \). The first term in the right-hand side of (8) can also be written as the time derivative of a function by using the way given in [9] as follows. It is shown in [9] that for a function \( f \) that is analytic at 0, partial integration shows that for time-dependent smooth functions \( u \) and \( v \),
\[
\langle f(hD)u, v \rangle - \langle u, f(-hD)v \rangle \text{ is a total derivative up to } \mathcal{O}(h^N) \text{ for arbitrary } N, \tag{9}
\]
where \( \langle \cdot, \cdot \rangle \) is Euclidean inner product. Moreover, it is true that
\[
\langle \dot{z}, A'(z)(L_1L_2^{-1}(e^{hD})z) \rangle = \langle A'(z)\dot{z}, L_1L_2^{-1}(e^{hD})z \rangle = \langle DA(z), L_1L_2^{-1}(e^{hD})z \rangle.
\]

Thence the first term in the right-hand side of (8) becomes
\[
\frac{1}{h}\left(\langle DA(z), L_1L_2^{-1}(e^{hD})z \rangle - \langle L_1L_2^{-1}(e^{hD})A(z), Dz \rangle\right),
\]
which is a total derivative up to \( \mathcal{O}(h^{N-1}) \) for arbitrary \( N \) by considering (9) with \( f(hD) = L_1L_2^{-1}(e^{hD})/(hD) \), \( u = DA(z) \) and \( v = Dz \). Clearly, it follows from (7) that \( f(-hD) = f(hD) \), which is used here. Meanwhile, this function is of magnitude \( \mathcal{O}(h^2) \), because \( L_1L_2^{-1}(e^{hD})z = \dot{z} + \mathcal{O}(h^2) \).

According to the above analysis, there exist \( h \)-independent functions \( E_{2j}(x, v) \) such that the function
\[
E_h(x, v) = E(x, v) + h^2E_2(x, v) + h^4E_4(x, v) + \cdots,
\]
truncated at the \( \mathcal{O}(h^N) \) term, satisfies \( \frac{d}{dt}E_h(z, \dot{z}) = \mathcal{O}(h^N) \) along solutions of the modified differential equation (6). The proof is complete.
4.2 Proof of Theorem 2

The proof is analogous to the previous proof when (6) is multiplied with \((Sz)\). It is noted that by using \(A'(z)Sz = SA(z)\) (see [9]), we have

\[
(Sz)^\dagger A'(z)(L_1L_2^{-1}(e^{hD})z) - (Sz)^\dagger L_1L_2^{-1}(e^{hD})A(z)
\]

\[
= (A'(z)Sz)^\dagger (L_1L_2^{-1}(e^{hD})z) + z^\dagger L_1L_2^{-1}(e^{hD})SA(z)
\]

\[
= (SA(z))^\dagger (L_1L_2^{-1}(e^{hD})z) + z^\dagger L_1L_2^{-1}(e^{hD})SA(z)
\]

\[
= \langle SA(z), L_1L_2^{-1}(e^{hD})z \rangle - \langle L_1L_2^{-1}(e^{-hD})SA(z), z \rangle,
\]

which is a total derivative up to \(O(h^N)\) for arbitrary \(N\). We remark that \(L_1L_2^{-1}(e^{hD}) = -L_1L_2^{-1}(e^{-hD})\) is used here. According to \(z^\dagger S(z \times B(z)) = -\frac{d}{dt} (z^\dagger SA(z))\) and \(z^\dagger \nabla U(z) = 0\), it is obtained that there exist \(h\)-independent functions \(M_2(x, v)\) such that the function

\[
M_h(x, v) = M(x, v) + h^2 M_2(x, v) + h^4 M_4(x, v) + \cdots,
\]

truncated at the \(O(h^N)\) term, satisfies \(\frac{d}{dt} M_h(z, \dot{z}) = O(h^N)\) along solutions of (6). This shows the result.

5 Long term analysis in a strong magnetic field (Proof of Theorems 3–4)

In this section, we will use the technique of modulated Fourier expansion for studying long-time conservation properties. Modulated Fourier expansion was firstly developed in [6] and was extended to systems with solution dependent frequency in [7, 10]. Using the novel modulated Fourier expansion with state-dependent frequencies and eigenvectors recently developed in [10], we will derive the expansion of the method TSM and show two almost-invariants of the modulated functions.

5.1 Modulated Fourier expansion

Proposition 1 For \(0 \leq nh \leq T_\epsilon\) with \(T_\epsilon = O(\epsilon)\), it is assumed that the numerical solution \(x_n\) of the method TSM (5) stays in a compact set \(K\) and

\[
\frac{h}{\epsilon} |B(x_{n+1/2})| \leq 2 \tan \left( \frac{C}{2N+2} \right) \text{ with } C < \pi
\]

for some integer \(N \geq 1\). Then the numerical solution \(x_{n+1/2}\) admits the following modulated Fourier expansion
\[ x_{n+1/2} = \sum_{|k| \leq N+1} e^{i k \phi(t)/\epsilon} \zeta^k(t) + O(\epsilon^2), \quad t = (n + \frac{1}{2})h, \]

where the phase function \( \phi(t) \) is given by

\[ \tan \left( \frac{1}{2} \eta \phi \right) = \frac{\eta}{2} |B(\zeta^0)|. \]  

(10)

The bounds of the functions \( \zeta^k(t) \) as well as their derivatives (up to order \( N \)) are

\[ \zeta^k(t) = O(e^{|k|}) \quad \text{forall } |k| \leq N + 1 \]

and further one has

\[ \zeta^0 \times B(\zeta^0) = O(\epsilon), \quad P_j(\zeta^0)\zeta^k = O(\epsilon^2) \quad \text{textforall } |k| = 1, j \neq k. \]

The functions \( \zeta^k(t) \) are unique up to \( O(e^{N+2}) \) and the constants symbolised by \( O \) independent of \( n \) and \( \epsilon \) as long as \( 0 \leq nh \leq T_\epsilon \), but depend on \( N, T \), the constants in (3), and the bounds of derivatives of \( A(x) \) and \( U(x) \). The orthogonal projections \( P_j \) onto the eigenspaces are referred to [10].

**Proof** The proof is analogous to the proof in Section 5 of [10] but with some necessary modifications. For brevity we only present the main differences and for the details we refer to [10].

As previous analysis, the method TSM (5) has the following scheme

\[ \frac{1}{h^2} L_1^2 L_2^{-2}(e^{hD})z_n = \frac{1}{e^h} A^{(c)}(z_n)(L_1 L_2^{-1}(e^{hD})z_n) - \frac{1}{e^h} L_1 L_2^{-1}(e^{hD})A(z_n) + F(z_n), \]

where \( z_n = \frac{x_n + x_{n+1}}{2} \). For the solution \( z_n \) we consider the following modulated Fourier expansion

\[ z_n \approx \sum_{k \in \mathbb{Z}} e^{i k \phi(t)/\epsilon} \zeta^k(t) = \sum_{k \in \mathbb{Z}} Y^k(t), \]

where \( Y^k(t) = e^{i k \phi(t)/\epsilon} \zeta^k(t), \quad t = t_{n+1/2} := \frac{t_n + t_{n+1}}{2}, \) and the functions \( \phi \) and \( \zeta^k \) depend on the stepsize \( h \) and \( \eta = h/\epsilon \).

For the operators \( \frac{1}{h} L_1 L_2^{-1}(e^{hD}) \) and \( \frac{1}{h^2} L_1^2 L_2^{-2}(e^{hD}) \), with careful computations it is obtained that

\[ \frac{1}{h} L_1 L_2^{-1}(e^{hD})Y^k(t) = e^{i k \phi(t)/\epsilon} \sum_{j \geq 0} e^{j-1} c_j^1 \frac{d^j}{dt^j} \zeta^k(t), \]

\[ \frac{1}{h^2} L_1^2 L_2^{-2}(e^{hD})Y^k(t) = e^{i k \phi(t)/\epsilon} \sum_{j \geq 0} e^{j-2} d_j^1 \frac{d^j}{dt^j} \zeta^k(t), \]

where \( c^0_{2j} = d^0_{2j+1} = 0 \) and \( c^0_{2j+1} = \alpha_{2j+1} \eta^{2j}, \quad d^0_{2j} = \beta_{2j} \eta^{2j-2} \). Here \( \alpha \) and \( \beta \) are the coefficients appearing in the following series.
The first coefficients for \( k \neq 0 \) are defined by

\[
2 \tanh(t/2) = \sum_{j \geq 0} \alpha_j t^j, \quad 4 \tanh^2(t/2) = \sum_{j \geq 0} \beta_j t^j.
\]

It is noted that these coefficients depend on \( /u1D716, /u1D702 \) and \( t \) via derivatives of \( /u1D719(t) \).

For the method TSM, from the following required condition given in [10]

\[
\text{the result (10) is obtained. The } e^{\pm 1}_{\pm 1} \text{ and } e^j_k \text{ presented in [10] are replaced by}
\]

\[
ge^{\pm 1}_{\pm 1} = \pm \frac{2i}{\eta} \tan \left( \frac{1}{2} k \eta \phi \right) \sec^2 \left( \frac{1}{2} k \eta \phi \right),
ge^j_k = -\frac{4}{\eta^2} \tan \left( \frac{1}{2} k \eta \phi \right) \left( \tan \left( \frac{1}{2} k \eta \phi \right) - j \tan \left( \frac{1}{2} \eta \phi \right) \right).
\]

\( H(t) = H(0) + O(\epsilon) \text{ for } 0 \leq t \leq T \epsilon, \)

\( H(t_n+1/2) = H(x_{n+1/2}, \nu_{n+1/2}) + O(\epsilon) \text{ for } nh \leq T \epsilon, \)

where the constants symbolised by \( O \) are independent of \( n, h \) and \( \epsilon \), but depends on \( N \).

\textbf{Proposition 2} Under the conditions of Proposition 1, there exists a function \( \mathcal{H}(\zeta) \) such that

\[
\mathcal{H}(\zeta)(t) = \mathcal{H}(\zeta)(0) + O(t^N) \text{ for } 0 \leq t \leq T \epsilon, \quad \mathcal{H}(\zeta)(t_{n+1/2}) = H_h(x_{n+1/2}, \nu_{n+1/2}) + O(\epsilon) \text{ for } nh \leq T \epsilon, \]

where the constants symbolised by \( O \) are independent of \( n, h \) and \( \epsilon \), but depends on \( N \).

\textbf{Proof} • Proof of the first statement. For \( |k| > N + 1 \), it is assumed that \( Y^k(t) = 0 \). The equation (12) for the modulation functions can be written as
where $A_j(Y)$ and $U(Y)$ are given by (see [10])

$$U(Y) = \sum_{0 \leq m \leq N+1, s(a)=0} \frac{U^{(m)}}{m!} (Y^0) Y^a,$$

$$A(Y) = \left( \sum_{0 \leq m \leq N+2, s(a)=k} \frac{A^{(m)}}{m!} (Y^0) Y^a \right)_{k \in \mathbb{Z}} = \left( A_k(Y) \right)_{k \in \mathbb{Z}}.$$

Multiplication of (12) with $(\dot{Y}^k)^*$ and summation over $k$ yields

$$\sum_k (\dot{Y}^k)^* \frac{1}{h^2} L_1^2 L_2^{-2} (\dot{e}h D) Y^k + \frac{1}{\epsilon} \sum_k \left( \frac{d}{dt} A_k(Y)^* \frac{L_1 L_2^{-1} (\dot{e}h D)}{h} Y^k \right)$$

$$- (\dot{Y}^k)^* \frac{L_1 L_2^{-1} (\dot{e}h D)}{h} A_k(Y) + \frac{d}{dt} U(Y) = O(\epsilon^N).$$

By the expansion (7) of the operator $\frac{1}{h^2} L_1^2 L_2^{-2}$ and the analysis given in Theorem 5.1 of [7], we know that the first sum is a total derivative. The second sum is a total differential by the proof of Theorem 1 given in this paper. Therefore, the left-hand side is a total derivative of function $H[\zeta]$ such that

$$\frac{d}{dt} H[\zeta] = O(\epsilon).$$

The first result of the theorem is shown.

- **Proof of the second statement.** In what follows, we prove the second statement of the theorem. To this end, one needs to determine the dominant part of

$$H[\zeta](t) = K[\zeta](t) + \mathcal{M}[\zeta](t) + \mathcal{U}(\zeta(t)),$$

where the time derivatives of $K, \mathcal{M}, \mathcal{U}$ equal the three corresponding terms on the left-hand side of (13).

Firstly, it is clear that

$$\mathcal{U}[\zeta] = U(\zeta^0) + O(\epsilon).$$

For $K[\zeta]$, we compute
\[ 
\sum_k (Y^k)^* \frac{1}{h^2} L_2^2 L_2^{-2} (e^{hD}) Y^k = \sum_k \left( \hat{\zeta}^k + \frac{ik\phi}{e} \right)^* \left( \sum_{l \geq 0} e^{l-2} \frac{d^l}{dt^l} \hat{\zeta}^k(t) \right) \\
= (\hat{\zeta}^0)^* \hat{\zeta}^0 + \sum_{k=\pm 1} \left( \left( \frac{ik\phi}{e} \right)^* \frac{1}{e^2} d_0^k \psi^k + (\hat{\zeta}^k)^* \frac{1}{e^2} d_0^k \psi^k + \left( \frac{ik\phi}{e} \right)^* \frac{1}{e^2} d_0^k \psi^k \right) + O(e) \\
= (\hat{\zeta}^0)^* \hat{\zeta}^0 + \frac{2d\phi}{e^2} (2 - \cos(\eta\phi)) \sec^4 \left( \frac{1}{2} \eta \phi \right) |\zeta| |^2 \\
+ \frac{4}{e^2 \eta^2} \tan \left( \frac{1}{2} \eta \phi \right) \left( \eta \phi \sec^2 \left( \frac{1}{2} \eta \phi \right) - \tan \left( \frac{1}{2} \eta \phi \right) \right) ((\zeta^1)^* \zeta^1 + (\zeta^1)^* \zeta^1) + O(e). 
\]

It can be checked that
\[ 
\frac{2}{\eta^2} \frac{d}{dt} \tan \left( \frac{1}{2} \eta \phi \right) \left( \eta \phi \sec^2 \left( \frac{1}{2} \eta \phi \right) - \tan \left( \frac{1}{2} \eta \phi \right) \right) = \phi \phi (2 - \cos(\eta\phi)) \sec^4 \left( \frac{1}{2} \eta \phi \right). 
\]

Therefore, we have
\[ 
\mathcal{K}[\zeta] = \frac{1}{2} |\zeta^0| |^2 + \frac{4 |\zeta^1| |^2}{e^2 \eta^2} \tan \left( \frac{1}{2} \eta \phi \right) \left( \eta \phi \sec^2 \left( \frac{1}{2} \eta \phi \right) - \tan \left( \frac{1}{2} \eta \phi \right) \right) + O(e). 
\]

We then turn to \( \mathcal{M}[\zeta] \). Since the term \( k = 0 \) is of size \( O(e) \), the dominating terms appear for \( k = \pm 1 \), which read
\[ 
\frac{1}{e} \sum_{k=\pm 1} \left( \frac{d}{dt} A_k(Y)^* \frac{L_1 L_2^{-1} (e^{hD})}{h} \hat{Y}^k - \hat{Y}^k)^* \frac{L_1 L_2^{-1} (e^{hD})}{h} \partial A_k(Y) \right) \\
= \frac{ik\phi}{e^2} (c_0^1 + c_0^{-1}) ((A'(\zeta^0) \zeta^1)^* \zeta^1 - (\zeta^1)^* A'(\zeta^0) \zeta^1) \\
+ \frac{1}{e^2} (c_0^1 - i\phi c_0^{-1}) (A'(\zeta^0) \zeta^1)^* \zeta^1 + (A'(\zeta^0) \zeta^1)^* \zeta^1 \\
-(\zeta^1)^* A'(\zeta^0) \zeta^1 - (\zeta^1)^* A'(\zeta^0) \zeta^1) + O(e). 
\]

It follows from [10] that
\[ 
(A'(\zeta^0) \zeta^1)^* \zeta^1 - (\zeta^1)^* A'(\zeta^0) \zeta^1 = i \left| B(\zeta^0) \right| \left| \zeta^1 \right| |^2 + O(e). 
\]

Moreover, according to (11), we have
\[ 
c_0^1 + c_0^{-1} = \eta \tan \left( \frac{1}{2} \eta \phi \right) \sec^2 \left( \frac{1}{2} \eta \phi \right) \phi + O(e^2), \\
c_0^1 - i\phi c_0^{-1} = i \phi \left( \tan \left( \frac{1}{2} \eta \phi \right) - \sec^2 \left( \frac{1}{2} \eta \phi \right) \right) + O(e) 
\]
and it can be checked that the following relation holds.
Based on these analysis, the dominating terms of $\mathcal{M}[\zeta]$ are

$$\mathcal{M}[\zeta] = \left( \frac{\tan \left( \frac{1}{2} \eta \phi \right)}{\frac{1}{2} \eta \phi} - \sec^2 \left( \frac{1}{2} \eta \phi \right) \right) \phi |B(\xi^0)| \frac{|\xi_1^1|^2}{\epsilon^2} + \mathcal{O}(\epsilon).$$

Therefore, $\mathcal{H}[\zeta]$ is obtained as follows

$$\mathcal{H}[\zeta](t) = \frac{1}{2} \left| \xi^0 \right|^2 + \frac{4|\xi_1^1|^2}{\epsilon^2 \eta^2} \tan \left( \frac{1}{2} \eta \phi \right) \left( \eta \phi \sec^2 \left( \frac{1}{2} \eta \phi \right) - \tan \left( \frac{1}{2} \eta \phi \right) \right)$$

$$+ \left( \frac{\tan \left( \frac{1}{2} \eta \phi \right)}{\frac{1}{2} \eta \phi} - \sec^2 \left( \frac{1}{2} \eta \phi \right) \right) \phi |B(\xi^0)| \frac{|\xi_1^1|^2}{\epsilon^2} + U(\xi^0) + \mathcal{O}(\epsilon).$$

On the other hand, we consider the dominant term in

$$E\left(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}\right) = \frac{1}{2} \left| v_{n+\frac{1}{2}} \right|^2 + U\left(x_{n+\frac{1}{2}}\right).$$

Inserting the modulated Fourier expansion into $x_{n+\frac{1}{2}}$ yields $x_{n+\frac{1}{2}} = \xi^0(t_{n+\frac{1}{2}}) + \mathcal{O}(\epsilon)$ and further $U(x_{n+\frac{1}{2}}) = U(\xi^0(t_{n+\frac{1}{2}})) + \mathcal{O}(\epsilon)$. It is assumed that the modulated Fourier expansion for $v_{n+\frac{1}{2}}$ is

$$v_{n+\frac{1}{2}} \approx \sum_{k \in \mathbb{Z}} e^{ik\phi(t)/\epsilon} g^k(t).$$

From

$$v_{n+\frac{1}{2}} = \frac{L_1 L_2^{-1}(e^{\epsilon \Delta})}{\hbar} x_{n+\frac{1}{2}} = \sum_{k \in \mathbb{Z}} \frac{L_1 L_2^{-1}(e^{\epsilon \Delta})}{\hbar} e^{ik\phi(t)/\epsilon} \xi^k(t),$$

it follows that

$$g^0 = \xi^0 + \mathcal{O}(\epsilon),$$

$$g^1 = \frac{1}{\epsilon} c_{0}^1 \xi^1 + \mathcal{O}(\epsilon) = \frac{i}{\epsilon \eta} 2 \tan \left( \frac{1}{2} \eta \phi \right) \xi^1 + \mathcal{O}(\epsilon),$$

$$g^{-1} = \frac{1}{\epsilon} c_{-0}^{-1} \xi^{-1} + \mathcal{O}(\epsilon) = -\frac{i}{\epsilon \eta} 2 \tan \left( \frac{1}{2} \eta \phi \right) \xi^{-1} + \mathcal{O}(\epsilon).$$

Thus, we have
\[ v_{n+\frac{1}{2}} = \dot{\zeta}_0 + \frac{i}{\hbar} 2 \tan \left( \frac{1}{2} \eta \phi \right) \left( \zeta_1^1 e^{i\phi(t)/\epsilon} - \zeta_{-1}^{-1} e^{-i\phi(t)/\epsilon} \right) + \mathcal{O}(\epsilon), \]

which yields that
\[ \frac{1}{2} \left| v_{n+\frac{1}{2}} \right|^2 = \frac{1}{2} \left| \dot{\zeta}_0 \right|^2 + \frac{4 \tan^2 \left( \frac{1}{2} \eta \phi \right) \left| \zeta_1^1 \right|^2}{\hbar^2} \]

and
\[ I(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) = \frac{4 \tan^2 \left( \frac{1}{2} \eta \phi \right) \left| \zeta_1^1 \right|^2}{\hbar^2} |B(\zeta^0)|. \]

Therefore, we obtain
\[ E(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) = \frac{1}{2} \left| \dot{\zeta}_0 \right|^2 + \frac{4 \tan^2 \left( \frac{1}{2} \eta \phi \right) \left| \zeta_1^1 \right|^2}{\hbar^2} + U \left( \zeta^0 \left( t_{n+\frac{1}{2}} \right) \right) + \mathcal{O}(\epsilon) \]
\[ = \frac{1}{2} \left| \dot{\zeta}_0 \right|^2 + |B(\zeta^0)| I(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) + U \left( \zeta^0 \left( t_{n+\frac{1}{2}} \right) \right) + \mathcal{O}(\epsilon). \]

By subtracting the expressions obtained for \( \mathcal{H}[\zeta](t_{n+\frac{1}{2}}) \) and \( E(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) \) from each other, one gets
\[ \mathcal{H}[\zeta](t_{n+\frac{1}{2}}) - E(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) = (\eta \phi \csc(\eta \phi) - 1) I(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) |B(\zeta^0)| + \mathcal{O}(\epsilon), \]

where (10) is used in the simplifications. The second statement is obtained immediately from this result.

According to the above results and following the analysis presented in [10] and Chap. XIII of [11], the statement of Theorem 3 is easily obtained.

### 5.3 Proof of Theorem 4

**Proposition 3** Under the conditions of Proposition 1, there exists a function \( \mathcal{I}[\zeta] \) such that

\[ \mathcal{I}[\zeta](t) = \mathcal{I}[\zeta](0) + \mathcal{O}(te^N) \quad \text{for } 0 \leq t \leq T_e, \]
\[ \mathcal{I}[\zeta](t_{n+1/2}) = I_h(x_{n+1/2}, v_{n+1/2}) + \mathcal{O}(\epsilon) \quad \text{for } nh \leq T_e, \]

where the constants symbolised by \( \mathcal{O} \) are independent of \( n, h \) and \( \epsilon \), but depends on \( N \).

**Proof**
• **Proof of the first statement.** Multiplication of (12) with $-ik(Y^k)^*$ and summation over $k$ yields

$$
- \sum_k ik(Y^k)^* \frac{1}{\hbar^2} L^2_1 L^2_2 (e^{hD}) Y^k + \frac{1}{\epsilon} \sum_k ik \left( A_k(Y)^* \frac{L_1 L^{-1}_2 (e^{hD})}{\hbar} Y^k \right) 

-(Y^k)^* \frac{L_1 L^{-1}_2 (e^{hD})}{\hbar} A_k(Y) = \mathcal{O}(\epsilon),
$$

where the results (4.43) and (4.44) of [10] are used here. Similarly to the analysis of previous section, it can be shown that the real part of this left-hand size is a total derivative. Therefore, there exists a function $\mathcal{I}[\zeta]$ such that $\frac{d}{dt} \mathcal{I}[\zeta] = \mathcal{O}(\epsilon)$. This proves the first statement of the theorem.

• **Proof of the second statement.** Concerning the dominant terms of $\mathcal{I}[\zeta]$, the left-hand size of (14) is zero for $k = 0$. For $k = \pm 1$, we can verify that the second sum is of size $\mathcal{O}(\epsilon)$. Thus, the dominant part of $\mathcal{I}[\zeta]$ only exist in the first sum for $k = \pm 1$. With this and the “magic formulas” on p. 508 of [11], we deduce that

Re(first sum of (14))

$$
- i \sum_k k \frac{d}{dt} \sum_{l \geq 0} \beta_{l} \hbar^{2l} \text{Im} \left[ (Y^k)^* (Y^k)^{(2l+1)} - (Y^k)^* (Y^k)^{(2l)} \right]

+ \cdots \pm \left( (Y^k)^{(l)} \right)^* (Y^k)^{(l+1)}.
$$

For $k \neq 0$, from Lemma 5.1 given in [7], it follows that

$$
\frac{1}{m!} \frac{d^m}{dt^m} Y^k(t) = \frac{1}{m!} e^{i\phi(t)} \left( \frac{i k}{\epsilon} \right)^m \text{e}^{i k \phi(t) / \epsilon} + O \left( \frac{1}{(m/M)!} \left( \frac{c}{\epsilon} \right)^{m-1-|k|} \right),
$$

where $c$ and the constant symbolised by $O$ are independent of $m \geq 1$ and $\epsilon$. By inserting this into $(-1)^r \frac{d^r}{dt^r} (Y^k(t))^* \frac{d^s}{dt^s} Y^k(t)$, it can be seen that the dominant term is to be the same whenever $r + s = 2l + 1$. Thus, it is clear that

$$
\left[ (Y^k)^* (Y^k)^{(2l+1)} - (Y^k)^* (Y^k)^{(2l)} + \cdots \pm (Y^k)^{(l)} (Y^k)^{(l+1)} \right]

= (l + 1) \left( \frac{i k}{\epsilon} \phi \right)^{2l+1} (\xi^k)^{l+1} + O \left( \frac{1}{(l/M)!} \left( \frac{c}{\epsilon} \right)^{2l-2|k|} \right).
$$

This implies that the total derivative of (15) is given by
Therefore, we obtain that
\[
\frac{-i}{\epsilon} \sum_{k} \frac{ik}{h} \sum_{l \geq 0} \left[ (-1)^l \beta_{2l}(l+1) \left( \frac{kh}{\epsilon} \phi \right)^{2l+1} (\tilde{\xi})^l \xi^k \right] + O(\epsilon)
\]
\[
= \frac{1}{eh} \sum_{k} \frac{k}{2} \sum_{l \geq 0} \left[ (-1)^l \beta_{2l}(2l+2) \left( \frac{kh}{\epsilon} \phi \right)^{2l+1} (\tilde{\xi})^l \xi^k \right] + O(\epsilon)
\]
\[
= \frac{1}{eh} \sum_{k} \frac{k}{2} 2 \tan \left( \frac{1}{2} \eta k \phi \right) \sec^2 \left( \frac{1}{2} \eta k \phi \right) |\xi|^2 + O(\epsilon)
\]
\[
= \frac{2}{eh} \frac{1}{2} 2 \tan \left( \frac{1}{2} \eta \phi \right) \sec^2 \left( \frac{1}{2} \eta \phi \right) |\xi|^2 + O(\epsilon)
\]
\[
= \frac{|\xi|^2}{e^2} \cos^2 \left( \frac{1}{2} \eta \phi \right) + O(\epsilon) = \frac{1}{\cos^2 \left( \frac{1}{2} \eta \phi \right)} I(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) + O(\epsilon).
\]
Therefore, we obtain that
\[
\mathcal{I}[\xi](t_{n+\frac{1}{2}}) = \frac{1}{\cos^2 \left( \frac{1}{2} \eta \phi \right)} I(x_{n+\frac{1}{2}}, v_{n+\frac{1}{2}}) + O(\epsilon)
\]
and this completes the proof. \(\square\)

By using the analysis presented in [10] and Chap. XIII of [11] again, Theorem 4 is proved.

### 6 Concluding remarks

The study of long-term behaviour for an integrator when applied to charged-particle dynamics is of great importance which has been received a great attention. In this paper, we first presented a two-step symmetric method for charged-particle dynamics and then analysed its long time behaviour not only in a normal magnetic field but also in a strong magnetic field. Backward error analysis and modulated Fourier expansion were used to prove the results. By the analysis of this paper, the long time conservations of the method were shown clearly for two cases of magnetic fields. In compared with the Boris method and the variational method researched recently in [10], the method shows some superiorities in the conservations over long times.

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