Journal of Mathematical Research with Applications
Jan., 2023, Vol. 43, No. 1, pp. 116–126
DOI:10.3770/j.issn:2095-2651.2023.01.013
Http://jmre.dlut.edu.cn

An Arbitrarily High-Order Energy-Preserving Scheme for the Lorentz Force System

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Abstract This letter is focused on proposing an arbitrarily high-order energy-preserving method for solving the charged-particle dynamics. After transforming the original Hamiltonian energy functional into a quadratic form by using the invariant energy quadratization method, symplectic Runge-Kutta method is used to construct a novel energy-preserving scheme to solve the Lorentz force system. The new scheme is not only energy-preserving, but also can be arbitrarily high-order. Numerical experiments are conducted to demonstrate the notable superiority of the new method with comparison to the well-known Boris method and another second-order energy-preserving method in the literature.

Keywords Lorentz force system; energy-preserving method; invariant energy quadratization method; symplectic Runge-Kutta method

MR(2020) Subject Classification 34A05; 34C14; 65L06

1. Introduction

In recent years, the plasma physics has developed rapidly, which provides new technologies and processes for the further development of sciences such as information, materials, environmental space, energy, geophysics, space physics and so on. Plasma is a collection of charged particles interacting with electromagnetic field, whose source can be outside or inside the plasma. The most basic physical process in the collective dynamics of magnetized plasma is the movement of charged particles under the influence of electromagnetic field [1].

Several important phenomena in plasma can be understood and analyzed in light of the single particle motion satisfying the Lorentz force equation, which can be cast into a Hamiltonian formulation [2,3]. The development of long-term numerical simulations on trajectories of charged particles has greatly facilitated the research of plasma dynamics. Among these efficient numerical simulations, non-geometric methods are always acting unsatisfactory, i.e., they cannot track the trajectory accurately during a long computation. Many works show that the standard fourth-order Runge-Kutta (RK) method, a popular explicit integrator, may lead to a wrong solution

Received March 3, 2022; Accepted June 26, 2022
Support by the National Natural Science Foundation of China (Grants Nos. 11801277; 11971242).
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trajectory due to its error accumulation after many time steps [4]. The application of geometric numerical methods to handle the dynamics of charged particles is a recent great advance, which often reveals better performance in long-term numerical simulations compared with traditional methods. The most representative methods are volume-preserving methods [5, 6], including the popular Boris method [7], symmetric multistep methods [8], variational symplectic methods [9] and symplectic methods [10, 11].

Numerical methods are called geometric methods or structure-preserving methods if they can conserve the intrinsic geometric properties of the system [12]. Feng and his collaborators found that the structures preserved above also contain physical conservation laws and algebraic properties in addition to geometric structure, which triggered the interest of many scholars [13, 14]. It could be generally stated that the energy is the most noticeable structure of a Hamiltonian system, i.e., the Hamiltonian function itself. This paper aims to construct an arbitrarily high-order energy-preserving algorithm for the Lorentz force system.

In recent years, there have been so many methods to construct energy-preserving algorithms for ordinary differential equations (ODEs), including discrete gradient methods [15, 16], discrete variational methods [17], discrete line integral methods [18, 19], Hamiltonian boundary value methods [20, 21] and line integral methods [22]. In view of the core idea of Baida [23] and Guillen [24] in the processing of the liquid crystal model, (invariant) energy quadratization (IEQ) method emerged as the times require, which created an interesting and meaningful topic when applying it to Hamiltonian system for getting an efficient and exactly energy-preserving algorithm. Please refer to [25, 26] and the references there in.

For the plasma physics, the conservation of energy remains crucial [27, 28], which motivates us to construct an energy-preserving scheme. In this paper, we will combine the IEQ method and the symplectic Runge-Kutta (RK) method to solve the Lorentz force system. First, introducing an auxiliary variable, the original Hamiltonian energy functional can be changed into a quadratic form. Then, applying the symplectic RK method for the new system obtained above yields a novel scheme. Compared with the EPIEQ scheme, a second-order energy-preserving scheme was proposed in [28], the new scheme proposed here is not only energy-preserving, but also can be arbitrarily high-order, which can simulate the motion of charged particles more efficiently.

The context of the paper is as follows. In Section 2, we transform the dynamics of charged particles in the electromagnetic field as a Hamiltonian system. In Section 3, an arbitrarily high-order energy-preserving scheme is obtained. We also prove the conservation of energy strictly afterwards. Numerical experiments are conducted in Section 4 in order to confirm the theoretical results of the proposed new scheme. The conclusion is given in Section 5 finally.

2. The motion under the Lorentz force system

In this section, we will briefly review the motion equation of the single charged particle first. A charged particle in an electromagnetic field is in accordance with the equation of motion

associated with the Lorentz force

$$m\ddot{\boldsymbol{x}} = q(\boldsymbol{E} + \dot{\boldsymbol{x}} \times \boldsymbol{B}), \quad \boldsymbol{x} \in \mathbb{R}^3, \tag{2.1}$$

where $\boldsymbol{x}$ represents the position of the charged particle, m and q denote the mass and charge, respectively. For the sake of simplicity, we assume that $\boldsymbol{B}$ and $\boldsymbol{E}$ are both static, so $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ and $\boldsymbol{E} = -\nabla\varphi$, where $\boldsymbol{A}$ and φ are the potentials.

Denote transformation

$$G : (\boldsymbol{x}, \boldsymbol{p}) \longrightarrow (\boldsymbol{x}, \boldsymbol{v}), \dot{\boldsymbol{x}} = \boldsymbol{v}, \boldsymbol{v} = \frac{1}{m}(\boldsymbol{p} - q\boldsymbol{A}(\boldsymbol{x})),$$

and then the system (2.1) can be cast into

$$\begin{cases} \dot{\boldsymbol{x}} = \boldsymbol{v}, \\ \dot{\boldsymbol{v}} = \dfrac{q}{m}(\boldsymbol{E}(\boldsymbol{x}) + \boldsymbol{v} \times \boldsymbol{B}(\boldsymbol{x})). \end{cases} \tag{2.2}$$

If we denote $\boldsymbol{z} = (\boldsymbol{x}^{\mathrm{T}}, \boldsymbol{v}^{\mathrm{T}})^{\mathrm{T}}$, the system (2.2) can be rewritten as

$$\dot{\boldsymbol{z}} = \boldsymbol{K}(\boldsymbol{z})\nabla H(\boldsymbol{z}), \tag{2.3}$$

with the Hamiltonian $H(\boldsymbol{z}) = \dfrac{m}{2}\boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} + q\varphi(\boldsymbol{x})$. The skew-symmetric matrix

$$\boldsymbol{K}(\boldsymbol{z}) = \begin{pmatrix} \boldsymbol{0} & \frac{1}{m}\boldsymbol{I} \\ -\frac{1}{m}\boldsymbol{I} & \frac{q}{m^2}\hat{\boldsymbol{B}}(\boldsymbol{x}) \end{pmatrix}$$

shows that the system is a Hamiltonian system with

$$\hat{\boldsymbol{B}}(\boldsymbol{x}) = \begin{pmatrix} 0 & B_3(\boldsymbol{x}) & -B_2(\boldsymbol{x}) \\ -B_3(\boldsymbol{x}) & 0 & B_1(\boldsymbol{x}) \\ B_2(\boldsymbol{x}) & -B_1(\boldsymbol{x}) & 0 \end{pmatrix}$$

defined by $\boldsymbol{B}(\boldsymbol{x}) = [B_1(\boldsymbol{x}), B_2(\boldsymbol{x}), B_3(\boldsymbol{x})]^{\mathrm{T}}$.

3. Invariant energy quadratization method for the Lorentz force system

It is well known that the IEQ method wants to transform the free energy into a quadratic form about a new variable by changing variables and the novel, equivalent system still retains a similar energy conservation law in terms of the new variables, which opens up new possibilities for constructing an energy-preserving scheme.

In this section, we will introduce how to use the the IEQ method and the symplectic RK method to solve the Hamiltonian system (2.3) for developing an arbitrarily high-order energy-preserving scheme in detail.

3.1. Invariant energy quadratization reformulation

Choose a suitable constant C_0 such that $q\varphi(\boldsymbol{x}) + C_0 > 0$ and we denote $H_1(\boldsymbol{z}) = \dfrac{m}{2}\boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} - C_0$, $H_2(\boldsymbol{z}) = q\varphi(\boldsymbol{x}) + C_0$, then $H(\boldsymbol{z}) = H_1(\boldsymbol{z}) + H_2(\boldsymbol{z})$. Introducing a Lagrange multiplier or auxiliary

variable $r(t;\boldsymbol{z}) = \sqrt{H_2(\boldsymbol{z})} = \sqrt{q\varphi(\boldsymbol{x}) + C_0}$, we recast the system (2.3) as the IEQ reformulated system

$$\begin{cases} \boldsymbol{z}_t = \boldsymbol{K}(\boldsymbol{z})(\nabla H_1(\boldsymbol{z}) + \dfrac{r}{\sqrt{H_2(\boldsymbol{z})}}\nabla H_2(\boldsymbol{z})), \\ r_t = \dfrac{1}{2\sqrt{H_2(\boldsymbol{z})}}\nabla H_2(\boldsymbol{z})^{\mathrm{T}}\boldsymbol{z}_t, \end{cases} \tag{3.1}$$

where the consistent initial condition is $r|_{t=0} = \sqrt{H_2(\boldsymbol{z}(0))} = \sqrt{q\varphi|_{t=0} + C_0}$.

Next, the relevant properties of the system will be given as follows.

Proposition 3.1 *The corresponding modified energy is*

$$\tilde{H}(\boldsymbol{z}, r) = \frac{m}{2}\boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} + r^2 - C_0 = H_1(\boldsymbol{z}) + r^2,$$

which can be preserved by the above system (3.1), i.e.,

$$\frac{d}{dt}\tilde{H}(\boldsymbol{z}, r) = 0.$$

Proof According to the definition of energy $\tilde{H}(\boldsymbol{z}, r)$ and the form of system (3.1), we have

$$\begin{aligned} \frac{d}{dt}\tilde{H}(\boldsymbol{z}, r) &= \frac{d}{dt}(H_1(\boldsymbol{z}) + r^2) = \nabla H_1(\boldsymbol{z})^{\mathrm{T}}\boldsymbol{z}_t + 2rr_t \\ &= \nabla H_1(\boldsymbol{z})^{\mathrm{T}}\boldsymbol{K}(\boldsymbol{z})(\nabla H_1(\boldsymbol{z}) + \frac{r}{\sqrt{H_2(\boldsymbol{z})}}\nabla H_2(\boldsymbol{z})) + 2r\frac{1}{2\sqrt{H_2(\boldsymbol{z})}}\nabla H_2(\boldsymbol{z})^{\mathrm{T}}\boldsymbol{z}_t \\ &= \nabla H_1(\boldsymbol{z})^{\mathrm{T}}\boldsymbol{K}(\boldsymbol{z})\frac{r}{\sqrt{H_2(\boldsymbol{z})}}\nabla H_2(\boldsymbol{z}) + \frac{r}{\sqrt{H_2(\boldsymbol{z})}}\nabla H_2(\boldsymbol{z})^{\mathrm{T}}\boldsymbol{K}(\boldsymbol{z})\nabla H_1(\boldsymbol{z}) \\ &= 0, \end{aligned}$$

due to the skew-symmetry of the matrix $\boldsymbol{K}(\boldsymbol{z})$. □

Remark 3.2 According to Proposition 3.1 and the definition of the energy above, we have

$$\tilde{H}(\boldsymbol{z}(t), r(t)) \equiv \tilde{H}(\boldsymbol{z}(0), r(0)) = H_1(\boldsymbol{z}(0)) + H_2(\boldsymbol{z}(0)) = H(\boldsymbol{z}(0)) \equiv H(\boldsymbol{z}(t))$$

in continuous state. So, $\tilde{H}(\boldsymbol{z}, r)$ is also the energy of the original Hamiltonian system (2.3).

3.2. Invariant energy quadratization Runge-Kutta method

After the introduction of the IEQ method, we will derive the symplectic RK method for the IEQ reformulated system (3.1) to get the arbitrarily high-order structure-preserving scheme.

Let b_i, a_{ij} $(i, j = 1, \ldots, s)$ be real numbers and $c_i = \sum_{j=1}^{s} a_{ij}$. For given $(\boldsymbol{z^n}, r^n)$, the intermediate values Z_i and R_i are first calculated by

$$\begin{aligned} \boldsymbol{Z_i} &= \boldsymbol{z^n} + \tau\sum_{j=1}^{s} a_{ij}\boldsymbol{k_j}, \\ R_i &= r^n + \tau\sum_{j=1}^{s} a_{ij}l_j, \end{aligned} \tag{3.2}$$

where $\boldsymbol{k_i} = \boldsymbol{K}(\boldsymbol{Z_i})(\nabla H_1(\boldsymbol{Z_i}) + \dfrac{R_i}{\sqrt{H_2(\boldsymbol{Z_i})}}\nabla H_2(\boldsymbol{Z_i}))$ and $l_i = \dfrac{1}{2\sqrt{H_2(\boldsymbol{Z_i})}}\nabla H_2(\boldsymbol{Z_i})^T\boldsymbol{k_i}$, respec-

tively. Then $(\boldsymbol{z^{n+1}}, r^{n+1})$ is updated via

$$\begin{aligned} \boldsymbol{z^{n+1}} &= \boldsymbol{z^n} + \tau \sum_{i=1}^{s} b_i \boldsymbol{k_i}, \\ r^{n+1} &= r^n + \tau \sum_{i=1}^{s} b_i l_i. \end{aligned} \tag{3.3}$$

Remark 3.3 The s-stage RK coefficients are usually displayed by a Butcher table [18]:

$$\begin{array}{c|c} \boldsymbol{c} & \boldsymbol{A} \\ \hline & \boldsymbol{b^{\mathrm{T}}} \end{array},$$

where $\boldsymbol{A} \in \mathbb{R}^s$ and $\boldsymbol{c} = \boldsymbol{Al}$ with $\boldsymbol{l} = (1, 1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^s$.

Remark 3.4 The new proposed schemes (3.2) and (3.3) are called the IEQ-RK scheme here.

We call an RK method the symplectic RK method if it can preserve quadratic first integrals, which is indeed its advantage. An RK method whose coefficients satisfy the following Lemma 3.5 is symplectic.

Lemma 3.5 ([18, Theorem 4.3 in Chapter VI]) *(S-conservative condition or symplectic condition). An RK scheme is S-conservative if and only if the symmetric coefficient matrix $\boldsymbol{M}$ with elements*

$$m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j, \quad i, j = 1, 2, \ldots, s \tag{3.4}$$

is the zero matrix.

Theorem 3.6 *The IEQ-RK schemes (3.2) and (3.3) preserve the energy $\tilde{H}(\boldsymbol{z}, r)$ of the Lorentz force system.*

Proof Denote $\boldsymbol{k_i} = ((\boldsymbol{k_i^x})^{\mathrm{T}}, (\boldsymbol{k_i^v})^{\mathrm{T}})^{\mathrm{T}}$, then according to $\boldsymbol{z} = (\boldsymbol{x}^{\mathrm{T}}, \boldsymbol{v}^{\mathrm{T}})^{\mathrm{T}}$ and Eqs. (3.2) and (3.3), we get

$$\begin{aligned} \boldsymbol{X_i} &= \boldsymbol{x^n} + \tau \sum_{j=1}^{s} a_{ij} \boldsymbol{k_j^x}, \\ \boldsymbol{V_i} &= \boldsymbol{v^n} + \tau \sum_{j=1}^{s} a_{ij} \boldsymbol{k_j^v}, \\ R_i &= r^n + \tau \sum_{j=1}^{s} a_{ij} l_j \end{aligned} \tag{3.5}$$

and

$$\begin{aligned} \boldsymbol{x^{n+1}} &= \boldsymbol{x^n} + \tau \sum_{i=1}^{s} b_i \boldsymbol{k_i^x}, \\ \boldsymbol{v^{n+1}} &= \boldsymbol{v^n} + \tau \sum_{i=1}^{s} b_i \boldsymbol{k_i^v}, \\ r^{n+1} &= r^n + \tau \sum_{i=1}^{s} b_i l_i, \end{aligned} \tag{3.6}$$

where

$$\begin{aligned}
\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{x}} &= \boldsymbol{V}_{\boldsymbol{i}}, \\
\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}} &= -\frac{R_i\sqrt{q}}{m\sqrt{\varphi(\boldsymbol{X}_{\boldsymbol{i}})}}\nabla\varphi(\boldsymbol{X}_{\boldsymbol{i}}) + \frac{q}{m}\hat{\boldsymbol{B}}(\boldsymbol{X}_{\boldsymbol{i}})\boldsymbol{V}_{\boldsymbol{i}}, \\
l_i &= \frac{\sqrt{q}}{2}\frac{(\nabla\varphi(\boldsymbol{X}_{\boldsymbol{i}}))^T\boldsymbol{V}_{\boldsymbol{i}}}{\sqrt{\varphi(\boldsymbol{X}_{\boldsymbol{i}})}}.
\end{aligned} \tag{3.7}$$

Because of Eq. (3.5), we have

$$\begin{aligned}
&\tilde{H}(\boldsymbol{z}^{\boldsymbol{n+1}}, r^{n+1}) - \tilde{H}(\boldsymbol{z}^{\boldsymbol{n}}, r^n) = H_1(\boldsymbol{z}^{\boldsymbol{n+1}}) - H_1(\boldsymbol{z}^{\boldsymbol{n}}) + (r^{n+1})^2 - (r^n)^2 \\
&= \frac{m}{2}(\boldsymbol{v}^{\boldsymbol{n+1}})^{\mathrm{T}}\boldsymbol{v}^{\boldsymbol{n+1}} - \frac{m}{2}(\boldsymbol{v}^{\boldsymbol{n}})^{\mathrm{T}}\boldsymbol{v}^{\boldsymbol{n}} + (r^{n+1})^2 - (r^n)^2.
\end{aligned} \tag{3.8}$$

The two terms on the right of the Eq. (3.8) are

$$\begin{aligned}
&\frac{m}{2}(\boldsymbol{v}^{\boldsymbol{n+1}})^{\mathrm{T}}\boldsymbol{v}^{\boldsymbol{n+1}} - \frac{m}{2}(\boldsymbol{v}^{\boldsymbol{n}})^{\mathrm{T}}\boldsymbol{v}^{\boldsymbol{n}} = \frac{m}{2}\Big(\boldsymbol{v}^{\boldsymbol{n}} + \tau\sum_{i=1}^{s} b_i\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}}\Big)^{\mathrm{T}}\Big(\boldsymbol{v}^{\boldsymbol{n}} + \tau\sum_{i=1}^{s} b_i\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}}\Big) - \frac{m}{2}(\boldsymbol{v}^{\boldsymbol{n}})^{\mathrm{T}}\boldsymbol{v}^{\boldsymbol{n}} \\
&= \frac{m}{2}\tau\sum_{i=1}^{s} b_i(\boldsymbol{v}^{\boldsymbol{n}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}} + \frac{m}{2}\tau\sum_{j=1}^{s} b_j(\boldsymbol{v}^{\boldsymbol{n}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}} + \frac{m}{2}\tau^2\sum_{i=1}^{s}\sum_{j=1}^{s} b_ib_j(\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}} \\
&= \frac{m}{2}\tau\sum_{i=1}^{s} b_i\Big(\boldsymbol{V}_{\boldsymbol{i}} - \tau\sum_{j=1}^{s} a_{ij}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}}\Big)^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}} + \frac{m}{2}\tau\sum_{j=1}^{s} b_j\Big(\boldsymbol{V}_{\boldsymbol{j}} - \tau\sum_{i=1}^{s} a_{ji}\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}}\Big)^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}} + \\
&\quad \frac{m}{2}\tau^2\sum_{i=1}^{s}\sum_{j=1}^{s} b_ib_j(\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}} \\
&= m\tau\sum_{i=1}^{s} b_i(\boldsymbol{V}_{\boldsymbol{i}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}} + \frac{m\tau^2}{2}\sum_{i=1}^{s}\sum_{j=1}^{s}(b_ib_j - b_ia_{ij} - b_ja_{ji})(\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}},
\end{aligned}$$

$$\begin{aligned}
&(r^{n+1})^2 - (r^n)^2 = \Big(r^n + \tau\sum_{i=1}^{s} b_il_i\Big)^2 - (r^n)^2 \\
&= \tau\sum_{i=1}^{s} b_ir^nl_i + \tau\sum_{j=1}^{s} b_jl_jr^n + \tau^2\sum_{i=1}^{s}\sum_{j=1}^{s} b_ib_jl_il_j \\
&= \tau\sum_{i=1}^{s} b_i\Big(R_i - \tau\sum_{j=1}^{s} a_{ij}l_j\Big)l_i + \tau\sum_{j=1}^{s} b_jl_j\Big(R_j - \tau\sum_{i=1}^{s} a_{ji}l_i\Big) + \tau^2\sum_{i=1}^{s}\sum_{j=1}^{s} b_ib_jl_il_j \\
&= 2\tau\sum_{i=1}^{s} b_iR_il_i + \tau^2\sum_{i=1}^{s}\sum_{j=1}^{s}(b_ib_j - b_ia_{ij} - b_ja_{ji})l_il_j,
\end{aligned}$$

respectively. Then, substituting Eq. (3.7) into these two formulas above, we have

$$\tilde{H}(\boldsymbol{z}^{\boldsymbol{n+1}}, r^{n+1}) - \tilde{H}(\boldsymbol{z}^{\boldsymbol{n}}, r^n) = \tau^2\sum_{i=1}^{s}\sum_{j=1}^{s}(b_ib_j - b_ia_{ij} - b_ja_{ji})(\frac{m}{2}(\boldsymbol{k}_{\boldsymbol{i}}^{\boldsymbol{v}})^{\mathrm{T}}\boldsymbol{k}_{\boldsymbol{j}}^{\boldsymbol{v}} + l_il_j).$$

When the S-conservative condition is satisfied, the IEQ-RK schemes (3.2) and (3.3) exactly preserves the energy, i.e.,

$$\tilde{H}(\boldsymbol{z}^{\boldsymbol{n+1}}, r^{n+1}) = \tilde{H}(\boldsymbol{z}^{\boldsymbol{n}}, r^n). \quad \square$$

4. Numerical experiments

Here, numerical experiments are conducted to indicate the efficiency of our proposed IEQ-RK scheme. Say concretely, we choose $s = 2$ and $s = 3$ in symplectic RK method and compare the scheme with the well-known Boris method [7] and the second-order EPIEQ method [28] to demonstrate the practicability, accuracy as well as energy conservation property of our proposed scheme.

Example 4.1 We will consider the 2D dynamics of the charged particle in an electromagnetic field which is static and non-uniform. By theoretic analysis, we know that the orbit of the charged particle is a spiral circle with constant radius. The larger circle corresponds to the $\nabla \cdot \boldsymbol{B}$ drift and the $\boldsymbol{E} \times \boldsymbol{B}$ drift of the steering center, and the smaller circle is the fast scale rotary motion [5].

For the charged-particle dynamics (2.1), we consider the scalar potential

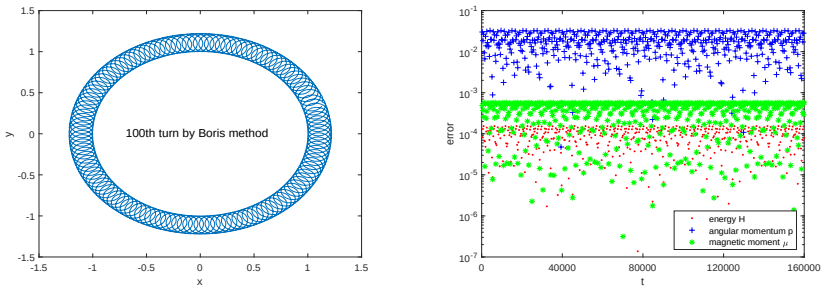
$$\varphi(\boldsymbol{x}) = \frac{1}{100\sqrt{x_1^2 + x_2^2}}$$

and the filed

$$\boldsymbol{B}(\boldsymbol{x}) = \nabla \times \frac{1}{3}\big(-x_2\sqrt{x_1^2 + x_2^2}, x_1\sqrt{x_1^2 + x_2^2}, 0\big)^{\mathrm{T}}.$$

The initial values are chosen as $\boldsymbol{x_0} = (0, -1, 0)^{\mathrm{T}}$ and $\boldsymbol{v_0} = (0.1, 0.01, 0)^{\mathrm{T}}$.

First, we make a comparison among the Boris method [7], the EPIEQ method [28] and the IEQ-RK method we proposed. We choose the stepsize $h = \pi/10$ and the results are shown in Figures 1–3.

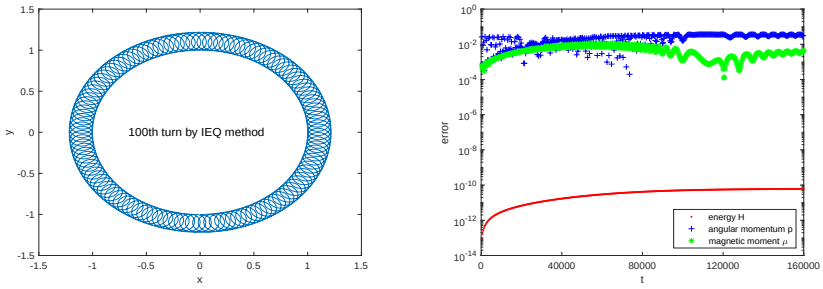


(a) (b)

Figure 1 The numerical results of Boris method with step $h = \pi/10$. (a) The orbit in the 100th turn; (b) Errors of the angular momentum p_ξ, the magnetic moment μ and the energy H for $t \in [0, 5 \times 10^5 h]$.

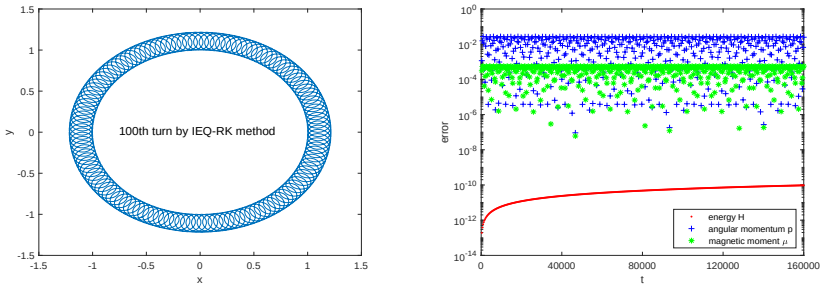
Figures 1–3 show the 100th turn and the errors of the angular momentum p_ξ, the magnetic moment μ and the energy H for $t \in [0, 5 \times 10^5 h]$ by these three methods, respectively. By comparing the three figures, we can see that the 100th turn by the three methods shows excellent agreement. For invariants' conservation, the IEQ-RK scheme proposed here and the EPIEQ method [28] both can exactly preserve energy while the Boris method [7] just can keep the error of energy between $10^{-5} \sim 10^{-4}$. What's more, the angular momentum p_ξ and the magnetic

moment μ can keep stable oscillation even reach 10^{-6} via the IEQ-RK scheme, which shows a better behaviour than the EPIEQ method [28].



(a) (b)

Figure 2 The numerical results of EPIEQ method with step $h = \pi/10$. (a) The orbit in the 100th turn; (b) Errors of the angular momentum p_ξ, the magnetic moment μ and the energy H for $t \in [0, 5 \times 10^5 h]$.



(a) (b)

Figure 3 The numerical results of IEQ-RK scheme with step $h = \pi/10$. (a) The orbit in the 100th turn; (b) Errors of the angular momentum p_ξ, the magnetic moment μ and the energy H for $t \in [0, 5 \times 10^5 h]$.

Then, in order to compute the order of convergence of the IEQ-RK scheme proposed here, we choose different stepsizes $h = 1/2^j$, where $j = 2, 3, 4, 5$. Here, the numerical solution of stepsize $h = 1/2^5$ is chosen as the exact solution because of the lack of analytical solution. We define the errors as follows

$$\|e(\boldsymbol{x})\|_\infty = \max_{1\le i\le 3} |x_N^i - \overline{x}_{N_1}^i|,$$
$$\|e(\boldsymbol{v})\|_\infty = \max_{1\le i\le 3} |v_N^i - \overline{v}_{N_1}^i|,$$

where x_N^i and v_N^i are the numerical solutions in $t = T$ with the stepsizes $h = 1/2^j$, where $j = 2, 3, 4$. $\overline{x}_{N_1}^i$ and $\overline{v}_{N_1}^i$ are solutions in $t = T$ with stepsize $h = 1/2^5$. Then we use the following formulas to calculate the order of convergence

$$\text{order}_{\boldsymbol{x}} = \frac{\log(\text{error}_{\boldsymbol{x}}^1/\text{error}_{\boldsymbol{x}}^2)}{\log 2},$$
$$\text{order}_{\boldsymbol{v}} = \frac{\log(\text{error}_{\boldsymbol{v}}^1/\text{error}_{\boldsymbol{v}}^2)}{\log 2},$$

where $\text{error}_{\boldsymbol{x}}^i$ and $\text{error}_{\boldsymbol{v}}^i$ $(i = 1, 2)$ represent the corresponding errors of $\boldsymbol{x}$ and $\boldsymbol{v}$, respectively.

We display the results in Table 1.

Table 1 confirms that the IEQ-RK scheme we proposed has fourth-order and six-order convergence when we choose $s = 2$ and $s = 3$, respectively. In fact, the IEQ-RK scheme can be arbitrary high-order as long as we take the bigger value of s, which shows that the order of convergence of IEQ-RK scheme we proposed is higher than the Boris method [7] and the EPIEQ method [28], since the Boris method and the EPIEQ method are both of second-order convergence.

	h	$1/2^2$	$1/2^3$	$1/2^4$
$s=2$	$\|e(x)\|_\infty$	5.1875×10^{-6}	3.2394×10^{-7}	1.9068×10^{-8}
	$\text{order}_{\boldsymbol{x}}$	—	**4.0012**	**4.0865**
	$\|e(v)\|_\infty$	5.2490×10^{-6}	3.2777×10^{-7}	1.9294×10^{-8}
	$\text{order}_{\boldsymbol{v}}$	—	**4.0013**	**4.0865**
$s=3$	$\|e(x)\|_\infty$	2.3415×10^{-9}	3.6645×10^{-11}	5.6402×10^{-13}
	$\text{order}_{\boldsymbol{x}}$	—	**5.9977**	**6.0217**
	$\|e(v)\|_\infty$	2.3644×10^{-9}	3.7003×10^{-11}	5.6952×10^{-13}
	$\text{order}_{\boldsymbol{v}}$	—	**5.9977**	**6.0217**

Table 1 Convergence order of the proposed IEQ-RK scheme for $T = 10s$

Remark 4.2 The numerical scheme (3.2)-(3.3) we proposed has the arbitrary high-order accuracy. In fact, the convergence order of our scheme is dependent on the order of the used symplectic RK method, that is, the order of implicit RK method which satisfies the S-conservative condition. While, if the s-stage implicit RK method based on Gauss quadrature formula is chosen, the Gauss Method has the $2s$ order according to [18, 29], whose orders of 4 and 6 are utilized in the above numerical experiments. The results of $2s-1$ or $2s-2$ order can be obtained if we choose the Radau Method or the Lobatto Method [18]. So, as we take bigger and bigger s, then the convergence order of our method gets higher and higher, which means that we can get the arbitrary high-order convergence.

All of the results indicate that the IEQ-RK scheme we proposed has excellent invariants-conservation property and a higher order of convergence.

Example 4.3 We consider the charged-particle dynamics (2.1) with another scalar potential [27]

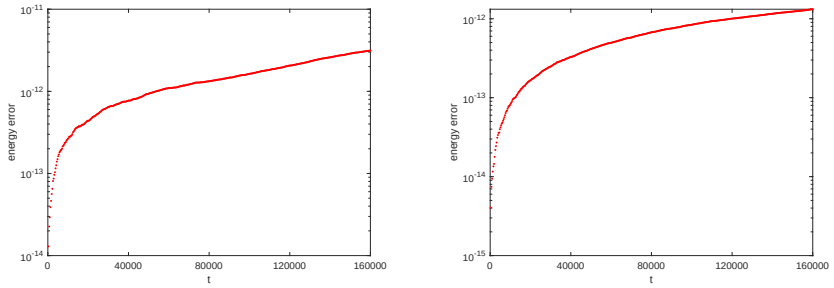
$$\varphi(\boldsymbol{x}) = \frac{1}{5}(x_1^4 + x_2^4 + x_3^4)$$

and the filed

$$\boldsymbol{B}(\boldsymbol{x}) = \nabla \times \frac{1}{4}(x_3^2 - x_2^2, x_3^2 - x_1^2, x_2^2 - x_1^2)^{\mathrm{T}} = \frac{1}{2}(x_2 - x_3, x_1 + x_3, x_2 - x_1)^{\mathrm{T}}.$$

What's more, we choose the initial values as $\boldsymbol{x_0} = (0, 1, 0)^{\mathrm{T}}$ and $\boldsymbol{v_0} = (0.09, 0.55, 0.3)^{\mathrm{T}}$ and the problem is calculated in the interval $[0, T]$. Same as Example 1, we take the step length $h = \pi/10$ and set $T = 5 \times 10^5 h$. Figure 4 shows the energy errors of IEQ-RK scheme, where (a) corresponds to $s = 2$ and (b) corresponds to $s = 3$.

In this case, we find the Hamiltonian $H(\boldsymbol{z})$ is not quadratic, but the energy still can be conserved very well using the proposed scheme IEQ-RK here. It is easy to see that the errors of energy oscillate near zero in the scale $10^{-14} \sim 10^{-11}$ and $10^{-15} \sim 10^{-12}$ for $s = 2$ and $s = 3$ calculated via the proposed IEQ-RK scheme, which indicates that the IEQ-RK scheme we proposed can preserve the energy conservation very well again.



(a) (b)

Figure 4 The energy errors of IEQ-RK scheme. (a) $s = 2$; (b) $s = 3$.

5. Conclusions

Several important phenomena in plasma can be described in the light of the single particle motion satisfying the Lorentz force equation, which can be expressed as a Hamiltonian formulation. In this paper, a new energy-preserving method is proposed to solve the Lorentz force system by combining the invariant energy quadratization method and the symplectic Runge-Kutta method. The proposed scheme is energy-preserving and can be arbitrarily high-order, which can efficiently simulate the motion of charged particles. Numerical results conducted verify the theoretical research.

Acknowledgements We thank the referees for their time and comments.

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