

Fourth-order energy-preserving exponential integrator for charged-particle dynamics in a strong constant magnetic field

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(Received 6 May 2020; accepted 8 October 2020; published 22 October 2020)

Charged-particle dynamics in a strong constant magnetic field can yield a fast gyromotion with high frequency around the center. Considering the superior of exponential integrators for highly oscillatory problems and the benefit of energy preservation of numerical integrators in solving the charged-particle dynamics, this paper is devoted to developing a fourth-order energy-preserving exponential integrator for the charged-particle dynamics in a strong constant magnetic field. To this end, we first rewrite the problem in the form of a semilinear Poisson system, to which the exponential average vector field (EAVF) method can be applied with energy preservation. Then, by deriving the truncated modified differential equation of the EAVF method, we propose a fourth-order energy-preserving exponential integrator according to the *modifying integrator* theory. Finally, numerical results soundly support the good energy preservation and high efficiency of the proposed fourth-order integrator in solving the problem considered in this paper.

DOI: [10.1103/PhysRevE.102.043315](https://doi.org/10.1103/PhysRevE.102.043315)

I. INTRODUCTION

Charged-particle dynamics in a strong magnetic field under the Lorentz force plays an important role in the understanding of plasmas physics. In this paper, we are concerned with the motion of a single charged particle (of unit mass and charge) in a strong constant magnetic field:

$$\ddot{x} = \dot{x} \times \frac{1}{\epsilon} \tilde{B} + G(x), \quad t \in [t_0, T], \quad x(t_0) = x_0, \quad \dot{x}(t_0) = \dot{x}_0, \quad (1)$$

where $x, \dot{x} \in \mathbb{R}^3$ are, respectively, the position and velocity of the particle, $\tilde{B} = (B_1, B_2, B_3)^T$ is a constant magnetic field, $G(x) = -\nabla_x U(x)$ is an electric field with the potential $U(x)$, and ϵ is a scaling parameter such that $0 < \epsilon \ll 1$. For a discussion of the scaling parameter ϵ , readers can refer to Refs. [1,2] for more details. As stated in Ref. [2], the small magnitude of ϵ indicates a fast gyromotion with high frequency around the center. Then the high frequency makes (1) become a highly oscillatory problem, for which numerical methods are usually challenging to construct. Except for the classical Boris method [3–5], numerical methods that can effectively solve this problem include symmetric multistep methods [6], volume-preserving algorithms [7,8], symplectic methods [9,10], and energy-preserving methods [11,12].

In fact, the system (1) can be formulated by a semilinear Poisson system. Let E be the identity matrix,

$$B = \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} \frac{1}{\epsilon} B & -E \\ E & 0 \end{pmatrix},$$

and $Q = \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix}$, then S is skew-symmetric and Q is symmetric. By using the notations $v = \dot{x}$ and $v_0 = \dot{x}_0$, the system (1) becomes

$$\begin{pmatrix} \dot{v} \\ \dot{x} \end{pmatrix} = S Q \begin{pmatrix} v \\ x \end{pmatrix} + S \begin{pmatrix} 0 \\ \nabla_x U(x) \end{pmatrix}, \quad x(t_0) = x_0, \quad v(t_0) = v_0, \quad (2)$$

which is a semilinear Poisson system with the energy

$$H(v, x) = \frac{1}{2} v^T v + U(x). \quad (3)$$

The exact solution of the system (2) can be expressed by the variation-of-constants formula [13] as follows:

$$\begin{aligned} x(t_0 + h) &= x_0 + h \varphi_1 \left(\frac{h}{\epsilon} B \right) v_0 + h^2 \int_0^1 (1 - \xi) \\ &\quad \cdot \varphi_1 \left((1 - \xi) \frac{h}{\epsilon} B \right) G(x(t_0 + \xi h)) d\xi, \\ v(t_0 + h) &= e^{\frac{h}{\epsilon} B} v_0 + h \int_0^1 e^{(1-\xi) \frac{h}{\epsilon} B} G(x(t_0 + \xi h)) d\xi, \end{aligned}$$

where the matrix-valued function φ_1 will be introduced in Sec. II.

In consideration of the small magnitude of ϵ and the semilinearity of (2), exponential integrators [14–16] are expected to have better performance than nonexponential integrators. This point has been supported by the good performance of the filtered Boris algorithm [13], the explicit symplectic exponential integrator [17,18], and the energy-preserving exponential integrator [19], which are essentially designed following from the variation-of-constants formula of (2). Moreover, as explained in Ref. [4], bounding the energy error is generally beneficial for the numerical solving of the

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charged-particle dynamics. In this sense, exponential integrators that can preserve the energy will be very promising for this problem. However, the present energy-preserving exponential integrator [19] has a limit accuracy only of second order. Higher-order energy-preserving exponential integrators for this problem are thus desirable.

In this paper, on noting the identity of the second-order exponential average vector field (EAVF) method [20] applied to (2) with the energy-preserving exponential integrator in Ref. [19], we aim at developing a fourth-order energy-preserving exponential integrator based on the *modifying integrator* theory [21] for modified differential equations. To this end, the rest of this paper is organized as follows. In Sec. II, by deriving the leading term of the local truncation error of the EAVF integrator (6), we present the details for how to construct the fourth-order energy-preserving exponential integrator. Section III is concerned with the numerical experiment, which shows the good energy preservation and high efficiency of the proposed fourth-order method in comparison with two nonexponential energy-preserving methods and the second-order EAVF integrator. Conclusions are drawn in the last section.

II. CONSTRUCTION OF THE FOURTH-ORDER ENERGY-PRESERVING EXPONENTIAL INTEGRATOR

We first introduce the matrix-valued functions of V :

$$\varphi_k(V) = \int_0^1 e^{(1-\theta)V} \frac{\theta^{k-1}}{(k-1)!} d\theta, \quad k \geq 1,$$

which admit the recurrence relation

$$\varphi_{k+1}(V) = \frac{\varphi_k(V) - \varphi_k(0)}{V}, \quad \varphi_0(V) = e^V. \quad (4)$$

To make sense for the singular case of V , the denominator of (4) should be considered as reducing the power of V by one rather than its inverse. Usually, the functions $\varphi_k(V)$ can be expressed in a formal series:

$$\varphi_k(V) = \sum_{j=0}^{\infty} \frac{V^j}{(j+k)!}, \quad k \in \mathbb{N}, \quad (5)$$

which is valid for both the nonsingular and singular cases of V . For the practical calculation of $\varphi_k(V)$, readers can refer to Ref. [22] for more details.

Let h be the step size. With the definition of $\varphi_k(V)$, the EAVF integrator can be formulated as

$$y_{n+1} = e^{hM} y_n + h\varphi_1(hM) \cdot \int_0^1 f((1-\xi)y_n + \xi y_{n+1}) d\xi, \quad (6)$$

which is proposed in Ref. [20] to solve the semilinear Poisson system

$$y'(t) = My + f(y), \quad y(t_0) = y_0 \in \mathbb{R}^d, \quad (7)$$

where $M = SQ$, $f(y) = S\nabla U(y)$, and S is skew-symmetric and Q is symmetric. This method is symmetric and can preserve the energy $H(y) = \frac{1}{2}y^\top Qy + U(y)$, i.e., $H(y_{n+1}) = H(y_n)$.

A. Truncated modified differential equation

In this subsection, we will derive the modified differential equation that is truncated at fourth order for the EAVF integrator (6). By setting $y_n = y(t_n)$ as the exact solution of (7) at time $t = t_n$, the Taylor expansion for the EAVF integrator (6) at $t = t_n$ yields the local truncation error

$$y_{n+1} - y(t_{n+1}) = \frac{h^3}{12}(MF + FM + FF) \cdot S \cdot (Qy + \nabla U(y)) + O(h^5), \quad (8)$$

where $F = \frac{\partial f}{\partial y}$ is the Jacobian of $f(y)$. Equation (8) gives

$$\tilde{g}_3(y) = \frac{1}{12}(MF + FM + FF) \cdot S \cdot (Qy + \nabla U(y)).$$

Let $\tilde{g}_3(y) = \widehat{S}(Qy + \nabla U(y))$, then we have

$$\begin{aligned} \widehat{S} &= \frac{1}{12}(MF + FM + FF) \cdot S \\ &= \frac{1}{12}(SQSUS + SUSQS + SUSUS), \end{aligned}$$

where $\mathcal{U} = \mathcal{U}(y)$ is the Hessian of $U(y)$. The skew symmetry of \widehat{S} follows from the symmetry of \mathcal{U} and the skew symmetry of S .

With the setting $g(y) = My + f(y)$, we denote Φ_g^h and φ_g^h , respectively, as the numerical flow of the EAVF integrator (6) applying to the problem (7) and the exact flow of the problem (7). From the theory of backward error analysis (see Chap. IX of Ref. [23]), Φ_g^h can be viewed as the exact flow of a modified differential equation satisfying

$$\tilde{y}' = \tilde{g}(\tilde{y}) = g(\tilde{y}) + h^2 \tilde{g}_3(\tilde{y}) + h^4 \tilde{g}_5(\tilde{y}) + \dots, \quad (9)$$

where $\tilde{g}_3(y)$ is just obtained previously, i.e., $\Phi_g^h(y) = \varphi_g^h(y)$. Furthermore, based on the *modifying integrator* theory [21] and noting the symmetry of the EAVF integrator (6), there also exists another modified differential equation,

$$\hat{y}' = \widehat{g}(\hat{y}) = g(\hat{y}) + h^2 g_3(\hat{y}) + h^4 g_5(\hat{y}) + \dots, \quad (10)$$

such that applying the EAVF formula (6) to (10) can yield the exact solution of (7), namely, $\Phi_g^h(y) = \varphi_g^h(y)$. Due to the symmetry of the EAVF integrator (6), the terms of the odd power of h , i.e., \tilde{g}_{2k} and g_{2k} for $k \geq 1$ vanish respectively in (9) and (10).

According to the relation between the truncation leading terms of $\tilde{g}(y)$ and $\widehat{g}(y)$ [Theorem 1.2 of Chap. IX on p. 340 of Ref. [23] and Eq. (6) in Ref. [21]], we have $g_3(y) = -\tilde{g}_3(y)$. Therefore, the truncation of $\widehat{g}(y)$ at fourth order reads

$$\begin{aligned} g^{[4]}(y) &= g(y) + h^2 g_3(y) + h^4 g_4(y) \\ &= \widetilde{S}(y)(Qy + \nabla U(y)), \end{aligned} \quad (11)$$

where $\widetilde{S}(y) = S - h^2 \widehat{S}(y)$. In consequence, the modified differential equation that is used for the construction of high-order method and truncated at fourth order can be expressed as follows:

$$y' = g^{[4]}(y) = \widetilde{S}(y)(Qy + \nabla U(y)), \quad y(t_0) = y_0, \quad (12)$$

where $\widetilde{S}(y)$ is skew-symmetric.

B. Fourth-order exponential integrator

Applying the second-order EAVF integrator to the modified differential equation (12) yields

$$y_{n+1} = e^{h\tilde{M}} y_n + h\varphi_1(h\tilde{M}) \cdot \tilde{S} \left(\frac{y_n + y_{n+1}}{2} \right) \cdot \int_0^1 \nabla U((1-\xi)y_n + \xi y_{n+1}) d\xi, \quad (13)$$

where $\tilde{M} = \tilde{S} \left(\frac{y_n + y_{n+1}}{2} \right) Q$, $\tilde{S} \left(\frac{y_n + y_{n+1}}{2} \right) = S - h^2 \hat{S} \left(\frac{y_n + y_{n+1}}{2} \right)$, and $\hat{S} \left(\frac{y_n + y_{n+1}}{2} \right)$ means evaluating \hat{S} at the point $\frac{y_n + y_{n+1}}{2}$. Based on the modifying integrator theory, it is obtained that the exponential integrator (13) is of order four for the system (2). Furthermore, the new integrator (13) can inherit the energy preservation and symmetry of the second-order EAVF integrator (13), which is the key feature of modifying integrators based on modified differential equations [21]. In fact, one can also prove the energy preservation and symmetry of (13) in a similar way as that for the EAVF integrator in Ref. [20], and the details are omitted here.

Now we turn to the simplification of the fourth-order energy-preserving integrator (13). For the system (2), we have $M = SQ = \begin{pmatrix} \frac{1}{\epsilon} B & 0 \\ E & 0 \end{pmatrix}$ and $f(z) = \begin{pmatrix} G(x) \\ 0 \end{pmatrix}$, which consequently

yield $F = \begin{pmatrix} 0 & \mathcal{V} \\ 0 & 0 \end{pmatrix}$ and $\hat{S} = \frac{1}{12} \begin{pmatrix} (B\mathcal{V} + \mathcal{V}B) & -\mathcal{V} \\ \mathcal{V} & 0 \end{pmatrix}$, where $\mathcal{V} = \mathcal{V}(x)$ is the negative Hessian of $U(x)$ with respect to x and thus are symmetric. It then follows that

$$\tilde{S} = S - h^2 \hat{S} = \begin{pmatrix} \frac{1}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) & -E + \frac{h^2}{12} \mathcal{V} \\ E - \frac{h^2}{12} \mathcal{V} & 0 \end{pmatrix},$$

and

$$\tilde{M} = \tilde{S}Q = \begin{pmatrix} \frac{1}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) & 0 \\ E - \frac{h^2}{12} \mathcal{V} & 0 \end{pmatrix}.$$

Therefore, the modified differential equation truncated at fourth order reads

$$\begin{pmatrix} \dot{v} \\ \dot{x} \end{pmatrix} = \begin{pmatrix} \frac{1}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) & 0 \\ E - \frac{h^2}{12} \mathcal{V} & 0 \end{pmatrix} \begin{pmatrix} v \\ x \end{pmatrix} + \begin{pmatrix} (E - \frac{h^2}{12} \mathcal{V})G(x) \\ 0 \end{pmatrix}. \quad (14)$$

According to the special form of \tilde{M} , the functions $\varphi_k(h\tilde{M})$ can be expressed as follows:

$$\varphi_k(h\tilde{M}) = \begin{pmatrix} \varphi_k \left(\frac{h}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) \right) & 0 \\ h(E - \frac{h^2}{12} \mathcal{V}) \cdot \varphi_{k+1} \left(\frac{h}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) \right) & \frac{1}{k!} E \end{pmatrix}, \quad k \in \mathbb{N},$$

due to the fact that $(h\tilde{M})^0 = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix}$, and

$$(h\tilde{M})^k = \begin{pmatrix} \left(\frac{h}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) \right)^k & 0 \\ h(E - \frac{h^2}{12} \mathcal{V}) \left(\frac{h}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B)) \right)^{k-1} & 0 \end{pmatrix}, \quad k \geq 1.$$

Since $G(x)$ is involved only with the variable x , instead of directly employing the original formula (13) with \tilde{S} and \tilde{M} , the fourth-order energy-preserving exponential integrator for the system (2) can be simplified as

$$\begin{aligned} x_{n+1} &= x_n + h \left(E - \frac{h^2}{12} \mathcal{V} \right) \cdot \varphi_1 \left(\frac{h}{\epsilon} \left(B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B) \right) \right) v_n \\ &\quad + h^2 \left(E - \frac{h^2}{12} \mathcal{V} \right) \cdot \varphi_2 \left(\frac{h}{\epsilon} \left(B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B) \right) \right) \cdot \left(E - \frac{h^2}{12} \mathcal{V} \right) \int_0^1 G((1-\xi)x_n + \xi x_{n+1}) d\xi, \\ v_{n+1} &= e^{\frac{h}{\epsilon} (B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B))} v_n + h\varphi_1 \left(\frac{h}{\epsilon} \left(B - \frac{h^2}{12} (B\mathcal{V} + \mathcal{V}B) \right) \right) \cdot \left(E - \frac{h^2}{12} \mathcal{V} \right) \int_0^1 G((1-\xi)x_n + \xi x_{n+1}) d\xi, \end{aligned} \quad (15)$$

where \mathcal{V} is evaluated at $\frac{x_n + x_{n+1}}{2}$.

It is easily verified that the EAVF integrator (6) applied to (2) is identical to the energy-preserving exponential method presented in Ref. [19] via the simplification procedure similar to (15). A comparison between the EAVF integrator (6) and the fourth-order energy-preserving exponential integrator (13) shows that (13) essentially can be regarded as a suitable modification with a small correction to (6). In this sense, we can yield that the fixed-point iteration is efficient for the fourth-order method (13) or (15) as well as the EAVF integrator (6) (see Ref. [20]).

Finally, it should be noticed that the direct Taylor expansion for the EAVF integrator (6) accompanying the

comparison between higher-order truncation terms of $\tilde{g}(y)$ and $\hat{g}(y)$ is invalid in the construction of higher-order (more than fourth order) energy-preserving exponential integrator, because the relation $g_{2k-1}(y) = -\tilde{g}_{2k-1}(y)$ does not hold for higher-order truncation terms with $k \geq 3$. In this case, the B-series approach along with the substitution law for bicolored trees is needed to find the truncated modified vector field $g^{[2k]}(y)$ for $k \geq 3$. More details on this theme are found in Ref. [21].

III. NUMERICAL EXPERIMENTS

In this section, we are concerned with numerical experiments to show the high efficiency and good energy

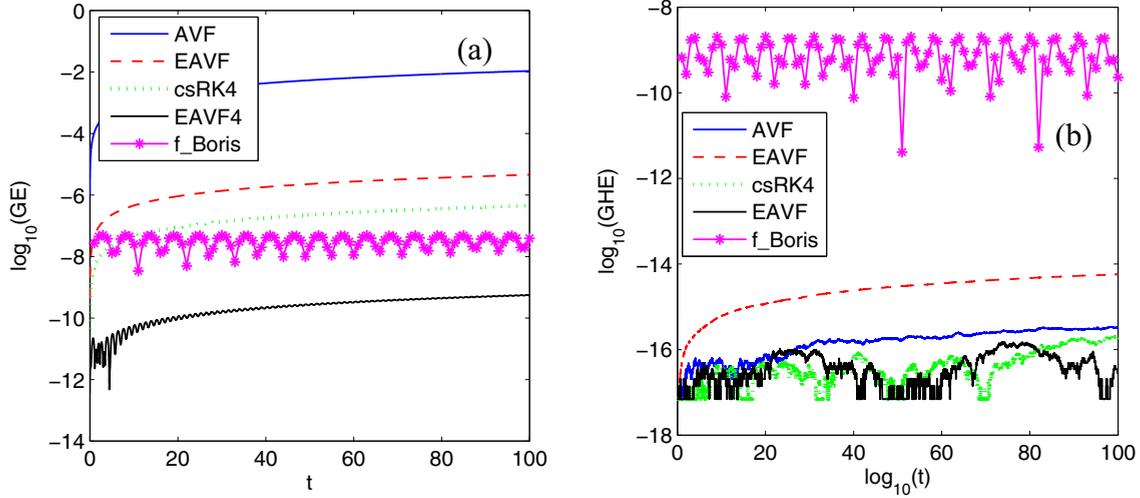


FIG. 1. The global errors (GE) and the global errors of energy (GHE) with $h = 0.01$.

preservation of the proposed fourth-order energy-preserving exponential integrator (15) in solving the charged particle dynamics. Note that a comparison between exponential integrators and the widely used Boris method has been made in Refs. [13,19]. Hence, in our numerical experiments we select only the following methods:

- (1) *AVF*: the average vector field method of order two [24]
- (2) *EAVF*: the exponential average vector field method (6) of order two [19,20]
- (3) *csRK4*: the energy-preserving continuous-stage Runge-Kutta method of order four [25]
- (4) *EAVF4*: the fourth-order energy-preserving exponential integrator (15) proposed in this paper
- (5) *f_Boris*: the filtered Boris method proposed in Ref. [13].

We first note that the filtered Boris method *f_Boris* is explicit, exponential, and volume-preserving, and of order two when applied to the system (1), which has been claimed in Ref. [13]. In addition, the other four methods are implicit and involved with the integral $\int_0^1 \dots d\sigma$ during the implementation. Once the function $G(x)$ is nonlinear on x , the integral in

these numerical integrators cannot be directly calculated. For this reason, we use the six-point Gauss-Legendre quadrature formula $(b_i, c_i)_{i=1}^6$ to numerically evaluate the integral. This idea has been naturally used in the literature [18–20,24,25]. As we have explained previously, the fixed-point iteration is used for the implementation of these implicit methods, and the tolerance error to stop the iteration is set as $\delta = 2 * eps \approx 4.4409 \times 10^{-16}$. The last point is that we carry out our numerical experiments using MATLAB R2012a on a Lenovo desktop Yangtian A6860f-10.

In the numerical experiment, the potential and the constant magnetic field are given as

$$U(x) = \frac{1}{100\sqrt{x_1^2 + x_2^2}}, \quad \tilde{B} = (0, 0, 1).$$

The initial values are selected as $x(0) = (0, 1, 0.1)^T$, $v(0) = (0.09, 0.05, 0.2)^T$ (the same as in Ref. [6]), and the small parameter is set $\epsilon = 0.1$. We solve this problem in the interval $t \in [0, 100]$ and regard the numerical solution obtained by EAVF with a very tiny step size as the reference solution.

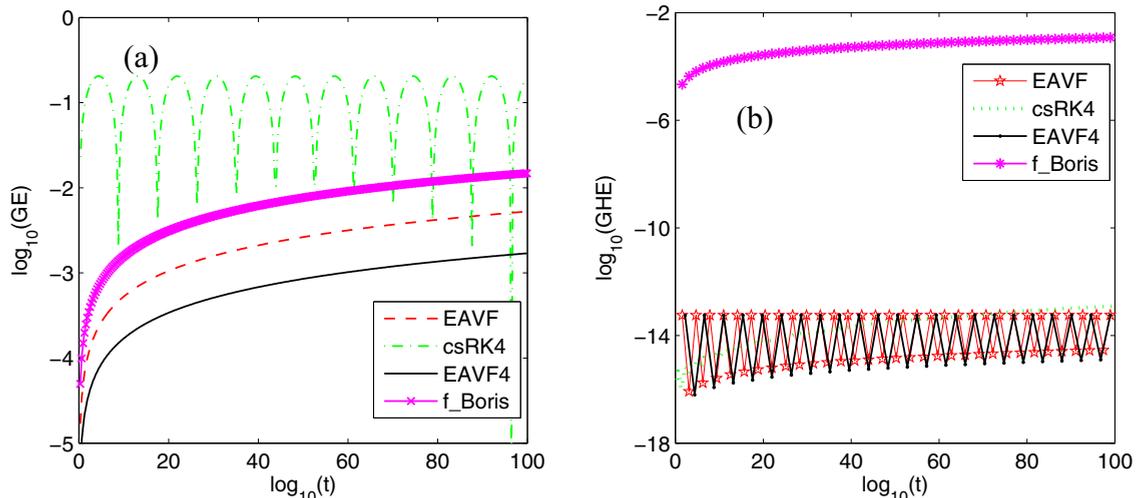


FIG. 2. The global errors (GE) and the global errors of energy (GHE) with a large step size $h = \pi\epsilon \approx 0.314$.

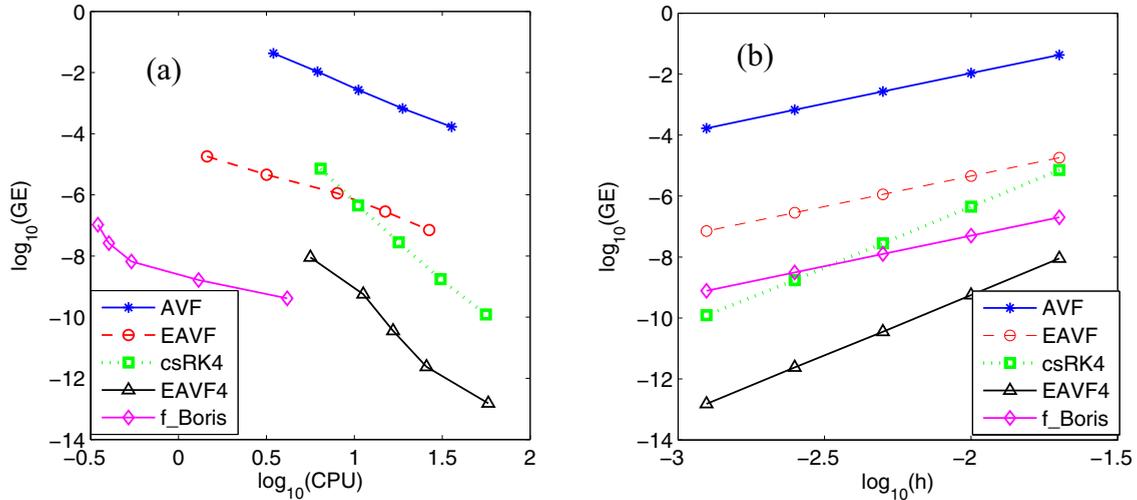


FIG. 3. The efficiency curves and the numerical convergence orders.

We display the numerical results with a small step size $h = 0.01$ in Fig. 1. It can be seen from Fig. 1(a) that the exponential integrators provide more accurate solutions than the same order nonexponential integrators, and the proposed exponential integrator EAVF4 has the best accuracy. Figure 1(b) displays the energy preservation of the five numerical integrators, from which it can be concluded that the four energy-preserving integrators (AVF, EAVF, csRK4, and EAVF4) have good energy preservation because their energy errors are of such a small magnitude of 10^{-14} or 10^{-16} , while the volume-preserving method f_Boris preserves the energy only with an accuracy of 10^{-9} . To exhibit the performance of these numerical method with large step size, we further display the numerical results with $h = \pi\epsilon \approx 0.314$ in Fig. 2, from which we can observe that the proposed method EAVF4 also works well with large step size and has the best accuracy in global errors. The results of AVF are not displayed in Fig. 2, because the fixed-point iteration for this method is no longer convergent. It should be emphasized that the energy errors of some energy-preserving integrators are not up to the roundoff error 10^{-16} but in the magnitude of 10^{-14} . This fact may be caused by an implementation issue of implicit methods that can sometimes cause a rapid accumulation of roundoff errors. More details about this issue can be found in Ref. [26].

Finally, we plot the efficiency curves in Fig. 3(a), which confirm the higher efficiency of exponential integrators by showing the global errors versus the consumed CPU times (in seconds). It is not surprising that f_Boris seems to be more efficient than AVF, EAVF, and csRK4, because it is an explicit method. Figure 3(b) shows that the numerical convergence orders of AVF, EAVF, csRK4, EAVF4, and f_Boris

are, respectively, 2.00, 2.00, 3.97, 3.96, and 2.01, which are consistent with their theoretical orders.

IV. CONCLUSIONS

Charged-particle dynamics in a strong constant magnetic field is widely used in plasma physics, and it can be expressed by a semilinear Poisson system whose linear part depends on the small scaling parameter $0 < \epsilon \ll 1$. Considering the semilinearity of the Poisson system, exponential integrators are preferred to solve this problem. In this paper, according to the relation between the truncation leading terms of $\tilde{g}(y)$ and $\hat{g}(y)$ that are used for different purposes, we derived the truncated modified differential equation of the EAVF integrator. Then a fourth-order exponential integrator was obtained by applying the EAVF formula to the truncated modified differential equation. It was proved that the proposed integrator is symmetric, energy-preserving, and of order four. Finally, numerical experiments support the good energy preservation and high efficiency of the proposed method, which confirms the theoretical analysis made in this paper.

ACKNOWLEDGMENTS

The authors sincerely thank the anonymous reviewers for their valuable suggestions, which helped improve this manuscript. This research is supported in part by the National Natural Science Foundation of China under Grants 11801377 and 11903022, the Natural Science Foundation of Jiangxi Province under Grants 20192BCBL23030 and 20192ACBL21053, and the Science and Technology Foundation of the Jiangxi Provincial Department of Education under Grants GJJ180884 and GJJ170937.

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