Explicit symplectic algorithms based on generating functions for charged particle dynamics

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Dynamics of a charged particle in the canonical coordinates is a Hamiltonian system, and the well-known symplectic algorithm has been regarded as the *de facto* method for numerical integration of Hamiltonian systems due to its long-term accuracy and fidelity. For long-term simulations with high efficiency, explicit symplectic algorithms are desirable. However, it is generally believed that explicit symplectic algorithms are only available for sum-separable Hamiltonians, and this restriction limits the application of explicit symplectic algorithms to charged particle dynamics. To overcome this difficulty, we combine the familiar sum-split method and a generating function method to construct second- and third-order explicit symplectic algorithms for dynamics of charged particle. The generating function method is designed to generate explicit symplectic algorithms for product-separable Hamiltonian with form of $H(\mathbf{x},\mathbf{p}) = \mathbf{p}_i f(\mathbf{x})$ or $H(\mathbf{x},\mathbf{p}) = \mathbf{x}_i g(\mathbf{p})$. Applied to the simulations of charged particle dynamics, the explicit symplectic algorithms based on generating functions demonstrate superiorities in conservation and efficiency.

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I. INTRODUCTION

Dynamics of charged particle in external or self-consistent electromagnetic fields plays a fundamental role in plasma physics, accelerator physics, astrophysics, space physics, and other branches of physics. One of the key components of first-principle-based particle simulations is the algorithm for advancing charged particles, which is an active research topic. The dynamics of a charged particle with the Lorentz force in the canonical coordinates $(\mathbf{x},\mathbf{p})$ is a canonical Hamiltonian system,

$$\frac{d\mathbf{Z}}{dt} = J^{-1}\nabla H(\mathbf{Z}) : \\ = \begin{cases} \frac{d\mathbf{x}}{dt} = \frac{1}{m}[\mathbf{p} - q\mathbf{A}(\mathbf{x})], \\ \frac{d\mathbf{p}}{dt} = -q\nabla\phi(\mathbf{x}) + \frac{q}{m}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T(\mathbf{p}-q\mathbf{A}), \end{cases} \tag{1}$$

where $\mathbf{Z} = (\mathbf{x}^T,\mathbf{p}^T)^T$ is a six-dimensional vector,

$$J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$$

is the canonical symplectic matrix, and

$$H(\mathbf{Z}) = \frac{1}{2m}[\mathbf{p} - q\mathbf{A}(\mathbf{x})]^2 + q\phi(\mathbf{x}) \tag{2}$$

is the Hamiltonian function. For canonical Hamiltonian system

$$\dot{\mathbf{Z}} = J^{-1}\nabla H(\mathbf{Z}), \quad \mathbf{Z} \in \mathbf{R}^{2k}, \quad \mathbf{Z}(t_0) = \mathbf{Z}_0, \tag{3}$$

it is well known that symplectic algorithms conserve the symplectic structure exactly and globally bound the energy error by a small number [1–14]. They have become the *de facto* standard for numerical integration of Hamiltonian systems with important applications in nonlinear dynamics, astrophysics, plasma physics, accelerator physics, and quantum physics. Recently, symplectic and geometric algorithms have been developed for noncanonical particle dynamics [15–28] and the infinite-dimensional particle-field systems [29–43] in plasma physics and accelerator physics. Root searching of implicit algorithms often require more computation resource than explicit algorithms. To improve the efficiency and accuracy of long-term simulations for systems with a large number, e.g., 10^9, of degrees of freedom, it is sometimes desirable to have explicit symplectic algorithms available. Splitting method has been proven to be an effective tool in constructing explicit symplectic algorithms [22,24,38,39,44–48]. The basic procedure is to decompose original system into solvable subsystems possessing the same geometric structure, then compose the geometric subalgorithms together to obtain the desired algorithms [13,44,49]. It is well known that for a Hamiltonian whose $\mathbf{p}$-dependence and $\mathbf{x}$-dependence can be separated as summands in a summation as follows:

$$H(\mathbf{Z}) = f(\mathbf{p}) + g(\mathbf{x}), \tag{4}$$

the splitting method can generate explicit symplectic algorithms of any orders [5,7]. The familiar leapfrog algorithm is an example of this method. We will call the form in Eq. (4) *sum-separable* and refer to this well-known splitting method as *sum-split method*. It is generally believed that if a Hamiltonian is not sum-separable as in Eq. (4), general explicit symplectic algorithms do not exist [11,13,14,44,47,50,51]. For dynamics of charged particle, sum-split method loses efficacy and cannot be applied directly to construct explicit symplectic algorithms, because the Hamiltonian Eq. (2) is not sum-separable. An explicit noncanonical symplectic algorithm has been developed by He *et al.* using sum-split method for charged particle dynamics in the noncanonical coordinates [25,37,40]. However, it requires numerical integration of the magnetic field along given paths, which can be nontrivial for certain

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complicated magnetic fields. In this paper, different from He's splitting algorithm, we combine the familiar sum-split method with a generating function method to construct explicit symplectic algorithms for dynamics of charged particles, which do not require numerical integration of the magnetic field.

The generating function method has been well developed to construct symplectic methods for a Hamiltonian system Eq. (3) [4,13,14]. It is well-known that there are four types of generating functions, i.e., $F_1(\mathbf{x},\mathbf{X})$, $F_2(\mathbf{P},\mathbf{x})$, $F_3(\mathbf{p},\mathbf{X})$, and $F_4(\mathbf{p},\mathbf{P})$, for constructing canonical transformation $(\mathbf{p},\mathbf{x}) \mapsto (\mathbf{P},\mathbf{X})$ [52]. However, in order to apply the generating functions to construct near-identity transformation for numerical algorithms, the first type of generating function $S_1(\mathbf{P},\mathbf{x})$ and the second type of generating function $S_2(\mathbf{p},\mathbf{X})$ are more suitable [4,13,14]. For the purpose of designing algorithms, a mixed kind of generating function in the form of $S_3((\mathbf{P}+\mathbf{p})/2,(\mathbf{X}+\mathbf{x})/2)$ have also been used [4,13,14]. The symplectic Euler method and midpoint method are included in this family. Generally speaking, symplectic methods based on all three types of generating functions are usually implicit. However, for *product-separable* Hamiltonians in the form of

$$H(\mathbf{Z}) = \mathbf{p}_i f(\mathbf{x}), \tag{5}$$

or

$$H(\mathbf{Z}) = \mathbf{x}_i g(\mathbf{p}), \tag{6}$$

explicit symplectic algorithms with accuracy of order 2 and 3 can be constructed by applying the first type of generating function and the second type of generating function, respectively. Here, $\mathbf{p}_i$ is the ith component of the vector $\mathbf{p}$, and $f(\mathbf{x})$ is a scalar function of $\mathbf{x}$. And $\mathbf{x}_i$ is the ith component of the vector $\mathbf{x}$, and $g(\mathbf{p})$ is a scalar function of $\mathbf{p}$. *Product-separable* means that the $\mathbf{x}$-dependency and $\mathbf{p}$-dependency can be separated as factors in a production. For dynamics of charged particle governed by Eq. (1), we sum-split the Hamiltonian Eq. (2) into five parts, two of which can be solved exactly. The other three parts are in the form of Eq. (5) and admit explicit symplectic algorithms based on the generating functions. Then combining the exact solution flows and explicit symplectic subalgorithms in various manners, explicit symplectic algorithms of different orders can be constructed.

The paper is organized as follows. In Sec. II, symplectic algorithms based on generating functions are introduced, and for the Hamiltonian systems with the forms of Eqs. (5) and (6), explicit symplectic algorithms are given. In Sec. III, we construct explicit symplectic algorithms of order 2 and 3 for charged particle dynamics based on generating functions. Numerical experiments are provided, and the superiority of the explicit symplectic algorithms relative to nonsymplectic Runge-Kutta methods and implicit symplectic methods is demonstrated in Sec. IV.

II. SYMPLECTIC METHOD BASED ON GENERATING FUNCTION

Symplectic methods based on generating functions have been well developed and applied in numerical simulations [4,13,14]. A generating function F satisfying $\mathbf{P}^T d\mathbf{X} - \mathbf{p}^T d\mathbf{x} = dF$ generates a canonical transformations $(\mathbf{p},\mathbf{x}) \mapsto (\mathbf{P},\mathbf{X})$, and in general there are four types of generating functions [52]. However, to obtain near-identity canonical transformations, the first type of generating function $S_1(\mathbf{P},\mathbf{x})$, the second type of generating function $S_2(\mathbf{p},\mathbf{X})$, and a mixed type $S_3((\mathbf{P}+\mathbf{p})/2,(\mathbf{X}+\mathbf{x})/2)$ have been used. They are determined by

$$\begin{aligned}
&\mathbf{X}^T d\mathbf{P} + \mathbf{p}^T d\mathbf{x} = d(\mathbf{P}^T\mathbf{x} + S_1(\mathbf{P},\mathbf{x})),\\
&\mathbf{P}^T d\mathbf{X} + \mathbf{x}^T d\mathbf{p} = d(\mathbf{p}^T\mathbf{X} - S_2(\mathbf{p},\mathbf{X})),\\
&(\mathbf{X}-\mathbf{x})^T d(\mathbf{P}+\mathbf{p}) - (\mathbf{P}-\mathbf{p})^T d(\mathbf{X}+\mathbf{x})\\
&\quad = 2d(S_3((\mathbf{P}+\mathbf{p})/2,(\mathbf{X}+\mathbf{x})/2)),
\end{aligned} \tag{7}$$

respectively, and the corresponding symplectic algorithms have been constructed [4,13,14]. The symplectic method based on the mixed type of generating function $S_3((\mathbf{P}+\mathbf{p})/2,(\mathbf{X}+\mathbf{x})/2)$ involves both old and new variables, and is usually implicit. Here, we construct symplectic methods based on the first type of generating function $S_1(\mathbf{P},\mathbf{x})$ and second type of generating function $S_2(\mathbf{p},\mathbf{X})$. The symplectic methods based on generating functions of the first type can be written as

$$\begin{aligned}
\mathbf{p}^{n+1} &= \mathbf{p}^n - \nabla_{\mathbf{x}} G(\mathbf{p}^{n+1},\mathbf{x}^n,\Delta t),\\
\mathbf{x}^{n+1} &= \mathbf{q}^n + \nabla_{\mathbf{p}} G(\mathbf{p}^{n+1},\mathbf{x}^n,\Delta t),
\end{aligned} \tag{8}$$

with the generating function

$$G(\mathbf{p},\mathbf{x},t) = tG_1(\mathbf{p},\mathbf{x}) + t^2 G_2(\mathbf{p},\mathbf{x}) + t^3 G_3(\mathbf{p},\mathbf{x}) + \cdots, \tag{9}$$

where

$$\begin{aligned}
G_1(\mathbf{p},\mathbf{x}) &= H(\mathbf{p},\mathbf{x}),\\
G_2(\mathbf{p},\mathbf{x}) &= \frac{1}{2}\left(\frac{\partial H}{\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{x}}\right)(\mathbf{p},\mathbf{x}),\\
G_3(\mathbf{p},\mathbf{x}) &= \frac{1}{6}\left[\frac{\partial^2 H}{\partial \mathbf{p}^2}\left(\frac{\partial H}{\partial \mathbf{x}}\right)^2 + \frac{\partial^2 H}{\partial \mathbf{p}\partial \mathbf{x}}\frac{\partial H}{\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{x}}\right.\\
&\quad \left. + \frac{\partial^2 H}{\partial \mathbf{x}^2}\left(\frac{\partial H}{\partial \mathbf{p}}\right)^2\right],\\
&\cdots\cdots.
\end{aligned} \tag{10}$$

Utilizing the truncated series,

$$G(\mathbf{p},\mathbf{x},t) = \sum_{i=1}^{r} t^i G_i(\mathbf{p},\mathbf{x}). \tag{11}$$

we obtain a symplectic method of order r [4,13,14]. The symplectic methods based on generating functions of the second type can be constructed similarly. Both types are usually implicit for general Hamiltonian systems. However, for product-separable Hamiltonian with the form of Eq. (5) or Eq. (6), second- and third-order symplectic algorithms based on generating functions can be constructed explicitly. Let's take Hamiltonian Eq. (5) as an example to demonstrate the explicit symplectic methods based on the generating functions. The corresponding second-order generating function of the first type is

$$G(\mathbf{p},\mathbf{x},t) = t\mathbf{p}_i f(\mathbf{x}) + \frac{t^2}{2}\mathbf{p}_i \frac{\partial f}{\partial \mathbf{x}_i} f(\mathbf{x}). \tag{12}$$

Then the explicit symplectic method of order 2 based on the first type of generating function is

$$\mathbf{p}^{n+1} = \mathbf{p}^n - \mathbf{p}_i^{n+1}\left[\Delta t \nabla_{\mathbf{x}} f(\mathbf{x}^n) + \frac{\Delta t^2}{2}\nabla_{\mathbf{x}}\left(\frac{\partial f}{\partial \mathbf{x}_i} f(\mathbf{x}^n)\right)\right],$$
$$\mathbf{x}_i^{n+1} = \mathbf{x}_i^n + \Delta t f(\mathbf{x}^n) + \frac{\Delta t^2}{2}\frac{\partial f}{\partial \mathbf{x}_i} f(\mathbf{x}^n). \tag{13}$$

For the product-separable Hamiltonian in the form of Eq. (6), explicit symplectic algorithms can be constructed similarly utilizing the second type of generating functions.

III. EXPLICIT SYMPLECTIC ALGORITHMS FOR CHARGED PARTICLE DYNAMICS

In this section, we will use the methods given in Sec. II to construct explicit symplectic algorithms for charged-particle dynamics determined by Eq. (1). It was commonly believed that this system does not admit any explicit symplectic algorithm, because the Hamiltonian given by Eq. (2) is not sum-separable. Now, we show how to construct explicit symplectic algorithms for it using the generating-function method and the familiar sum-split method. We sum-split the Hamiltonian function into five parts as

$$H(\mathbf{x},\mathbf{p}) = H_1 + H_2 + H_3 + H_4 + H_5, \tag{14}$$

where

$$H_1 = \frac{1}{2m}\mathbf{p}^2, \quad H_2 = \frac{q^2}{2m}\mathbf{A}(\mathbf{x})^2 + q\phi(\mathbf{x}),$$
$$H_3 = -\frac{q}{m}\mathbf{A}(\mathbf{x})^T(p_1,0,0)^T = -\frac{q}{m}\mathbf{A}_1(\mathbf{x})p_1,$$
$$H_4 = -\frac{q}{m}\mathbf{A}(\mathbf{x})^T(0,p_2,0)^T = -\frac{q}{m}\mathbf{A}_2(\mathbf{x})p_2,$$
$$H_5 = -\frac{q}{m}\mathbf{A}(\mathbf{x})^T(0,0,p_3)^T = -\frac{q}{m}\mathbf{A}_3(\mathbf{x})p_{3.} \tag{15}$$

The corresponding subsystems generated by these sub-Hamiltonians are

$$S_1 := \begin{cases} \frac{d\mathbf{x}}{dt} = \frac{1}{m}\mathbf{p}, \\ \frac{d\mathbf{p}}{dt} = \mathbf{0}, \end{cases}$$
$$S_2 := \begin{cases} \frac{d\mathbf{x}}{dt} = \mathbf{0}, \\ \frac{d\mathbf{p}}{dt} = -\frac{q^2}{m}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T \mathbf{A} - q\nabla\phi(\mathbf{x}), \end{cases}$$
$$S_3 := \begin{cases} \frac{d\mathbf{x}}{dt} = -\frac{q}{m}(\mathbf{A}_1(\mathbf{x}),0,0)^T, \\ \frac{d\mathbf{p}}{dt} = \frac{q}{m}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T(p_1,0,0)^T, \end{cases}$$
$$S_4 := \begin{cases} \frac{d\mathbf{x}}{dt} = -\frac{q}{m}(0,\mathbf{A}_2(\mathbf{x}),0)^T, \\ \frac{d\mathbf{p}}{dt} = \frac{q}{m}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T(0,p_2,0)^T, \end{cases}$$
$$S_5 := \begin{cases} \frac{d\mathbf{x}}{dt} = -\frac{q}{m}(0,0,\mathbf{A}_3(\mathbf{x}),)^T, \\ \frac{d\mathbf{p}}{dt} = \frac{q}{m}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T(0,0,p_3)^T. \end{cases} \tag{16}$$

For subsystems S_1 and S_2, exact solutions can be computed explicitly as

$$\varphi_1(t) := \begin{cases} \mathbf{x}(t) = \mathbf{x}_0 + t\frac{1}{m}\mathbf{p}_0, \\ \mathbf{p}(t) = \mathbf{p}_0, \end{cases}$$
$$\varphi_2(t) := \begin{cases} \mathbf{x}(t) = \mathbf{x}_0, \\ \mathbf{p}(t) = \mathbf{p}_0 - t\frac{q^2}{m}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T \mathbf{A}\mid_{\mathbf{x}=\mathbf{x}_0} - qt\nabla\phi(\mathbf{x}_0). \end{cases} \tag{17}$$

The sub-Hamiltonians of the remaining three subsystems S_3, S_4, and S_5 are all product-separable as in Eq. (5). Let's take the subsystem S_3 associated with the sub-Hamiltonian $H_3(\mathbf{p},\mathbf{x}) = -\frac{q}{m}p_1\mathbf{A}_1(\mathbf{x})$ as an example to demonstrate our method. In terms of Cartesian components, the subsystem S_3 is

$$S_3 := \begin{cases} \frac{dx}{dt} = -\frac{q}{m}\mathbf{A}_1(\mathbf{x}), \\ \frac{dp_1}{dt} = \frac{q}{m}\frac{\partial \mathbf{A}_1}{\partial x}p_1, \\ \frac{dp_2}{dt} = \frac{q}{m}\frac{\partial \mathbf{A}_1}{\partial y}p_1, \\ \frac{dp_3}{dt} = \frac{q}{m}\frac{\partial \mathbf{A}_1}{\partial z}p_1. \end{cases} \tag{18}$$

The symplectic method of order 2 based on generating function can be obtained,

$$\mathbf{p}^{n+1} = \mathbf{p}^n - \nabla_{\mathbf{x}}G(\mathbf{p}^{n+1},\mathbf{x}^n,\Delta t),$$
$$\mathbf{x}^{n+1} = \mathbf{x}^n + \nabla_{\mathbf{p}}G(\mathbf{p}^{n+1},\mathbf{x}^n,\Delta t), \tag{19}$$

where the truncated generating function of order 2 is

$$G(\mathbf{p},\mathbf{x},\Delta t) = \Delta t H_3(\mathbf{p},\mathbf{x}) + \frac{\Delta t^2}{2}(\nabla_{\mathbf{p}}H_3 \cdot \nabla_{\mathbf{x}}H_3)(\mathbf{p},\mathbf{x}),$$
$$= -\Delta t\frac{q}{m}p_1\mathbf{A}_1(\mathbf{x}) + \frac{\Delta t^2}{2}\frac{q^2}{m^2}p_1\frac{\partial \mathbf{A}_1}{\partial x}\mathbf{A}_1(\mathbf{x}). \tag{20}$$

Thus, the second-order symplectic methods for S_3 is

$$\psi_3^{\Delta t} = \begin{cases} x^{n+1} = x^n - \Delta t\frac{q}{m}\mathbf{A}_1(x^n,y^n,z^n) + \frac{\Delta t^2}{2}\frac{q^2}{m^2}\mathbf{A}_1(x^n,y^n,z^n)\frac{\partial \mathbf{A}_1}{\partial x}(x^n,y^n,z^n), \\ p_1^{n+1} = p_1^n + p_1^{n+1}\left[\Delta t\frac{q}{m}\frac{\partial \mathbf{A}_1}{\partial x} - \frac{\Delta t^2}{2}\frac{q^2}{m^2}\frac{\partial \mathbf{A}_1}{\partial x}\frac{\partial \mathbf{A}_1}{\partial x} - \frac{\Delta t^2}{2}\frac{q^2}{m^2}\mathbf{A}_1\frac{\partial^2 \mathbf{A}_1}{\partial x\partial x}\right](x^n,y^n,z^n), \\ p_2^{n+1} = p_2^n + p_1^{n+1}\left[\Delta t\frac{q}{m}\frac{\partial \mathbf{A}_1}{\partial y} - \frac{\Delta t^2}{2}\frac{q^2}{m^2}\frac{\partial \mathbf{A}_1}{\partial x}\frac{\partial \mathbf{A}_1}{\partial y} - \frac{\Delta t^2}{2}\frac{q^2}{m^2}\mathbf{A}_1\frac{\partial^2 \mathbf{A}_1}{\partial x\partial y}\right](x^n,y^n,z^n), \\ p_3^{n+1} = p_3^n + p_1^{n+1}\left[\Delta t\frac{q}{m}\frac{\partial \mathbf{A}_1}{\partial z} - \frac{\Delta t^2}{2}\frac{q^2}{m^2}\frac{\partial \mathbf{A}_1}{\partial x}\frac{\partial \mathbf{A}_1}{\partial z} - \frac{\Delta t^2}{2}\frac{q^2}{m^2}\mathbf{A}_1\frac{\partial^2 \mathbf{A}_1}{\partial x\partial z}\right](x^n,y^n,z^n), \end{cases} \tag{21}$$

which is an explicit method, but not symmetric. For subsystems S_4 and S_5, second-order explicit symplectic methods $\psi_4^{\Delta t}$ and $\psi_5^{\Delta t}$ are constructed similarly. Composing the exact solutions and the symplectic numerical flows of the five subsystems, we obtain the following explicit symplectic method for charged particle dynamics with the accuracy of order 1,

$$\Psi_{\Delta t}^1 = \varphi_1^{\Delta t} \circ \varphi_2^{\Delta t} \circ \psi_3^{\Delta t} \circ \psi_4^{\Delta t} \circ \psi_5^{\Delta t}. \tag{22}$$

To improve the accuracy of explicit symplectic algorithms based on generating function, one of methods is to compose $\Psi_{\Delta t}^1$ and its adjoint $(\Psi_{\Delta t}^1)^* = (\Psi_{-\Delta t}^1)^{-1}$, and obtain

$$\left(\Psi_{\Delta t}^2\right)' = \varphi_1^{\Delta t/2} \circ \varphi_2^{\Delta t/2} \circ \psi_3^{\Delta t/2} \circ \psi_4^{\Delta t/2} \circ \psi_5^{\Delta t/2} \circ \left(\psi_5^{\Delta t/2}\right)^*$$
$$\circ\left(\psi_4^{\Delta t/2}\right)^* \circ \left(\psi_3^{\Delta t/2}\right)^* \circ \left(\varphi_2^{\Delta t/2}\right)^* \circ \left(\varphi_1^{\Delta t/2}\right)^*, \tag{23}$$

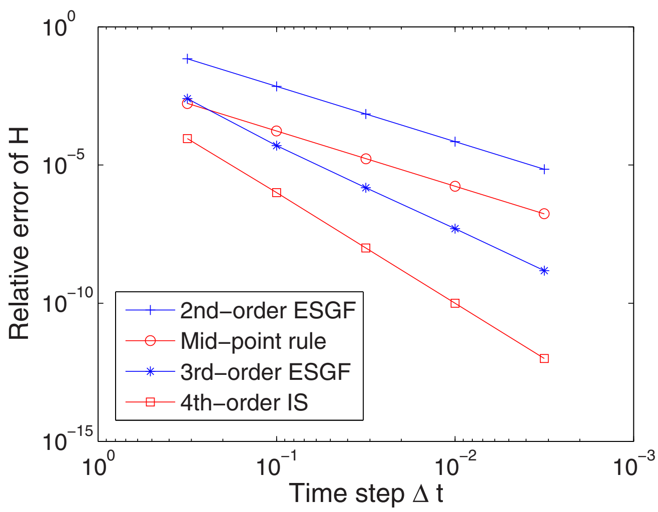

FIG. 1. Convergence rate of the energy error for four symplectic methods. It verifies that $\Psi^2_{\Delta t}$ is indeed a second-order method and $\Psi^3_{\Delta t}$ is a third-order method.

which is symmetric, i.e., $[(\Psi^2_{\Delta t})^{'}]^* = (\Psi^2_{\Delta t})^{'}$. The symmetric numerical algorithms are of even order, so $(\Psi^2_{\Delta t})^{'}$ is at least second order. However, for the subnumerical solutions $\psi_i^{\Delta t/2}$,$(i = 3,4,5)$, their adjoints are not explicit, neither is $(\Psi^2_{\Delta t})^{'}$. To construct explicit algorithms, we replace $(\psi_i^{\Delta t/2})^*$ by $\psi_i^{\Delta t/2}$ in Eq. (23), and obtain

$$\begin{aligned}\Psi^2_{\Delta t} = {} & \varphi_1^{\Delta t/2} \circ \varphi_2^{\Delta t/2} \circ \psi_3^{\Delta t/2} \circ \psi_4^{\Delta t/2} \\ & \circ \psi_5^{\Delta t} \circ \psi_4^{\Delta t/2} \circ \psi_3^{\Delta t/2} \circ \varphi_2^{\Delta t/2} \circ \varphi_1^{\Delta t/2},\end{aligned} \tag{24}$$

which is also of order 2. The proof is given in the Appendix. Since all the subalgorithms preserve the canonical symplectic structure, $\Psi^1_{\Delta t}$ and $\Psi^2_{\Delta t}$ preserve the canonical symplectic structure naturally. Of course, it is possible to increase the accuracy of the numerical methods by various compositions [13,44]. For example, a third-order algorithm can be obtained by the following composition method using $\Psi^2_{\Delta t}$,

$$\Psi^3_{\Delta t} = \Psi^2_{a\Delta t} \circ \Psi^2_{b\Delta t} \circ \Psi^2_{a\Delta t}, \tag{25}$$

where $a = \frac{1}{2-2^{1/3}}$ and $b = 1 - 2a$. To numerically verify the orders of $\Psi^2_{\Delta t}$ and $\Psi^3_{\Delta t}$, we now apply $\Psi^2_{\Delta t}$, $\Psi^3_{\Delta t}$, the second-order implicit midpoint method and a fourth-order implicit symplectic method to simulate the dynamics of charged particle in the magnetic field of a tokamak (see next section). Here, the fourth-order implicit symplectic method is generated by symmetric composition of the second-order implicit midpoint method. The relative errors of Hamiltonian as functions of time step Δt for these methods are plotted in Fig. 1, which verifies that $\Psi^2_{\Delta t}$ is indeed a second-order method and $\Psi^3_{\Delta t}$ is a third-order method.

IV. NUMERICAL EXAMPLES

To numerically test the explicit symplectic algorithms developed, we simulate the dynamics of a 3.5 MeV α particle, which is a product of D-T fusion, in the magnetic field of a tokamak. We will compare the second-order explicit symplectic (ES2) method $\Psi^2_{\Delta t}$ developed with the second-order implicit symplectic midpoint (IS2) method and the forth-order nonsymplectic Runge-Kutta (RK4) method. Numerical results will demonstrate the superb properties of explicit symplectic methods in terms of accuracy, efficiency, and preserving energy over long-term simulations.

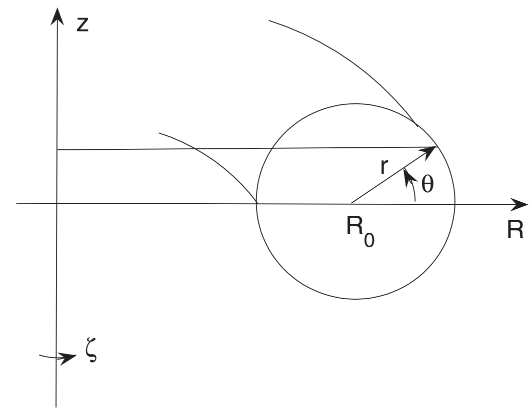

FIG. 2. Two-dimensional tokamak geometry with circular concentric flux surfaces.

The axisymmetric tokamak geometry is illustrated in Fig. 2. A model vector potential of the magnetic field is

$$\mathbf{A} = \frac{B_0 r^2}{2Rq} e_\zeta - \ln\left(\frac{R}{R_0}\right)\frac{R_0 B_0}{2} e_z + \frac{B_0 R_0 z}{2R} e_R, \tag{26}$$

where $R = \sqrt{x^2 + y^2}$ is the major radius coordinate, R_0 is the major radius, B_0 is the magnetic field on axis, the constant q is the safety factor, and $\zeta = \arctan(\frac{x}{y})$ is the toroidal coordinate of the torus. In this example, we take $R_0 = 3m$ and $B_0 = 1T$ with $q = 2$.

The initial position and velocity of the α particle are $\mathbf{x}_0 = (3.15,0,0)m$ and $\mathbf{v}_0 = (0.016,0.04,0)c$, where c is the speed of light, and the simulation time-step is set to be $\Delta t = 0.2\times 10^{-8}s$. Displayed in Fig. 3 is the comparison of transit orbits calculated by the nonsymplectic forth-order Runge-Kutta (RK4) method, second-order implicit symplectic midpoint (IS2) method, and the explicit second symplectic (ES2) algorithm $\Psi^2_{\Delta t}$. It is expected that the orbit consists of a fast, small-scale gyromotion due to Lorentz force, and a slow, large-scale transit motion induced by the inhomogeneity of the magnetic field. In Fig. 3, the small circles of a few centimeters are the fast gyromotion, and the large circles about half a meter in size in the RZ plane is the large-scale transit dynamics. Figure 3(a) shows that the orbit obtained by the nonsymplectic RK4 method after 1.998×10^7 time steps is not accurate any more, while the orbits calculated by the IS2 method in Fig. 3(b) and ES2 algorithm $\Psi^2_{\Delta t}$ in Fig. 3(c) are accurate for all time steps and form closed transit orbits. The long-term energy by nonsymplectic method gradually decreases without bound due to numerical errors. On the contrary, for the symplectic integrators, the energy errors are bounded by a small number for all time. This fact is clearly demonstrated in Fig. 3(d), where normalized energy for the three algorithms are plotted.

To illustrate the efficiency of the explicit symplectic algorithms developed, the CPU time used by the three methods

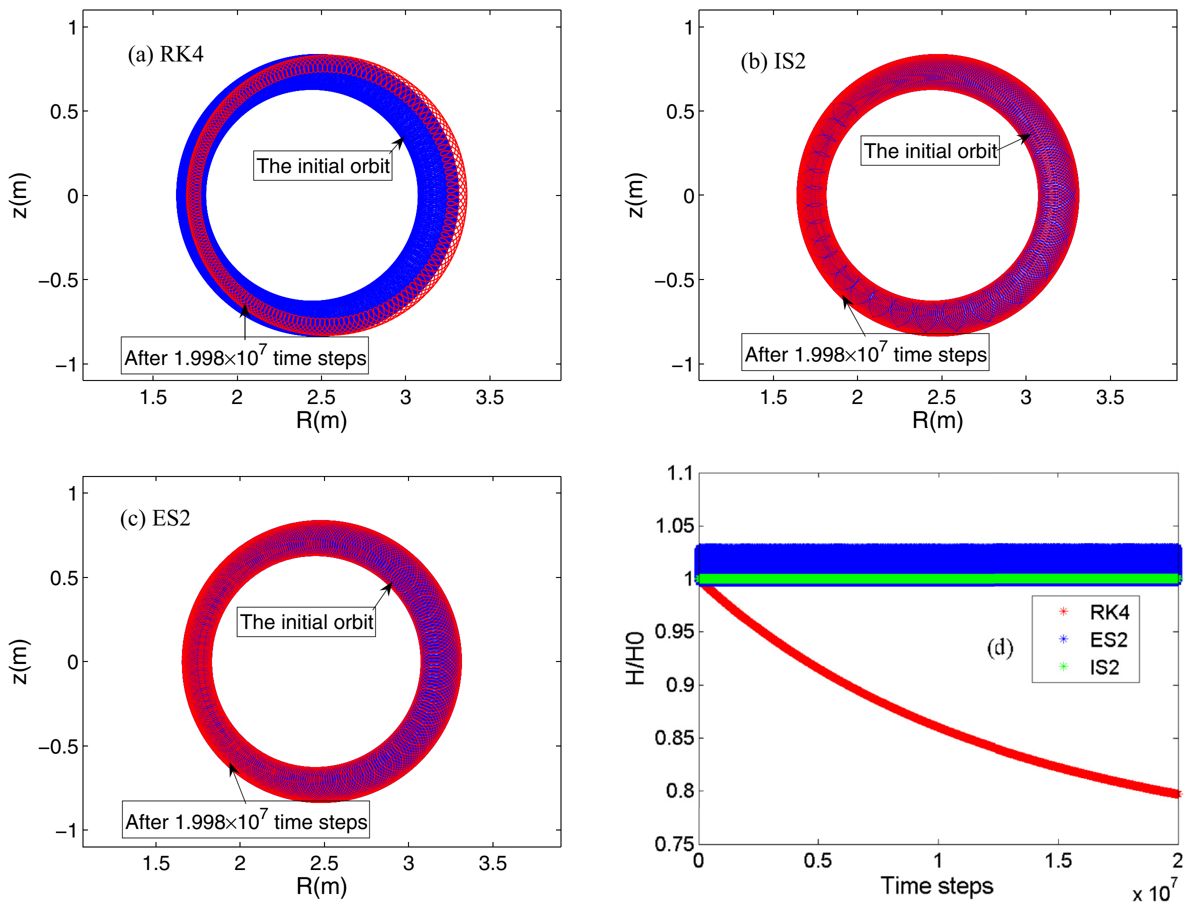

FIG. 3. Simulations of long-term dynamics of a 3.5 MeV α particle in a tokamak. The initial orbits are plotted using blue lines, and the orbits after 1.998×10^7 steps are plotted using red lines. (a) Numerical orbit obtained by a nonsymplectic RK4 method. (b) The orbit obtained by the IS2 method. (c) The numerical orbit by the ES2 method $\Psi^2_{\Delta t}$. (d) The normalized energy H/H_0 of three methods are plotted as functions of simulation time step.

for calculating the charged particle dynamics is listed in Table I. The numerical calculation consists of 10^6 time steps, and is carried using on a Inter Core i5-4200U CPU. It is clear that the ES2 algorithm $\Psi^2_{\Delta t}$ is much more efficient than the IS2 algorithm.

V. CONCLUSION

In this paper, we have constructed explicit symplectic algorithms for dynamics of charged particle by combining the familiar sum-split method with a specially designed generating function method. The newly developed algorithms are expected to significantly extend the applicability of symplectic algorithms to physics problems that contain a large number of degrees of freedom and require accuracy, fidelity, and efficiency of long-term dynamics, such as the classical particle-field system described by the Vlasov-Maxwell equations [53].

TABLE I. CPU time used by the three algorithms for charged particle dynamics in a tokamak.

	RK4	IS2	ES2
CPU time	324s	3446s	1212s

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APPENDIX

We will prove the explicit algorithm $\Psi^2_{\Delta t}$ given by Eq. (24) is a second-order method for the Hamiltonian

$$H(\mathbf{x},\mathbf{p}) = \tfrac{1}{2}[\mathbf{p}-\mathbf{A}(\mathbf{x})]^2 + \phi(\mathbf{x}). \tag{A1}$$

To simplify the notation, we have taken $m = 1$ and $q = 1$. There are three steps in the proof.

Step 1: To prove $\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}$ is a numerical method of order 2 for the sub-Hamiltonian system with Hamiltonian

$$H^1(\mathbf{x},\mathbf{p}) = -\mathbf{p}_1\mathbf{A}_1(\mathbf{x}) - \mathbf{p}_2\mathbf{A}_2(\mathbf{x}) - \mathbf{p}_3\mathbf{A}_3(\mathbf{x}). \tag{A2}$$

Since $\psi_{2+i}^{\Delta t}$, $i=1,2,3$, is numerical method of order 2 for Hamiltonian system generated by $H_{2+i}=-\mathbf{p}_i\mathbf{A}_i(\mathbf{x})$, it can be rewritten as

$$\psi_{2+i}^{\Delta t}(\mathbf{x}^0,\mathbf{p}^0)=\left(I+\Delta t\begin{pmatrix}-\mathbf{A}_i\mathbf{e}_i\\ \mathbf{p}_i\nabla\mathbf{A}_i\end{pmatrix}+\frac{\Delta t^2}{2}\begin{pmatrix}\frac{\partial\mathbf{A}_i}{\partial\mathbf{x}_i}\mathbf{A}_i\mathbf{e}_i\\ \mathbf{p}_i\left(\frac{\partial\mathbf{A}_i}{\partial\mathbf{x}_i}\nabla\mathbf{A}_i-\mathbf{A}_i\nabla\frac{\partial\mathbf{A}_i}{\partial\mathbf{x}_i}\right)\end{pmatrix}+O(\Delta t^3)\right)(\mathbf{x}^0,\mathbf{p}^0),\tag{A3}$$

where $\mathbf{e}_i$ is the unit vector in the ith Cartesian direction. The composition method $\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}$ can be obtained using the iterations step by step as follows:

$$\begin{aligned}
&\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left(I+\frac{\Delta t}{2}\begin{pmatrix}-\mathbf{A}_1\mathbf{e}_1\\ \mathbf{p}_1\nabla\mathbf{A}_1\end{pmatrix}+\frac{\Delta t^2}{8}\begin{pmatrix}\frac{\partial\mathbf{A}_1}{\partial\mathbf{x}_1}\mathbf{A}_1\mathbf{e}_1\\ \mathbf{V}_{11}\end{pmatrix}+O(\Delta t^3)\right)\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left(I+\frac{\Delta t}{2}\begin{pmatrix}-\mathbf{A}_1\mathbf{e}_1-\mathbf{A}_2\mathbf{e}_2\\ \mathbf{p}_2\nabla\mathbf{A}_2+\mathbf{p}_1\nabla\mathbf{A}_1\end{pmatrix}+O(\Delta t^3)\right)\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&\quad+\frac{\Delta t^2}{8}\begin{pmatrix}\frac{\partial\mathbf{A}_1}{\partial\mathbf{x}_1}\mathbf{A}_1\mathbf{e}_1+\frac{\partial\mathbf{A}_2}{\partial\mathbf{x}_2}\mathbf{A}_2\mathbf{e}_2+2\frac{\partial\mathbf{A}_1}{\partial\mathbf{x}_2}\mathbf{A}_2\\ \sum_{i=1}^2\mathbf{V}_{ii}+2\mathbf{V}_{21}\end{pmatrix}\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left(I+\frac{\Delta t}{2}\begin{pmatrix}-\mathbf{A}_1\mathbf{e}_1-\mathbf{A}_2\mathbf{e}_2-2\mathbf{A}_3\mathbf{e}_3\\ \mathbf{p}_2\nabla\mathbf{A}_2+\mathbf{p}_1\nabla\mathbf{A}_1+2\mathbf{p}_3\nabla\mathbf{A}_3\end{pmatrix}+O(\Delta t^3)\right)\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&\quad\times\frac{\Delta t^2}{8}\begin{pmatrix}\frac{\partial\mathbf{A}_1}{\partial\mathbf{x}_1}\mathbf{A}_1\mathbf{e}_1+\frac{\partial\mathbf{A}_2}{\partial\mathbf{x}_2}\mathbf{A}_2\mathbf{e}_2+2\frac{\partial\mathbf{A}_1}{\partial\mathbf{x}_2}\mathbf{A}_2\mathbf{e}_1+4\frac{\partial\mathbf{A}}{\partial\mathbf{x}_3}\mathbf{A}_3\\ \sum_{i=1}^2\mathbf{V}_{ii}+4\mathbf{V}_{33}+4\mathbf{V}_{32}+4\mathbf{V}_{31}+2\mathbf{V}_{21}\end{pmatrix}\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left(I+\frac{\Delta t}{2}\begin{pmatrix}-\mathbf{A}_1\mathbf{e}_1-2\mathbf{A}_2\mathbf{e}_2-2\mathbf{A}_3\mathbf{e}_3\\ 2\mathbf{p}_2\nabla\mathbf{A}_2+\mathbf{p}_1\nabla\mathbf{A}_1+2\mathbf{p}_3\nabla\mathbf{A}_3\end{pmatrix}+O(\Delta t^3)\right)\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&\quad+\frac{\Delta t^2}{8}\begin{pmatrix}\frac{\partial\mathbf{A}_1}{\partial\mathbf{x}_1}\mathbf{A}_1\mathbf{e}_1+4\frac{\partial\mathbf{A}}{\partial\mathbf{x}_2}\mathbf{A}_2+4\frac{\partial\mathbf{A}}{\partial\mathbf{x}_3}\mathbf{A}_3\\ \mathbf{V}_{11}+4\mathbf{V}_{22}+4\mathbf{V}_{33}+4\mathbf{V}_{32}+4\mathbf{V}_{31}+4\mathbf{V}_{21}+4\mathbf{V}_{23}\end{pmatrix}\psi_3^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left(I+\Delta t\begin{pmatrix}-\mathbf{A}\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{p}\end{pmatrix}+\frac{\Delta t^2}{2}\begin{pmatrix}\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\mathbf{A}\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{p}-\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)_x^T\mathbf{A}\mathbf{p}\end{pmatrix}+O(\Delta t^3)\right)(\mathbf{x}^0,\mathbf{p}^0),
\end{aligned}\tag{A4}$$

where $\mathbf{V}_{ij}=\mathbf{p}_i\frac{\partial\mathbf{A}_i}{\partial\mathbf{x}_j}\nabla\mathbf{A}_j-\mathbf{p}_j\mathbf{A}_i\nabla\frac{\partial\mathbf{A}_j}{\partial\mathbf{x}_i}$. This shows that the $\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}$ is of order 2.

Step 2: To prove $\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}$ is of order 2 for the sub-Hamiltonian system with Hamiltonian

$$H^2(\mathbf{x},\mathbf{p})=-\mathbf{p}_1\mathbf{A}_1(\mathbf{x})-\mathbf{p}_2\mathbf{A}_2(\mathbf{x})-\mathbf{p}_3\mathbf{A}(\mathbf{x})+\tfrac{1}{2}\mathbf{A}^2(\mathbf{x})+\phi(\mathbf{x}).\tag{A5}$$

As proved in Step 1, the iteration $\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}$ is of order 2, and

$$\varphi_2^{\Delta t}(\mathbf{x}^0,\mathbf{p}^0)=\left[I-\Delta t\begin{pmatrix}0\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{A}+\nabla\phi\end{pmatrix}\right](\mathbf{x}^0,\mathbf{p}^0).\tag{A6}$$

The following calculation shows that $\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}$ has accuracy of order 2,

$$\begin{aligned}
&\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left[I-\frac{\Delta t}{2}\begin{pmatrix}0\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{A}+\nabla\phi\end{pmatrix}\right]\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left[I+\Delta t\begin{pmatrix}-\mathbf{A}\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{p}-\frac{1}{2}\left(\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{A}+\nabla\phi\right)\end{pmatrix}+O(\Delta t^3)\right]\varphi_2^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&\quad+\frac{\Delta t^2}{2}\begin{pmatrix}\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\mathbf{A}\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{p}-\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)_x^T\mathbf{A}\mathbf{p}+\nabla_{xx}\left(\frac{\mathbf{A}^2}{2}\right)\mathbf{A}+\nabla_{xx}\phi\mathbf{A}\end{pmatrix}\varphi_2^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&=\left[I+\Delta t\begin{pmatrix}-\mathbf{A}\\ \left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{p}-\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)^T\mathbf{A}-\nabla\phi\end{pmatrix}+O(\Delta t^3)\right](\mathbf{x}^0,\mathbf{p}^0)
\end{aligned}$$

$$+\frac{\Delta t^2}{2}\begin{pmatrix} \frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{A} \\ \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\mathbf{p} - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T_x \mathbf{A}\mathbf{p} + \nabla_{xx}\left(\frac{\mathbf{A}^2}{2}\right)\mathbf{A} + \nabla_{xx}\phi\mathbf{A}\end{pmatrix}(\mathbf{x}^0,\mathbf{p}^0)$$
$$+\frac{\Delta t^2}{2}\begin{pmatrix} 0 \\ -\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\left(\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\mathbf{A} + \nabla\phi\right)\end{pmatrix}(\mathbf{x}^0,\mathbf{p}^0). \tag{A7}$$

Step 3: To prove $\varphi_1^{\Delta t/2}\circ\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}\circ\varphi_1^{\Delta t/2}$ is of order 2 for the Hamiltonian Eq. (A1). The iteration $\varphi_1^{\Delta t}$ is

$$\varphi_1^{\Delta t}(\mathbf{x}^0,\mathbf{p}^0) = \left(I + \Delta t\begin{pmatrix}\mathbf{p}\\0\end{pmatrix}\right)(\mathbf{x}^0,\mathbf{p}^0). \tag{A8}$$

Combining with the second-order iteration $\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}$ proved in Step 2, we obtain

$$\begin{aligned}\Psi^2_{\Delta t} &= \varphi_1^{\Delta t/2}\circ\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}\circ\varphi_1^{\Delta t/2}\\
&= \left(I + \Delta t\begin{pmatrix}\mathbf{p}\\0\end{pmatrix}\right)\varphi_2^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\psi_4^{\Delta t/2}\circ\psi_5^{\Delta t}\circ\psi_4^{\Delta t/2}\circ\psi_3^{\Delta t/2}\circ\varphi_2^{\Delta t/2}\circ\varphi_1^{\Delta t/2}(\mathbf{x}^0,\mathbf{p}^0)\\
&= \left(I + \Delta t\begin{pmatrix}\mathbf{p}-\mathbf{A}\\ \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\mathbf{p} - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\mathbf{A} - \nabla\phi\end{pmatrix} + O(\Delta t^3)\right)(\mathbf{x}^0,\mathbf{p}^0) + \frac{\Delta t^2}{2}\begin{pmatrix}\left(\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T - \frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)(\mathbf{p}-\mathbf{A}) - \nabla\phi\\ \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\mathbf{p} + \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T_x(\mathbf{p}-\mathbf{A})\mathbf{p}\end{pmatrix}(\mathbf{x}^0,\mathbf{p}^0)\\
&\quad + \frac{\Delta t^2}{2}\begin{pmatrix}0\\ -\nabla_{xx}\left(\frac{\mathbf{A}^2}{2}+\phi\right)(\mathbf{p}-\mathbf{A}) - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\left(\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\mathbf{A} + \nabla\phi\right)\end{pmatrix}(\mathbf{x}^0,\mathbf{p}^0),\end{aligned} \tag{A9}$$

which shows that $\Psi^2_{\Delta t}$ is a second-order method.

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