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Symplectic properties research for finite element methods of Hamiltonian system

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Abstract

In this paper, we first apply properties of the wedge product and continuous finite element methods to prove that the linear, quadratic element methods are symplectic algorithms to the linear Hamiltonian systems, i.e., the symplectic condition $dp_{j+1} \wedge dq_{j+1} = dp_j \wedge dq_j$ is preserved exactly and the linear element method is an approximately symplectic integrator to nonlinear Hamiltonian systems, i.e., $dp_{j+1} \wedge dq_{j+1} = dp_j \wedge dq_j + O(h^2)$, as well as energy conservative.

Keywords: Hamiltonian systems, continuous finite element methods, energy conservative, wedge product, symplectic algorithm.

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1. Introduction

Hamiltonian system is a kind of important mechanical systems. It has a symplectic structure which has strong geometric properties of a dynamical system and maintain the total energy $H(q,p)$ which means the phase-space points (q,p) are allowed on the constant energy hypersurface satisfying $H(q,p) = E$. It is natural to look for those discretization systems which preserve as much as possible the characteristic properties of the original continuous systems. Traditional algorithms, such as classical R-K method [4,5], Adams method etc. except some occasions are nonsymplectic, eventually lead to greatly distortions. Symplectic geometry is the mathematical foundation of Hamiltonian systems. Authors in [4–15] constructed the symplectic methods to solve the Hamiltonian system and got good results.

Consider the autonomous Hamiltonian systems:

$$\frac{dp^{(i)}}{dt} = -\frac{\partial H}{\partial q^{(i)}}, \; \frac{dq^{(i)}}{dt} = \frac{\partial H}{\partial p^{(i)}}, \; i = 1,2,\dots,n, \tag{1.1}$$

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where $p = (p^{(1)}, p^{(2)}, \ldots, p^{(n)})^T$, $q = (q^{(1)}, q^{(2)}, \ldots, q^{(n)})^T$, 'T' is matrix transpose. In applications to mechanics, q represents the space coordinates, p the momenta, and H is the energy of systems.

Let $z = (p, q)^T$, $\frac{\partial H}{\partial z} = H_z \in R^{2n}$. Then (1.1) can be written as

$$\frac{dz}{dt} = J^{-1}\frac{\partial H}{\partial z}, \quad J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}. \tag{1.2}$$

I_n is the $n \times n$ identity matrix, $J^T = J^{-1} = -J$.

Let Ψ be a diffeomorphism of R^{2n}:

$$z = \begin{pmatrix} p \\ q \end{pmatrix} \to \Psi(z) = \begin{bmatrix} \Psi^{(1)}(z) \\ \cdot \\ \cdot \\ \cdot \\ \Psi^{(2n)}(z) \end{bmatrix} = \begin{bmatrix} \hat{p}(p, q) \\ \hat{q}(p, q) \end{bmatrix}.$$

Definition 1.1. A smooth map Ψ on the phase space R^{2n} is called a symplectic map or canonical map if its Jacobi $\Psi_z(z)$ satisfies:

$$[\Psi_z(z)]^T J \Psi_z(z) = J$$

for all z in the domain of definition of Ψ [4].

Equation (1.1) or (1.2) be defined in phase space R^{2n} with a standard symplectic structure given by the non-singular anti-symmetric closed differential 2-form

$$\omega = \sum_{i=1}^{n} dz^{(i)} \wedge dz^{(n+i)} = \sum_{i=1}^{n} dp^{(i)} \wedge dq^{(i)} = dp \wedge dq.$$

Ψ is called a symplectic transformation if Ψ preserves the 2-form ω

$$\sum_{i=1}^{n} d\hat{p}^{(i)} \wedge d\hat{q}^{(i)} = \sum_{i=1}^{n} dp^{(i)} \wedge dq^{(i)}.$$

This is equivalent to the condition that [4]

$$(\frac{\partial \Psi}{\partial z})^T J (\frac{\partial \Psi}{\partial z}) = J.$$

Thus conservation of symplecticness, under a transformation $\hat{p} = \Phi^1(p, q)$, $\hat{q} = \Phi^2(p, q)$ reduces to the statement

$$d\hat{p} \wedge d\hat{q} = dp \wedge dq,$$

where $d\hat{p} = \Phi^1_p(p, q)dp + \Phi^1_q(p, q)dq$, $d\hat{q} = \Phi^2_p(p, q)dp + \Phi^2_q(p, q)dq$.

Definition 1.2. A numerical method is symplectic integrator if the symplecticness condition $dp_{j+1} \wedge dq_{j+1} = dp_j \wedge dq_j$ is preserved exactly [11].

Wedge product is a differential 2-form, with the following properties:

1. skew-symmetry:

$$da \wedge db = -db \wedge da; \tag{1.3}$$

2. bilinearity:

$$\text{for } \alpha, \beta \in R, \quad da \wedge (\alpha db + \beta dc) = \alpha da \wedge db + \beta da \wedge dc;$$

3. rule of matrix multiplication (as a consequence of Property 2 and the definition)

$$da \wedge (Adb) = (A^T da) \wedge db, \quad \text{for any } \; n \times n \; \text{ matrix } \; A; \tag{1.4}$$

4.

$$\text{if } \; A \; \text{ is a symmetric matrix, then } \; da \wedge (Ada) = 0, \tag{1.5}$$

where da, db, and dc are n-vectors of differential one-forms on R^n.

The definition $\Psi_z(z)^T J \Psi_z(z) = J$ is not always the most convenient approach to check the symplecticness of a given map Ψ. The wedge product notation can be combined with implicit differentiation, which makes it a powerful tool to verify symplecticness of an implicitly given transformation Ψ. Leimkuhler and Reich in [11] utilized the wedge product and composition method proving that Euler-A, Euler-B, implicit midpoint method for the general Hamiltonian and the second-order Stormer-Verlet methods for the special case of a separable Hamiltonian are canonically symplectic. Sanz-Serna [14], Sanz-Serna and Calvo [15], Lasagni [10], and Suris [17] utilized the wedge product and tensor product to prove the conditions of the parameters a_{ij} and b_i are $b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, i, j = 1, \ldots, s$ for a s-stage symplectic Runge-Kutta method. So the wedge product is also an important method to study symplectic geometry algorithm of Hamiltonian system.

Symplectic algorithm is a difference method that preserves the structure of the system. However, most numerical methods can't maintain the two properties: symplectic and energy conservation simultaneously in general according to Ge-Marsde theorem [6]. Symplectic algorithm can preserves symplectic properties, but only obtain approximate energy conservation for nonlinear Hamiltonian system.

Many scholars pointed out that the energy conservation is more important at certain times, see [8, 16]. So we turn to the finite element method (FEM). It is founded that the continuous FEM always preserves the energy [18], thus we need only to discuss symplectic properties. In this paper, we apply continuous FEM and properties of the wedge product to prove that the linear, quadratic element methods are symplectic algorithms to the linear Hamiltonian systems, i.e.the symplectic condition $dp_{j+1} \wedge dq_{j+1} = dp_j \wedge dq_j$ is preserved exactly and the linear element method is an approximately symplectic integrator to nonlinear Hamiltonian systems, i.e., $dp_{j+1} \wedge dq_{j+1} = dp_j \wedge dq_j + O(h^2)$.

2. Continuous FEM for Hamiltonian system

Consider the first-order ordinary differential equation with initial value in the interval $I = [0, T]$

$$\frac{du}{dt} = u' = f(t, u), u(0) = u_0.$$

Set $\triangle^h : t_0 = 0 < t_1 < t_2 < \cdots < t_N = T$ as partition of I, with interval $I_j = (t_j, t_{j+1}), h_j = t_{j+1} - t_j$. Define the m-th degree continuous finite element space [2, 3]

$$S^h = \{w \mid w \in C(I), w \mid_{I_j} \in P_m\},$$

where P_m is a m-th degree polynomial. Each m-degree polynomial in interval I_j has m + 1 parameters, but only m freedoms, as its starting value at point t_j is given. Define m-th degree continuous finite element $U \in S^h$ satisfying

$$\int_{I_j} (U' - f(t, U)) v dt = 0, \quad v \in P_{m-1}, U(0) = u_0,$$

i.e., it is orthogonal to arbitrary P_{m-1} in I_j. Taking $v \in S^h$, its derivate $v' \in P_{m-1}$. In practical computation, take $v = (t - t_j)^i, i = 0, 1, 2, \ldots, m-1$.

Lemma 2.1 ([3]). *The m-th degree continuous finite element of ordinary differential equation has superconvergence in nodes* t_j

$$(u - U)(t_j) = O(h^{2m}) \parallel u \parallel_{m+1,\infty}.$$

In (1.2), the m-th degree continuous finite element $Z = \begin{bmatrix} P \\ Q \end{bmatrix}$ of z satisfies orthogonal relation:

$$\int_{I_j} (Z' - J^{-1}H_z)v^{'}dt = 0, Z(0) = z_0. \tag{2.1}$$

Taking $v = \begin{bmatrix} Q \\ P \end{bmatrix}$, we obtain:

$$\int_{I_j} (P' + H_q(P,Q))Q'dt = 0, P(0) = p_0, \quad \int_{I_j} (Q' - H_p(P,Q))P'dt = 0, Q(0) = q_0.$$

It follows from the above two equations that:

$$\int_{I_j} (H_pP' + H_qQ')dt = \int_{I_j} \frac{d}{dt}H(P,Q)dt = 0.$$

Hence, in each nodes t_j, we prove that:

$$H(P(t_j), Q(t_j)) = H(P(t_{j-1}), Q(t_{j-1})) = \cdots = H(P(0), Q(0)) = H(p_0, q_0).$$

So we can prove that

Lemma 2.2 ([18]). *Applying arbitrary degree continuous finite element to solve Hamilton equation, it maintains energy conservation, i.e.,* $H(P(t_j), Q(t_j)) = H(p_0, q_0)$.

3. The wedge product notation applied in the linear element methods

Consider the linear Hamiltonian system,

$$\frac{dz}{dt} = J^{-1}Lz, Z(0) = z_0,$$

where $H(z) = \frac{1}{2}z^TLz,\ L^T = L = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}$, and A, B are $n \times n$ symmetric matrices. Thus the canonical equation as follows

$$\frac{dp}{dt} = -C^Tp - Bq, \ \frac{dq}{dt} = Ap + Cq.$$

Utilizing linear FEM in the interval $I_j = [t_j, t_{j+1}]$:

$$\int_{I_j} \frac{dP}{dt} * 1dt = -\int_{I_j} (C^TP + BQ) * 1dt, \quad \int_{I_j} \frac{dQ}{dt} * 1dt = \int_{I_j} (AP + CQ) * 1dt, \tag{3.1}$$

where the linear element of p is $P = \frac{t-t_{j+1}}{t_j-t_{j+1}}P_j + \frac{t-t_j}{t_{j+1}-t_j}P_{j+1}$ and q is $Q = \frac{t-t_{j+1}}{t_j-t_{j+1}}Q_j + \frac{t-t_j}{t_{j+1}-t_j}Q_{j+1}$.

Integral (3.1)

$$\begin{aligned} P_{j+1} - P_j &= -\frac{h_j}{2}(C^T(P_j + P_{j+1}) + B(Q_j + Q_{j+1})), \\ Q_{j+1} - Q_j &= \frac{h_j}{2}(A(P_j + P_{j+1}) + C(Q_j + Q_{j+1})), j = 0, 1, \dots, N-1. \end{aligned} \tag{3.2}$$

By taking differential of (3.2) we can write

$$\begin{aligned} dP_{j+1} - dP_j &= -\frac{h_j}{2}(C^T(dP_j + dP_{j+1}) + B(dQ_j + dQ_{j+1})), \\ dQ_{j+1} - dQ_j &= \frac{h_j}{2}(A(dP_j + dP_{j+1}) + C(dQ_j + dQ_{j+1})). \end{aligned} \tag{3.3}$$

From (3.3), we can obtain

$$(I+\frac{h_jC^T}{2})dP_{j+1}+\frac{h_jB}{2}dQ_{j+1}=(I-\frac{h_jC^T}{2})dP_j-\frac{h_jB}{2}dQ_j, \quad (3.4)$$

$$-\frac{h_jA}{2}dP_{j+1}+(I-\frac{h_jC}{2})dQ_{j+1}=\frac{h_jA}{2}dP_j+(I+\frac{h_jC}{2})dQ_j, \quad (3.5)$$

by taking wedge products with dQ_{j+1} and dP_{j+1}, respectively. With symmetric properties of A and B and according to (1.5)

$$\frac{h_jB}{2}dQ_{j+1}\wedge dQ_{j+1}=0,-\frac{h_jA}{2}dP_{j+1}\wedge dP_{j+1}=0,$$

thus

$$(I+\frac{h_jC^T}{2})dP_{j+1}\wedge dQ_{j+1}=(I-\frac{h_jC^T}{2})dP_j\wedge dQ_{j+1}-\frac{h_jB}{2}dQ_j\wedge dQ_{j+1},$$
$$(I-\frac{h_jC}{2})dQ_{j+1}\wedge dP_{j+1}=\frac{h_jA}{2}dP_j\wedge dP_{j+1}+(I+\frac{h_jC}{2})dQ_j\wedge dP_{j+1}.$$

By subtracting the above equations we have

$$\begin{aligned}2dP_{j+1}\wedge dQ_{j+1}=&(I-\frac{h_jC^T}{2})dP_j\wedge dQ_{j+1}-\frac{h_jB}{2}dQ_j\wedge dQ_{j+1}\\&-\frac{h_jA}{2}dP_j\wedge dP_{j+1}-(I+\frac{h_jC}{2})dQ_j\wedge dP_{j+1}.\end{aligned} \quad (3.6)$$

Similarly, If we take the wedge product of (3.4) with dQ_j and (3.5) with dP_j, then subtract

$$\begin{aligned}2dP_j\wedge dQ_j=&(I+\frac{h_jC^T}{2})dP_{j+1}\wedge dQ_j+\frac{h_jB}{2}dQ_{j+1}\wedge dQ_j\\&+\frac{h_jA}{2}dP_{j+1}\wedge dP_j-(I-\frac{h_jC}{2})dQ_{j+1}\wedge dP_j.\end{aligned} \quad (3.7)$$

Based on (1.3), (1.4), (3.6), and (3.7), we prove the following equation

$$dP_{j+1}\wedge dQ_{j+1}=dP_j\wedge dQ_j.$$

Theorem 3.1. *The linear finite element method for the linear Hamiltonian systems is a symplectic algorithm, i.e., the symplectic condition* $dp_{j+1}\wedge dq_{j+1}=dp_j\wedge dq_j$ *is preserved exactly.*

4. The wedge product notation applied in the quadratic element methods

Utilizing quadratic element methods in the interval $I_j=[t_j,t_{j+1}]$:

$$\begin{aligned}\int_{I_j}\frac{dP}{dt}*1dt&=-\int_{I_j}(C^TP+BQ)*1dt,\\ \int_{I_j}\frac{dQ}{dt}*1dt&=\int_{I_j}(AP+CQ)*1dt,\\ \int_{I_j}\frac{dP}{dt}*(t-t_j)dt&=-\int_{I_j}(C^TP+BQ)*(t-t_j)dt,\\ \int_{I_j}\frac{dQ}{dt}*(t-t_j)dt&=\int_{I_j}(AP+CQ)*(t-t_j)dt,\end{aligned} \quad (4.1)$$

where the quadratic element of p is

$$P=\frac{(t-t_{j+1})(t-t_{j+\frac{1}{2}})}{(t_j-t_{j+1})(t_j-t_{j+\frac{1}{2}})}P_j+\frac{(t-t_{j+1})(t-t_j)}{(t_{j+\frac{1}{2}}-t_{j+1})(t_{j+\frac{1}{2}}-t_j)}P_{j+\frac{1}{2}}+\frac{(t-t_{j+\frac{1}{2}})(t-t_j)}{(t_{j+1}-t_{j+\frac{1}{2}})(t_{j+1}-t_j)}P_{j+1}$$

and q is

$$Q=\frac{(t-t_{j+1})(t-t_{j+\frac{1}{2}})}{(t_j-t_{j+1})(t_j-t_{j+\frac{1}{2}})}Q_j+\frac{(t-t_{j+1})(t-t_j)}{(t_{j+\frac{1}{2}}-t_{j+1})(t_{j+\frac{1}{2}}-t_j)}Q_{j+\frac{1}{2}}+\frac{(t-t_{j+\frac{1}{2}})(t-t_j)}{(t_{j+1}-t_{j+\frac{1}{2}})(t_{j+1}-t_j)}Q_{j+1}$$

in I_j.

Integral (4.1)

$$\begin{aligned}
P_{j+1}-P_j&=-\frac{h_j}{2}(C^T(\frac{P_j}{3}+\frac{4P_{j+1/2}}{3}+\frac{P_{j+1}}{3})+B(\frac{Q_j}{3}+\frac{4Q_{j+1/2}}{3}+\frac{Q_{j+1}}{3})),\\
Q_{j+1}-Q_j&=\frac{h_j}{2}(A(\frac{P_j}{3}+\frac{4P_{j+1/2}}{3}+\frac{P_{j+1}}{3})+C(\frac{Q_j}{3}+\frac{4Q_{j+1/2}}{3}+\frac{Q_{j+1}}{3})),\\
\frac{5P_{j+1}}{6}-\frac{P_j}{6}-\frac{2P_{j+1/2}}{3}&=-\frac{h}{4}(C^T(\frac{4P_{j+1/2}}{3}+\frac{2P_{j+1}}{3})+B(\frac{4Q_{j+1/2}}{3}+\frac{2Q_{j+1}}{3})),\\
\frac{5Q_{j+1}}{6}-\frac{Q_j}{6}-\frac{2Q_{j+1/2}}{3}&=\frac{h}{4}(A(\frac{4P_{j+1/2}}{3}+\frac{2P_{j+1}}{3})+C(\frac{4Q_{j+1/2}}{3}+\frac{2Q_{j+1}}{3})).
\end{aligned}\tag{4.2}$$

By taking differential of (4.2) we have

$$\frac{2h_jC^T}{3}dP_{j+1/2}+(I+\frac{h_jC^T}{6})dP_{j+1}+\frac{2h_jB}{3}dQ_{j+1/2}+\frac{h_jB}{6}dQ_{j+1}=(I-\frac{h_jC^T}{6})dP_j-\frac{h_jB}{6}dQ_j,\tag{4.3}$$

$$-\frac{2h_jA}{3}dP_{j+1/2}-\frac{h_jA}{6}dP_{j+1}-\frac{2h_jC}{3}dQ_{j+1/2}+(I-\frac{h_jC}{6})dQ_{j+1}=\frac{h_jA}{6}dP_j+(I+\frac{h_jC}{6})dQ_j,\tag{4.4}$$

$$(-\frac{2I}{3}+\frac{h_jC^T}{3})dP_{j+1/2}+(\frac{5I}{6}+\frac{h_jC^T}{6})dP_{j+1}+\frac{h_jB}{3}dQ_{j+1/2}+\frac{h_jB}{6}dQ_{j+1}=\frac{dP_j}{6},\tag{4.5}$$

$$-\frac{h_jA}{3}dP_{j+1/2}-\frac{h_jA}{6}dP_{j+1}+(-\frac{2I}{3}-\frac{h_jC}{3})dQ_{j+1/2}+(\frac{5I}{6}-\frac{h_jC}{6})dQ_{j+1}=\frac{dQ_j}{6}.\tag{4.6}$$

By taking wedge product of (4.3) with dQ_{j+1}, and (4.4) with dP_{j+1}, then subtract

$$\begin{aligned}
2dP_{j+1}\wedge dQ_{j+1}=&-\frac{2h_jC^T}{3}dP_{j+1/2}\wedge dQ_{j+1}-\frac{2h_jB}{3}dQ_{j+1/2}\wedge dQ_{j+1}-\frac{2h_jA}{3}dP_{j+1/2}\wedge dP_{j+1}\\
&-\frac{2h_jC}{3}dQ_{j+1/2}\wedge dP_{j+1}+(I-\frac{h_jC^T}{6})dP_j\wedge dQ_{j+1}-\frac{h_jB}{6}dQ_j\wedge dQ_{j+1}\\
&-\frac{h_jA}{6}dP_j\wedge dP_{j+1}-(I+\frac{h_jC}{6})dQ_j\wedge dP_{j+1}.
\end{aligned}\tag{4.7}$$

Similarly, we take the wedge product of (4.3) with dQ_j and (4.4) with dP_j, then subtract

$$\begin{aligned}
2dP_j\wedge dQ_j=&\frac{2h_jC^T}{3}dP_{j+1/2}\wedge dQ_j+\frac{2h_jB}{3}dQ_{j+1/2}\wedge dQ_j+\frac{2h_jA}{3}dP_{j+1/2}\wedge dP_j\\
&+\frac{2h_jC}{3}dQ_{j+1/2}\wedge dP_j+(I+\frac{h_jC^T}{6})dP_{j+1}\wedge dQ_j+\frac{h_jB}{6}dQ_{j+1}\wedge dQ_j\\
&+\frac{h_jA}{6}dP_{j+1}\wedge dP_j-(I-\frac{h_jC}{6})dQ_{j+1}\wedge dP_j.
\end{aligned}\tag{4.8}$$

By subtracting (4.8) from (4.7) we have

$$\begin{aligned}
dP_j\wedge dQ_j-dP_{j+1}\wedge dQ_{j+1}=&\frac{h_jC^T}{3}dP_{j+1/2}\wedge dQ_j+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_j\\
&+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_j+\frac{h_jC}{3}dQ_{j+1/2}\wedge dP_j+\frac{h_jC^T}{3}dP_{j+1/2}\wedge dQ_{j+1}\\
&+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_{j+1}+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_{j+1}\\
&+\frac{h_jC}{3}dQ_{j+1/2}\wedge dP_{j+1}.
\end{aligned}\tag{4.9}$$

By taking wedge product of (4.5) with dQ_j, (4.6) with dP_j, then subtract:

$$\begin{aligned}\frac{1}{3}dP_j\wedge dQ_j=&(-\frac{2I}{3}+\frac{h_jC^T}{3})dP_{j+1/2}\wedge dQ_j+(\frac{5I}{6}+\frac{h_jC^T}{6})dP_{j+1}\wedge dQ_j\\&+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_j+\frac{h_jB}{6}dQ_{j+1}\wedge dQ_j+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_j+\frac{h_jA}{6}dP_{j+1}\wedge dP_j\\&+(\frac{2I}{3}+\frac{h_jC}{3})dQ_{j+1/2}\wedge dP_j-(\frac{5I}{6}-\frac{h_jC}{6})dQ_{j+1}\wedge dP_j.\end{aligned}\tag{4.10}$$

By subtracting (4.8) from (4.10) we have

$$\begin{aligned}\frac{5}{3}dP_j\wedge dQ_j=&(\frac{2I}{3}+\frac{h_jC^T}{3})dP_{j+1/2}\wedge dQ_j+\frac{I}{6}dP_{j+1}\wedge dQ_j+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_j\\&+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_j+(-\frac{2I}{3}+\frac{h_jC}{3})dQ_{j+1/2}\wedge dP_j-\frac{I}{6}dQ_{j+1}\wedge dP_j.\end{aligned}\tag{4.11}$$

By taking wedge product of (4.5) with dQ_{j+1}, (4.6) with dP_{j+1}, then subtract, we have

$$\begin{aligned}-\frac{5}{3}dP_{j+1}\wedge dQ_{j+1}=&(-\frac{2I}{3}+\frac{h_jC^T}{3})dP_{j+1/2}\wedge dQ_{j+1}+(\frac{2I}{3}+\frac{h_jC}{3})dQ_{j+1/2}\wedge dP_{j+1}\\&+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_{j+1}+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_{j+1}\\&-\frac{I}{6}dP_j\wedge dQ_{j+1}+\frac{I}{6}dQ_j\wedge dP_{j+1}.\end{aligned}\tag{4.12}$$

By adding the above two equations (4.11) and (4.12):

$$\begin{aligned}&\frac{5}{3}dP_j\wedge dQ_j-\frac{5}{3}dP_{j+1}\wedge dQ_{j+1}\\&=(\frac{2I}{3}+\frac{h_jC^T}{3})dP_{j+1/2}\wedge dQ_j+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_j\\&\quad+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_j+(-\frac{2I}{3}+\frac{h_jC}{3})dQ_{j+1/2}\wedge dP_j+(-\frac{2I}{3}+\frac{h_jC^T}{3})dP_{j+1/2}\wedge dQ_{j+1}\\&\quad+(\frac{2I}{3}+\frac{h_jC}{3})dQ_{j+1/2}\wedge dP_{j+1}+\frac{h_jB}{3}dQ_{j+1/2}\wedge dQ_{j+1}+\frac{h_jA}{3}dP_{j+1/2}\wedge dP_{j+1}.\end{aligned}$$

Utilizing (4.9), we can prove that:

$$dP_j\wedge dQ_j-dP_{j+1}\wedge dQ_{j+1}=dP_{j+\frac{1}{2}}\wedge dQ_j-dQ_{j+\frac{1}{2}}\wedge dP_j-dP_{j+\frac{1}{2}}\wedge dQ_{j+1}+dQ_{j+\frac{1}{2}}\wedge dP_{j+1}.\tag{4.13}$$

By taking wedge product of (4.3) with $dQ_{j+1/2}$, (4.4) with $dP_{j+1/2}$, then subtract.

$$\begin{aligned}&-dP_{j+1/2}\wedge dQ_j+dQ_{j+\frac{1}{2}}\wedge dP_j+dP_{j+\frac{1}{2}}\wedge dQ_{j+1}-dQ_{j+\frac{1}{2}}\wedge dP_{j+1}=\\&\frac{h_jC^T}{6}dP_{j+\frac{1}{2}}\wedge dQ_{j+1}+\frac{h_jB}{6}dQ_{j+\frac{1}{2}}\wedge dQ_{j+1}+\frac{h_jA}{6}dP_{j+\frac{1}{2}}\wedge dP_{j+1}+\frac{h_jC}{6}dQ_{j+\frac{1}{2}}\wedge dP_{j+1}\\&\frac{h_jC^T}{6}dP_{j+\frac{1}{2}}\wedge dQ_j+\frac{h_jB}{6}dQ_{j+\frac{1}{2}}\wedge dQ_j+\frac{h_jA}{6}dP_{j+\frac{1}{2}}\wedge dP_j+\frac{h_jC}{6}dQ_{j+\frac{1}{2}}\wedge dP_j.\end{aligned}\tag{4.14}$$

$$\begin{aligned}&-dP_{j+1/2}\wedge dQ_j+dQ_{j+\frac{1}{2}}\wedge dP_j+dP_{j+\frac{1}{2}}\wedge dQ_{j+1}-dQ_{j+\frac{1}{2}}\wedge dP_{j+1}\\&=\frac{h_jC^T}{6}dP_{j+\frac{1}{2}}\wedge dQ_{j+1}+\frac{h_jB}{6}dQ_{j+\frac{1}{2}}\wedge dQ_{j+1}+\frac{h_jA}{6}dP_{j+\frac{1}{2}}\wedge dP_{j+1}+\frac{h_jC}{6}dQ_{j+\frac{1}{2}}\wedge dP_{j+1}\\&\quad+\frac{h_jC^T}{6}dP_{j+\frac{1}{2}}\wedge dQ_j+\frac{h_jB}{6}dQ_{j+\frac{1}{2}}\wedge dQ_j+\frac{h_jA}{6}dP_{j+\frac{1}{2}}\wedge dP_j+\frac{h_jC}{6}dQ_{j+\frac{1}{2}}\wedge dP_j.\end{aligned}$$

Combining (4.9) and (4.13), we obtain:

$$-dP_j \wedge dQ_j + dP_{j+1} \wedge dQ_{j+1} = \frac{dP_j \wedge dQ_j}{2} - \frac{dP_{j+1} \wedge dQ_{j+1}}{2},$$

i.e., $dP_{j+1} \wedge dQ_{j+1} = dP_j \wedge dQ_j$. We can prove the following theorem.

Theorem 4.1. *The quadratic finite element method for the linear Hamiltonian systems is a symplectic algorithm, i.e., the symplectic condition* $dp_{j+1} \wedge dq_{j+1} = dp_j \wedge dq_j$ *is preserved exactly.*

5. The wedge product notation applied in the nonlinear Hamiltonian system

Consider the general canonical system $H(q,p)$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}, \frac{dq}{dt} = \frac{\partial H}{\partial p}.$$

In interval $I_j = [t_j, t_{j+1}]$:

$$\int_{I_j} \frac{dP}{dt} * 1dt = -\int_{I_j} \frac{\partial H}{\partial q} * 1dt, \quad \int_{I_j} \frac{dQ}{dt} * 1dt = \int_{I_j} \frac{\partial H}{\partial p} * 1dt, j = 0, 1, \dots, N-1. \tag{5.1}$$

Integral (5.1)

$$\begin{aligned} P_{j+1} - P_j &= -\frac{h_j}{2} \int_{-1}^{1} \frac{\partial H}{\partial q}\Big|_{p=\frac{1-x}{2}P_j + \frac{1+x}{2}P_{j+1}, q=\frac{1-x}{2}Q_j + \frac{1+x}{2}Q_{j+1}} dx, \\ Q_{j+1} - Q_j &= \frac{h_j}{2} \int_{-1}^{1} \frac{\partial H}{\partial p}\Big|_{p=\frac{1-x}{2}P_j + \frac{1+x}{2}P_{j+1}, q=\frac{1-x}{2}Q_j + \frac{1+x}{2}Q_{j+1}} dx. \end{aligned} \tag{5.2}$$

By taking differentials of the equations (5.2),

$$dP_{j+1} - dP_j = -\frac{h_j}{2} \int_{-1}^{1} (H_{qp}(\frac{1-x}{2} dP_j + \frac{1+x}{2} dP_{j+1}) + H_{qq}(\frac{1-x}{2} dQ_j + \frac{1+x}{2} dQ_{j+1}))dx, \tag{5.3}$$

$$dQ_{j+1} - dQ_j = \frac{h_j}{2} \int_{-1}^{1} (H_{pp}(\frac{1-x}{2} dP_j + \frac{1+x}{2} dP_{j+1}) + H_{pq}(\frac{1-x}{2} dQ_j + \frac{1+x}{2} dQ_{j+1}))dx, \tag{5.4}$$

where $H_{pp}^T = H_{pp}$, $H_{qq}^T = H_{qq}$, $H_{pq}^T = H_{qp}$. By taking the wedge product of (5.3) with dQ_{j+1} and (5.4) with dP_{j+1}, we have

$$\begin{aligned} dP_{j+1} \wedge dQ_{j+1} - dP_j \wedge dQ_{j+1} = -\frac{h_j}{2} \int_{-1}^{1} (H_{qp}(\frac{1-x}{2} dP_j \wedge dQ_{j+1} + \frac{1+x}{2} dP_{j+1} \wedge dQ_{j+1}) \\ + H_{qq}\frac{1-x}{2} dQ_j \wedge dQ_{j+1})dx, \end{aligned} \tag{5.5}$$

$$\begin{aligned} dQ_{j+1} \wedge dP_{j+1} - dQ_j \wedge dP_{j+1} = \frac{h_j}{2} \int_{-1}^{1} (H_{pp}\frac{1-x}{2} dP_j \wedge dP_{j+1} \\ + H_{pq}(\frac{1-x}{2} dQ_j \wedge dP_{j+1} + \frac{1+x}{2} dQ_{j+1} \wedge dP_{j+1}))dx. \end{aligned} \tag{5.6}$$

By subtracting (5.5) from (5.6):

$$\begin{aligned} 2dP_{j+1} \wedge dQ_{j+1} = dP_j \wedge dQ_{j+1} - dQ_j \wedge dP_{j+1} - \frac{h_j}{2} \int_{-1}^{1} (H_{qp}\frac{1-x}{2} dP_j \wedge dQ_{j+1} \\ + H_{qq}\frac{1-x}{2} dQ_j \wedge dQ_{j+1} + H_{pp}\frac{1-x}{2} dP_j \wedge dP_{j+1} + H_{pq}\frac{1-x}{2} dQ_j \wedge dP_{j+1})dx. \end{aligned} \tag{5.7}$$

Similarly, by taking wedge product of (5.3) with dQ_j, (5.4) with dP_j, then subtract

$$\begin{aligned}2dP_j\wedge dQ_j &= dP_{j+1}\wedge dQ_j - dQ_{j+1}\wedge dP_j + \frac{h_j}{2}\int_{-1}^{1}(H_{pp}\frac{1+x}{2}dP_{j+1}\wedge dP_j \\ &+ H_{pq}\frac{1+x}{2}dQ_{j+1}\wedge dP_j + H_{qp}\frac{1+x}{2}dP_{j+1}\wedge dQ_j + H_{qq}\frac{1+x}{2}dQ_{j+1}\wedge dQ_j)dx.\end{aligned} \tag{5.8}$$

By subtracting (5.8) from (5.7) we have

$$\begin{aligned}2dP_j\wedge dQ_j - 2dP_{j+1}\wedge dQ_{j+1} &= \frac{h_j}{2}\int_{-1}^{1}x(H_{pp}dP_{j+1}\wedge dP_j \\ &+ H_{pq}dQ_{j+1}\wedge dP_j + H_{qp}dP_{j+1}\wedge dQ_j + H_{qq}dQ_{j+1}\wedge dQ_j)dx.\end{aligned} \tag{5.9}$$

Utilizing (5.3) and properties of wedge product, we obtain

$$\begin{aligned}&\frac{h_j}{2}\int_{-1}^{1}xH_{pp}dP_{j+1}\wedge dP_j dx \\ &= \frac{h_j}{2}\int_{-1}^{1}xH_{pp}(dP_j - \frac{h_j}{2}\int_{-1}^{1}(H_{qp}(\frac{1-x}{2}dP_j + \frac{1+x}{2}dP_{j+1}) \\ &\quad + H_{qq}(\frac{1-x}{2}dQ_j + \frac{1+x}{2}dQ_{j+1}))dx)\wedge dP_j dx \\ &= -\frac{h_j^2}{4}(\int_{-1}^{1}xH_{pp}dx\int_{-1}^{1}H_{qp}\frac{1-x}{2}dxdP_j\wedge dP_j + \int_{-1}^{1}xH_{pp}dx\int_{-1}^{1}H_{qp}\frac{1+x}{2}dxdP_{j+1}\wedge dP_j \\ &\quad + \int_{-1}^{1}xH_{pp}dx\int_{-1}^{1}H_{qq}\frac{1-x}{2}dxdQ_j\wedge dP_j + \int_{-1}^{1}xH_{pp}dx\int_{-1}^{1}H_{qq}\frac{1+x}{2}dxdQ_{j+1}\wedge dP_j) \\ &= O(h^2).\end{aligned}$$

Similarly, based on (5.9), utilizing (5.3), (5.4), and properties of wedge product, We can prove the following equation

$$dP_{j+1}\wedge dQ_{j+1} = dP_j\wedge dQ_j + O(h^2).$$

We can prove the following theorem.

Theorem 5.1. *The linear finite element method of the nonlinear Hamiltonian systems is an approximately symplectic method which have accurate of second to their symplectic condition, i.e.,* $dp_{j+1}\wedge dq_{j+1} = dp_j\wedge dq_j + O(h^2)$.

In particular, to linear Hamiltonian systems $H(z) = \frac{1}{2}z^TLz, H_{pp} = A,\ H_{pq} = C,\ H_{qq} = B$, then

$$\int_{-1}^{1}xH_{pp}dP_{j+1}\wedge dP_j dx = \int_{-1}^{1}xA dP_{j+1}\wedge dP_j dx = 0.$$

Based on (5.9), we can prove $dP_j\wedge dQ_j = dP_{j+1}\wedge dQ_{j+1}$, i.e., the linear finite element methods for the linear Hamiltonian systems is a symplectic algorithm.

6. Numerical experiments

Consider nonlinear Hamiltonian system

$$H(q,p) = K(p) + V(q),$$

where $K(p) = 2p_1^2 + p_2^2$ is the kinetic energy, $V(q)$ is the potential energy,

$$V(q) = 5\pi^2(D^2 - 5D + 6.5) + 4D^{-1} + 0.5\pi^2(|\ q_2\ | -1.5)^2 + |\ q_2\ |^{-1}, D = (q_1^2+q_2^2)^{1/2}.$$

The classical Hamiltonian canonical equation is ([4]),

$$\frac{dp_1}{dt} = -\frac{\partial V}{\partial q_1}, \frac{dp_2}{dt} = -\frac{\partial V}{\partial q_2}, \frac{dq_1}{dt} = \frac{\partial K}{\partial p_1}, \frac{dp_2}{dt} = \frac{\partial K}{\partial p_2}.$$

It is the motion of A_2B triatomic molecules within the C_{2v} symmetry. We take the Cartesian coordinate system yOz, with origin at the center of mass O, and the z axis is the C_2 axis, the coordinates of the two A atoms and B atom is $A(y_1, z_1), A(y_2, z_2), B(y_3, z_3)$. The generalized coordinates $q_1 = y_1 - y_2, q_2 = z_1 - 2z_3 + z_2$, the generalized momentum $p_1 = 0.25\frac{dq_1}{dt}, p_2 = 0.5\frac{dq_2}{dt}$. Construction of efficient schemes suitable for molecular dynamics applications is an important task. Since very long integration times are required for molecular dynamics simulations, many numerical methods have been developed but the most effective for use in molecular dynamics simulations should have superior long-term stability properties, energy conservation, and permit a large integration time step [1].

We consider the second order symplectic difference scheme (2SS) ([4])

$$z_{k+1} = z_k + hJ^{-1}H_z(\frac{z_{k+1} + z_k}{2}).$$

The 4-stage, 4th-order explicit symplectic difference scheme (4SS)

$$\begin{aligned} H(p, q) &= T(p) + V(q), \alpha = (2 - 2^{\frac{1}{3}})^{-1}, \beta = 1 - 2\alpha, \\ p_1 &= p^n - c_1 h(\frac{\partial V(q)}{\partial q})_{q^n}, q_1 = q^n + d_1 h(\frac{\partial T(p)}{\partial p})_{p_1}, \\ p_2 &= p^n - c_2 h(\frac{\partial V(q)}{\partial q})_{q_1}, q_2 = q^n + d_2 h(\frac{\partial T(p)}{\partial p})_{p_2}, \\ p_3 &= p^n - c_3 h(\frac{\partial V(q)}{\partial q})_{q_2}, q_3 = q^n + d_3 h(\frac{\partial T(p)}{\partial p})_{p_3}, \\ p^{n+1} &= p^n - c_4 h(\frac{\partial V(q)}{\partial q})_{q_3}, q_{n+1} = q^n + d_4 h(\frac{\partial T(p)}{\partial p})_{p^{n+1}}, \end{aligned}$$

where $c_1 = c_4 = \frac{\alpha}{2}, c_2 = c_3 = \frac{\alpha+\beta}{2}, d_1 = d_2 = \alpha, d_3 = \beta, d_4 = 0$.

Taking initial conditions $q_1(0) = 3,\ q_2(0) = 3/2,\ p_1(0) = 0,\ p_2(0) = 0$, then energy $H = 50.1951$, stepsize $h = 0.01$. Respectively we utilize the linear finite element method (1FEM), 2SS, 4SS, and 4RK to compute the classical trajectories of an A_2B type molecule in phase spaces and energy error $H_h - H$ as follows in Figs 1-7.

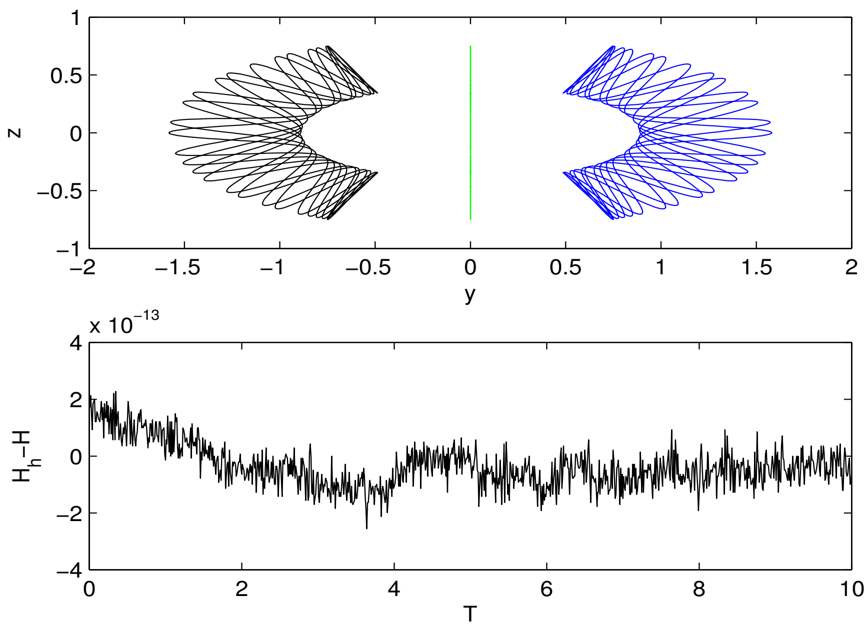

Figure 1: 1FEM, computing $K = 10^3$ step, integral interval $T = [0, 10]$, the initial 1000 nodes classical trajectories in phase space and energy error curve.

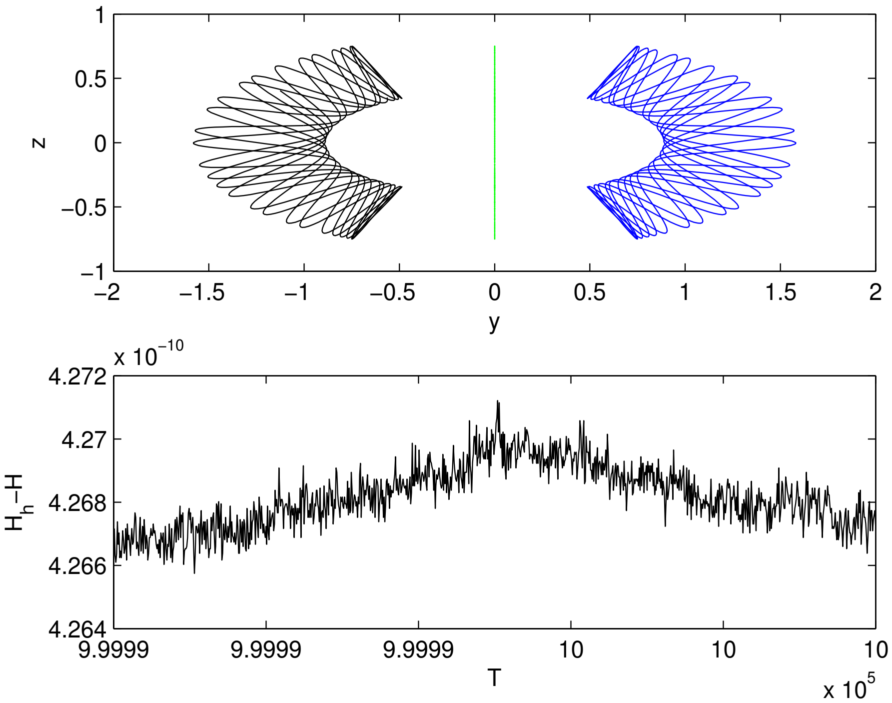

Figure 2: 1FEM, computing $K = 10^8$ step, integral interval $T = [0, 10^6]$, the final 1000 nodes classical trajectories in phase space and energy error curve.

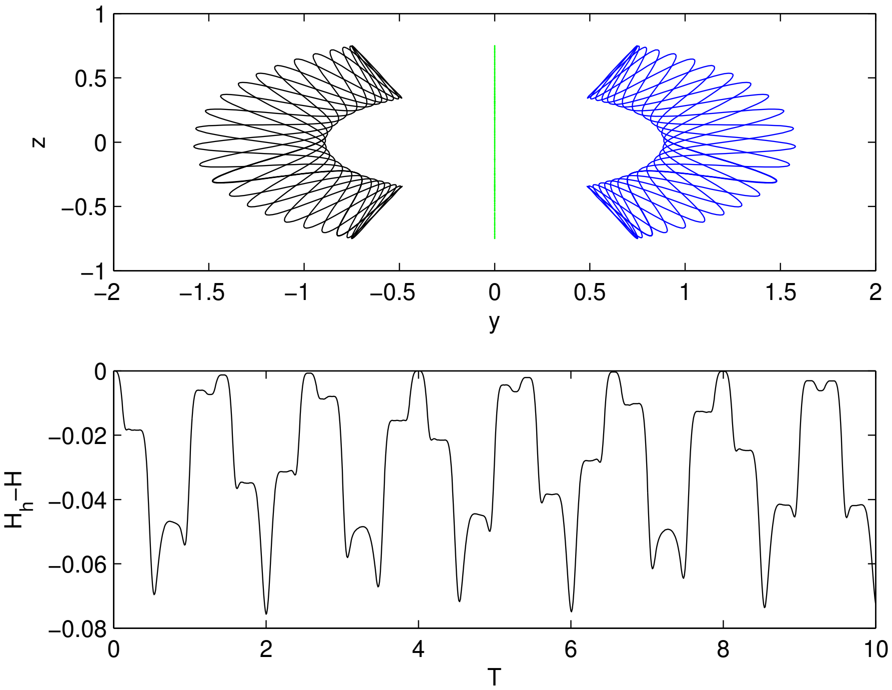

Figure 3: 2SS, computing $K = 10^3$ step, integral interval $T = [0, 10]$, the initial 1000 nodes classical trajectories in phase space and energy error curve.

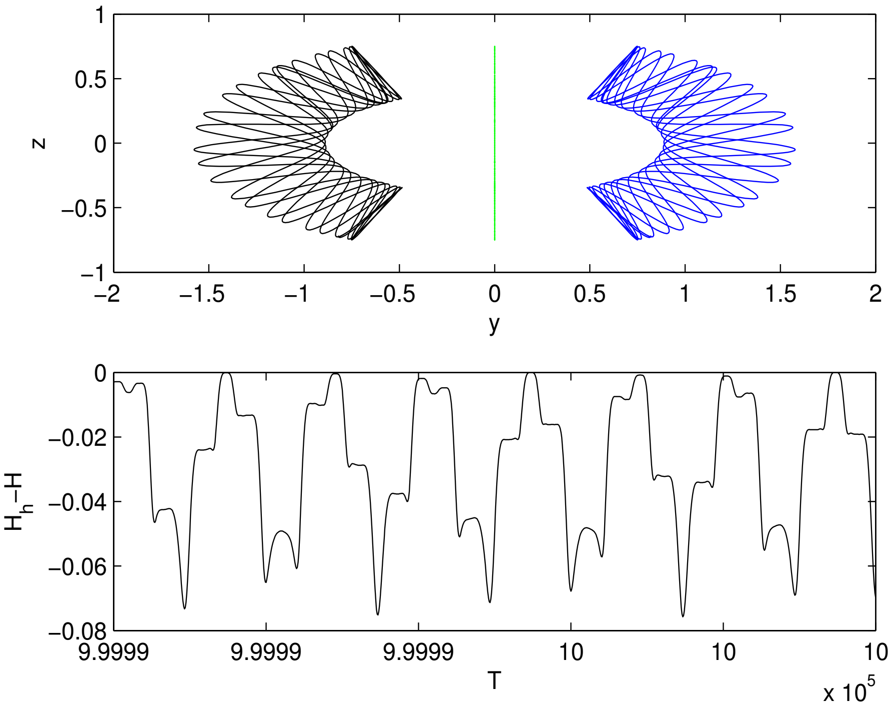

Figure 4: 2SS, computing $K = 10^8$ step, integral interval $T = [0, 10^6]$, the final 1000 nodes classical trajectories in phase space and energy error curve.

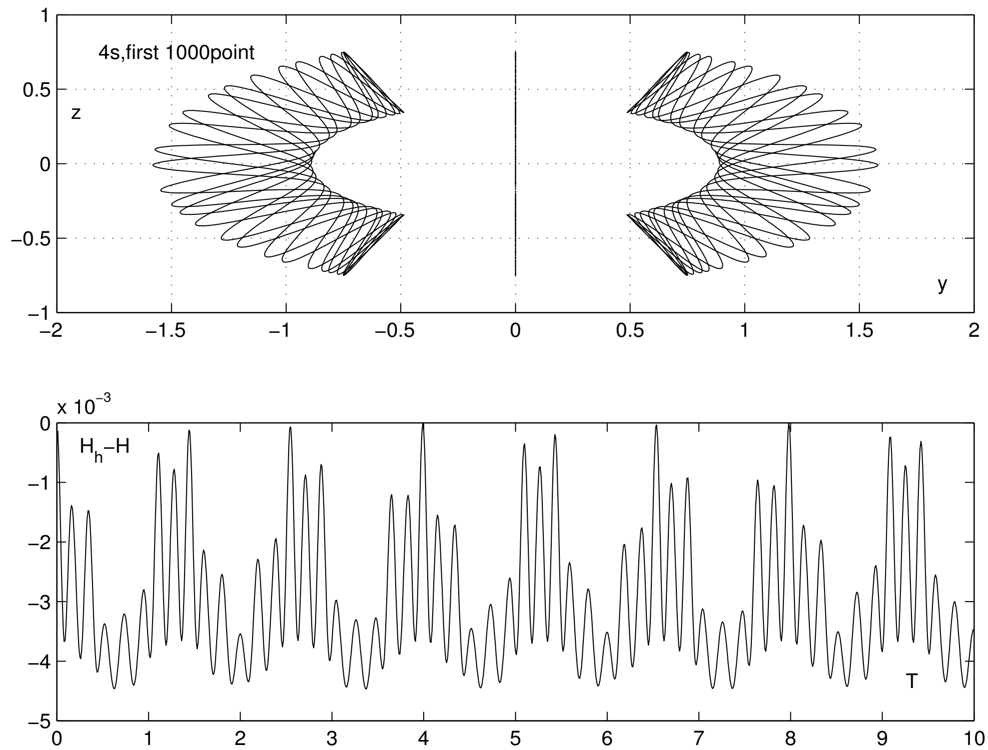

Figure 5: 4SS, computing $K = 10^3$ step, integral interval $T = [0, 10]$, the initial 1000 nodes classical trajectories in phase space and energy error curve.

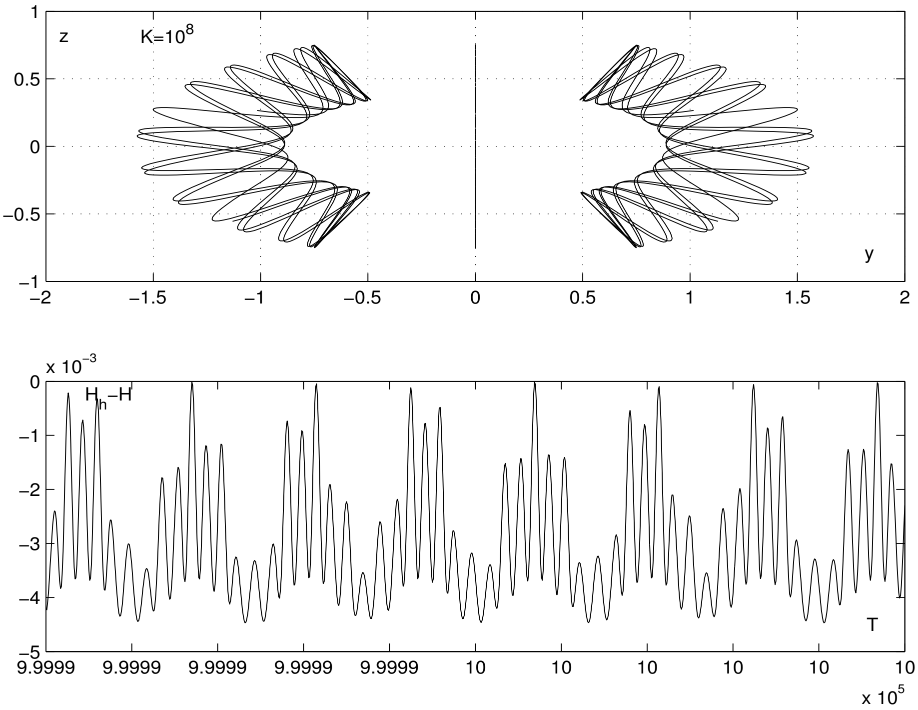

Figure 6: 4SS, computing $K = 10^8$ step, integral interval $T = [0, 10^6]$, the final 1000 nodes classical trajectories in phase space and energy error curve.

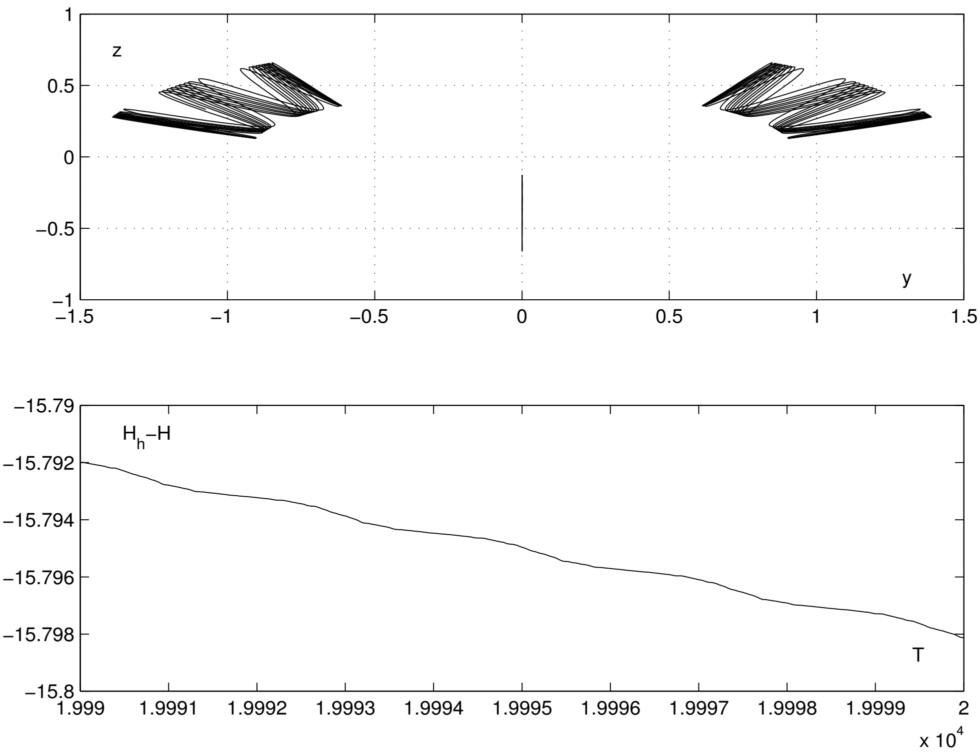

Figure 7: 4RK, computing $K = 2 \times 10^6$ step, integral interval $T = [0, 20000]$, the final 1000 nodes classical trajectories in phase space and energy error curve.

It is observed from Figs 1-7 that the numerical results computed by 1FEM are in good agreement with the theoretical analysis, the atom B and two atoms A in A_2B type molecule vibrate quasi-periodically and the phase space are not squeezed together Figs 1 and 2, which indicates that 1FEM can long-time preserve the high accuracy approximation to symplectic structure which just as the symplectic difference method Figs 3-6. However, the numerical results computed by the Runge-Kutta method are not symplectic method, the vibrational range of A_2B type molecule shrinks. The energy error computed by the linear element methods is only 10^{-10} when $T = 1000000$, but the energy deviation is comparatively larger by symplectic difference scheme, energy error up to $10^{-2}(2SS)$ and $10^{-3}(4SS)$. It can preserve these basic properties of molecular dynamics.

7. Conclusion

The above analysis shows that combing with the wedge product we prove the finite element methods is approximately preserves the symplectic structure to the general Hamiltonian system. It is a reliable method for long time simulations the Hamiltonian system and also provide a better ideas to research the Hamiltonian system.

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