Uniformly accurate structure-preserving algorithms for nonlinear Hamiltonian systems with highly oscillatory solution

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Abstract

Uniformly accurate algorithms and structure-preserving algorithms constitute two interesting classes of numerical methods. In this paper, we combine these two kinds of methods for solving Hamiltonian systems with highly oscillatory solution and the obtained algorithms respect the advantage of each method. Two kinds of algorithms are presented to preserve the symplecticity and energy of the Hamiltonian systems. Moreover, the algorithms are shown to be uniformly accurate for the highly oscillatory structure. A numerical experiment is carried out to support the theoretical results by showing the performance of the obtained algorithms.

Keywords: Hamiltonian system, highly oscillatory solution, symplectic algorithms, energy-preserving algorithms, uniformly accurate methods.

MSC: 65L05, 65L20, 65L70, 65P10.

1 Introduction

It is known that nonlinear Hamiltonian systems are ubiquitous in science and engineering applications. In numerical simulation of evolutionary problems, one of the most difficult problems is to deal with highly oscillatory problems. This paper is devoted to the following damped second-order differential equation

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

where \( x(t) \in \mathbb{R}^d \), \( \tilde{B} \) is a \( d \times d \) skew symmetric matrix, and \( F(x) = -\nabla_x U(x) \) is the negative gradient of a real-valued function \( U(x) \) whose second derivatives are continuous. In this work, we focus on the study of \( 0 < \varepsilon \ll 1 \) which means that the solution of this dynamic is “highly oscillatory”. For the dimension, it is required that \( d \geq 2 \) since when \( d = 1 \), \( \tilde{B} \) is a zero matrix and the system becomes a second-order ODE \( \ddot{x}(t) = F(x(t)) \) without highly oscillatory solution. Denote by \( v = \dot{x} \) and then the energy of this dynamic is given by

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

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We note further that with \( p = v - \frac{1}{2\varepsilon} \dot{B} x \), the equation (1) can be transformed into a Hamiltonian system with the non-separable Hamiltonian

\[
H(x, p) = \frac{1}{2} \left| p + \frac{1}{2\varepsilon} \dot{B} x \right|^2 + U(x).
\]

Hamiltonian systems with highly oscillatory solution frequently occur in physics and engineering such as charged-particle dynamics, classical and quantum mechanics, and molecular dynamics. Their numerical computation contains numerous enduring challenges. In the recent few decades, geometric numerical integration also called as structure-preserving algorithm for differential equations has received more and more attention. This kind of algorithms is designed to respect the structural invariants and geometry of the considered system. This idea has been used by many researchers to derive different structure-preserving algorithms (see, e.g. 11, 23). For the Hamiltonian system (3), there are two remarkable features: the symplecticity of its flow and the conservation of the Hamiltonian. Consequently, for a numerical algorithm, these two features should be respected as much as possible in the spirit of geometric numerical integration.

One typical example of system (1) is charged-particle dynamics in a strong and uniform magnetic field, which has been studied by many researchers. Usually the numerical methods used to treat this system can be summarized in the following three categories.

a) The primitive numerical methods usually depend on the knowledge of certain other characteristics of the solution besides high-frequency oscillation and structure preservation such as the Boris method 1 as well as its further researches 8, 15. This method does not perform well for highly oscillatory systems and cannot preserve any structure of the system.

b) Some recent methods are devoted to the structure preservation such as the volume-preserving algorithms 14, symplectic methods 13, 24, symmetric methods 9 and energy-preserving methods 19, 2, 16, 17. In 10, the long time near-conservation property of a variational integrator was analyzed under \( 0 < \varepsilon \ll 1 \). All of these methods can preserve or nearly preserve some structure of the considered system. However, these methods mentioned above do not pay attention to the high-frequency oscillation and the convergence of these methods is not uniformly accurate for \( \varepsilon \). When \( \varepsilon \to 0 \), these methods usually lose accuracy.

c) Accuracy is often an important consideration for highly oscillatory systems over long-time intervals. Some new methods with uniform accuracy for \( \varepsilon \) have been proposed and analysed recently. The authors in 12 improved asymptotic behaviour of the Boris method and derived a filtered Boris algorithm under a maximal ordering scaling. Some multiscale schemes have been proposed such as the asymptotic preserving schemes 6, 7 and the uniformly accurate schemes 3, 4. Although these powerful numerical methods have very good performance in accuracy, structure (nearly) preservation usually cannot be achieved.

Based on the above points, it is a natural question to ask on whether one can design a numerical method for (1) such that it is uniformly accurate for \( \varepsilon \) and can exactly preserve some structure simultaneously. A kind of energy-preserving method without convergent analysis was given in 21. It will be shown in this paper that this method has a uniform accuracy which has not been studied in 21. Very recently, the authors in 22 present first-order uniformly accurate methods with energy or volume preservation. However, only first-order methods are proposed there and higher order ones with energy or other structure preservation have not been developed. A numerical method combining high-order uniform accuracy and structure preservation has more challenges and importance.
In this paper, we will derive two kinds of algorithms to preserve the symplecticity and energy, respectively. For symplectic algorithms, their near energy conservation over long times will be analysed. Moreover, all the algorithms will be shown to have second-order uniform accuracy for $0 < \varepsilon \ll 1$ in $x$. The remainder of this paper is organised as follows. In Section 2, we formulate two kinds of algorithms. The main results of these algorithms are given in Section 3 and a numerical experiment is carried out there to numerically show the performance of the algorithms. The proofs of the main results are presented in Sections 4-6 one by one. The last section includes some concluding remarks.

2 Numerical algorithms

Before deriving effective algorithms for the system (1), we first present its exact solution as follows.

**Theorem 2.1** (See [12].) The exact solution of system (1) can be expressed as

\[
\begin{align*}
  x(t_n + h) &= x(t_n) + h\varphi_1(h\Omega)v(t_n) + h^2 \int_0^1 (1 - \tau)\varphi_1((1 - \tau)h\Omega)F(x(t_n + h\tau))d\tau, \\
  v(t_n + h) &= \varphi_0(h\Omega)v(t_n) + h \int_0^1 \varphi_0((1 - \tau)h\Omega)F(x(t_n + h\tau))d\tau,
\end{align*}
\]

where $\Omega = \frac{1}{h}x$, $h$ is a stepsize and the $\varphi$-functions are defined by (see [15])

\[
\varphi_0(z) = e^z, \quad \varphi_k(z) = \int_0^1 e^{(1-\sigma)z} \frac{\sigma^{k-1}}{(k-1)!} d\sigma, \quad k = 1, 2, \ldots.
\]

In what follows, we present two kinds of algorithms which will correspond to symplectic algorithms and energy-preserving algorithms, respectively.

**Algorithm 2.2** Define an $s$-stage adapted exponential algorithm by:

\[
\begin{align*}
  X_i &= x_n + c_i h\varphi_1(c_i h\Omega)v_n + h^2 \sum_{j=1}^s \alpha_{ij}(h\Omega)F(X_j), \quad i = 1, 2, \ldots, s \\
  x_{n+1} &= x_n + h\varphi_1(h\Omega)v_n + h^2 \sum_{i=1}^s \beta_i(h\Omega)F(X_i), \quad (4) \\
  v_{n+1} &= \varphi_0(h\Omega)v_n + h \sum_{i=1}^s \gamma_i(h\Omega)F(X_i),
\end{align*}
\]

where $\alpha_{ij}(h\Omega), \beta_i(h\Omega), \gamma_i(h\Omega)$ are bounded functions of $h\Omega$.

As some examples, we present four explicit algorithms. We firstly consider

\[
\begin{align*}
  s &= 1, \quad c_1 = \frac{1}{2}, \quad \beta_1 = b_1 (1 - c_1)\varphi_1((1 - c_1)h\Omega), \quad \gamma_1 = b_1 \varphi_0((1 - c_1)h\Omega).
\end{align*}
\]

This method is denoted by $M1$. For $s = 2$, choosing

\[
\begin{align*}
  c_1 &= 0, \quad c_2 = 1, \quad \alpha_{21} = \frac{1}{2}\varphi_1(h\Omega), \quad \beta_1 = \alpha_{21}, \quad \beta_2 = 0, \quad \gamma_1 = \frac{1}{2}\varphi_0(h\Omega), \quad \gamma_2 = 1
\end{align*}
\]

yields another method, which is called as $M2$. If we consider

\[
\begin{align*}
  \beta_1 &= b_1 (1 - c_1)\varphi_1((1 - c_1)h\Omega), \\
  \gamma_1 &= b_1 \varphi_0((1 - c_1)h\Omega), \\
  \beta_2 &= b_2 (1 - c_2)\varphi_1((1 - c_2)h\Omega), \\
  \gamma_2 &= b_2 \varphi_0((1 - c_2)h\Omega), \\
  \alpha_{21} &= a_{21} (c_2 - c_1)\varphi_1((c_2 - c_1)h\Omega)
\end{align*}
\]

with $b_1 = b_2 = \frac{1}{3}, a_{21} = \frac{1}{2}, c_1 = \frac{1}{2}, c_2 = \frac{3}{2}$, this method is referred to $M3$. We can also make other choice of $b_1 = \frac{1}{3}, b_2 = \frac{2}{3}, a_{21} = \frac{1}{3}, c_1 = \frac{1}{6}, c_2 = \frac{7}{6}$ and then the obtained method is denoted by $M4$. 

3
Algorithm 2.3 An s-degree continuous-stage adapted exponential algorithm is defined as

\[
X_\tau = x_n + hC_\tau(h) v_n + h^2 \int_0^1 A_{\tau\sigma}(h) F(X_\sigma) d\sigma, \quad 0 \leq \tau \leq 1,
\]

\[
x_{n+1} = x_n + h\varphi_1(h) v_n + h^2 \int_0^1 B_\tau(h) F(X_\tau) d\tau,
\]

\[
v_{n+1} = \varphi_0(h) v_n + h \int_0^1 B_\tau(h) F(X_\tau) d\tau,
\]

where \(X_\tau\) is a polynomial of degree \(s\) with respect to \(\tau\) satisfying \(X_0 = x_n, X_1 = x_{n+1}\). \(C_\tau, B_\tau, B_\tau\) and \(A_{\tau\sigma}\) are polynomials which depend on \(h\). The \(C_\tau(h)\) satisfies \(C_\tau(c_i) = c_i \varphi_1(c_i h)\), where \(c_i\) with \(i = 1, \ldots, s + 1\) are the fitting nodes, and one of them is required to be one.

As an example, we consider \(s = 1, c_1 = 0, c_2 = 1\) and choose

\[C_\tau(h) = (1 - \tau) I + \tau \varphi_1(h), \quad A_{\tau\sigma}(h) = \tau \varphi_2(h), \quad B_\tau(h) = \varphi_2(h), \quad B_\tau(h) = \varphi_1(h).\]

This obtained algorithm can be rewritten as

\[
x_{n+1} = x_n + h\varphi_1(h) v_n + h^2 \varphi_2(h) \int_0^1 F(x_n + \sigma(x_{n+1} - x_n)) d\sigma,
\]

\[
v_{n+1} = \varphi_0(h) v_n + h \int_0^1 \varphi_1(h) v_n + h \varphi_1(h) \int_0^1 F(x_n + \sigma(x_{n+1} - x_n)) d\sigma,
\]

which is denoted by M5.

Remark 2.4 It is noted that M5 has been given in [27] but its convergence has not been studied there. In this paper, we will analyse the convergence of each algorithm. It will be shown that M1-M5 are of order two and have a uniform convergence in \(\varepsilon\) for \(0 < \varepsilon \ll 1\). Meanwhile, it is noted that for both algorithms given above, higher order methods can be constructed but we do not go further here for brevity.

3 Main results and a numerical test

The main results of this paper are given by the following four theorems. The first three theorems are about structure preservations and the last one is for uniform accuracy.

Theorem 3.1 (Symplecticity of M1-M4.) Consider the methods M1-M4 with \(p_{n+1} = v_{n+1} - \frac{1}{2n} B x_{n+1}\). Then for the non-separable Hamiltonian (3), the map \((x_n, p_n) \rightarrow (x_{n+1}, p_{n+1})\) determined by these methods is symplectic.

Theorem 3.2 (Energy preservation of M5 [27].) For the method M5, it preserves the energy (2) exactly, i.e. \(E(x_{n+1}, v_{n+1}) = E(x_n, v_n), n = 0, 1, \ldots\).

Theorem 3.3 (Long time energy conservation of M1-M3.) Consider the following assumptions.

- It is assumed that the initial values \(x_0\) and \(\dot{x}_0\) are bounded such that the energy \(E\) is bounded independently of \(\varepsilon\) along the solution.
• We assume that the considered numerical solution stays in a compact set.
• A lower bound on the stepsize $h/\varepsilon \geq c_0 > 0$ is required.
• Assume that the numerical non-resonance condition is true
  \[ |\sin(\frac{h}{2}(k \cdot \hat{\Omega}))| \geq c\sqrt{h} \quad \text{for} \quad k \in \mathbb{Z} \setminus M \quad \text{with} \quad |k| \leq N \]

  for some $N \geq 2$ and $c > 0$. The notations used here are referred to the last part of Section 3.

For the symplectic methods M1-M3, it holds that
\[
E(x_n, v_n) = E(x_0, v_0) + \mathcal{O}(h)
\]
for $0 \leq nh \leq h^{-N+1}$. The constant symbolized by $\mathcal{O}$ is independent of $n, h, \varepsilon$, but depends on $N, T$ and the constants in the assumptions.

Remark 3.4 It is noted that although $M_4$ is symplectic, it does not have the above energy conservation property. The reason is that it is not a symmetric method. From the proof given in Section 4, it will be seen that symmetry plays an important role in the analysis.

Theorem 3.5 (Convergence of M1-M5.) For the symplectic methods M1-M4 and the energy-preserving method M5, the global errors are bounded by

conditional convergence: $|x_n - x(t_n)| + |v_n - v(t_n)| \lesssim h^2/\varepsilon$, \hspace{1cm} (8a)

unconditional convergence: $|x_n - x(t_n)| \lesssim h^2$, \hspace{1cm} (8b)

where $0 < nh \leq T$. Here we denote $A \lesssim B$ for $A \leq CB$ with a generic constant $C > 0$ independent of $h$ or $n$ or $\varepsilon$.

As an illustrative numerical experiment, we consider the charged particle system of (8) with an additional factor $1/\varepsilon$ and a constant magnetic field. The system can be expressed by (8) with $d = 3$, where the potential $U(x) = x_1^2 - x_2^3 + x_1^2/5 + x_2^2 + x_3^4$ and $\hat{B} = \begin{pmatrix} 0 & 0.2 & 0.2 \\ -0.2 & 0 & 1 \\ -0.2 & -1 & 0 \end{pmatrix}$. The initial values are chosen as $x(0) = (0.6, 1, -1)^T$ and $v(0) = (-1, 0.5, 0.6)^T$. We take $\varepsilon = 0.05, 0.005$ and apply M1-M5 as well as the symplectic Euler method (denoted by SE) to this problem on $[0, 0.1, 000]$ with $h = 0.05$. The same standard fixed point iteration is used for implicit schemes and we set $10^{-16}$ as the error tolerance and $10$ as the maximum number of iterations. The relative errors $ERR := \left(\frac{E(x_n, v_n) - E(x_0, v_0)}{E(x_0, v_0)}\right)$ of the energy are displayed in Figures 1-2. Then the problem is solved on $[0, 1]$ with $h = 1/2^i$ for $i = 6, \ldots, 12$. The global errors
\[
err_1 := \frac{|x_n - x(t_n)|}{|x(t_n)|}, \quad err_2 := \frac{|v_n - v(t_n)|}{|v(t_n)|}, \quad err_i := \frac{|x_n - x(t_n)|}{|x(t_n)|}
\]
for different $\varepsilon$ are shown in Figures 3-4, respectively. It is noted that we use the result of standard ODE45 method in MATLAB with an absolute and relative tolerance equal to $10^{-12}$ as the true solution. Finally, in order to illustrate the efficiency of the proposed methods, we solve this system till $T = 10$. The efficiency of each method (the error $err_2$ versus the CPU time) is displayed in
Based on these results, we have the following observations.

a) M1-M3 have near energy conservation over long times, M5 preserves the energy very well but M4 shows a bad energy conservation (Figures 1-2).

b) M1-M5 have a conditional convergence as stated by (8a) (Figure 3) and further have an unconditional second-order convergence in x (Figure 4).

c) All the methods presented in this paper behave better than the symplectic Euler method. Moreover, the computational cost of the new methods is not too much compared with the symplectic Euler method (Figure 5).

In the following three sections, we will prove Theorems 3.1, 3.3-3.5, respectively. In each proof, we will firstly consider \( d = 3 \) for brevity and then show that how to extend the analysis to other \( d \) with some necessary modifications.

4 Proof of symplecticity (Theorem 3.1)

- Transformed system and methods.

According to the skew-symmetric matrix \( \tilde{B} \), it is clear that there exists a unitary matrix \( P \) and a diagonal matrix \( \Lambda \) such that \( \tilde{B} = \Lambda \Lambda^{-1} \tilde{B} \), where \( \Lambda = \text{diag}(-||\tilde{B}||i, 0, ||\tilde{B}||i) \). With the linear change of variable

\[
\tilde{x}(t) = P^H x(t), \quad \tilde{v}(t) = P^H v(t),
\]
the system (1) can be rewritten as

$$
\begin{align*}
\dot{X} &= \left( \begin{array}{c}
\tilde{x} \\
\tilde{v}
\end{array} \right) = \left( \begin{array}{cc}
0 & I \\
0 & \tilde{\Omega}
\end{array} \right) \left( \begin{array}{c}
\tilde{x} \\
\tilde{v}
\end{array} \right) + \left( \begin{array}{c}
0 \\
\tilde{F}(\tilde{x})
\end{array} \right), \\
\tilde{x}_0 &= \left( \begin{array}{c}
P^H x_0 \\
P^H \dot{x}_0
\end{array} \right),
\end{align*}
$$

(10)

where $\tilde{\Omega} = \text{diag}(\tilde{\omega}, 0, \tilde{\omega})$ with $\tilde{\omega} = \frac{|\tilde{B}|}{\varepsilon}$ and $\tilde{F}(\tilde{x}) = P^H F(P\tilde{x}) = -\nabla U(P\tilde{x})$. In this paper, we denote the vector $x$ by $x = (x^{-1}, x^0, x^1)^T$ and the same notation is used for all the vectors in $\mathbb{R}^3$ or $\mathbb{C}^3$. According to (10) and the property of the unitary matrix $P$, one has that

$$
\tilde{x}^{-1} = (\tilde{x}^{-1}), \quad \tilde{v}^{-1} = (\tilde{v}^{-1}), \quad \tilde{x}^0, \quad \tilde{v}^0 \in \mathbb{R}.
$$

(11)

The energy of this transformed system (10) is given by

$$
E(x, \tilde{v}) = \frac{1}{2} |P\tilde{v}|^2 + U(P\tilde{x}) = \frac{1}{2} |\tilde{v}|^2 + U(\tilde{x}) := \tilde{E}(\tilde{x}, \tilde{v}).
$$

For this transformed system, we can modify the schemes of M1-M5 accordingly. For example, the scheme (4) has a transformed form for (10)

$$
\begin{align*}
\tilde{X}_i &= \tilde{x}_n + c_i h \varphi_1(c_i h \tilde{\Omega}) \tilde{v}_n + h^2 \sum_{j=1}^s \alpha_{ij} h \tilde{\Omega} \tilde{F}(\tilde{X}_j), \quad i = 1, 2, \ldots, s, \\
\tilde{x}_{n+1} &= \tilde{x}_n + h \varphi_1(h \tilde{\Omega}) \tilde{v}_n + h^2 \sum_{i=1}^s \beta_i h \tilde{\Omega} \tilde{F}(\tilde{X}_i), \\
\tilde{v}_{n+1} &= \varphi_0(h \tilde{\Omega}) \tilde{v}_n + h \sum_{i=1}^s \gamma_i h \tilde{\Omega} \tilde{F}(\tilde{X}_i).
\end{align*}

(12)
We summarise the relationships as follows:

The conditional errors of $M_3$

The conditional errors of $M_4$

The conditional errors of $M_5$

Figure 3: The conditional errors against $h^i$ (the slope of the dotted line is two).

We prove that (see [11])

\[ \sum_{i=1}^{J-1} \frac{1}{h} d_i \Delta x_i = \frac{1}{h} \sum_{i=1}^{J-1} d_i \Delta x_i. \]
We compute

\[
\sum_{J=-1}^{1} d x_{n+1}^J \land d p_{n+1}^J = \sum_{J=-1}^{1} d \tilde{x}_{n+1}^J \land d \tilde{p}_{n+1}^J = \sum_{J=-1}^{1} d (\tilde{P} \tilde{x}_{n+1}^J) \land d (P \tilde{p}_{n+1}^J)
\]

\[
= \sum_{J=-1}^{1} \left( d \sum_{i=-1}^{1} (\tilde{P} J+2, i+2 \tilde{x}_{n+1}^i) \right) \land \left( d \sum_{k=-1}^{1} (P J+2, k+2 p_{n+1}^k) \right)
\]

\[
= \sum_{J=-1}^{1} \left( \sum_{i=-1}^{1} (\tilde{P} J+2, i+2 \tilde{x}_{n+1}^i) \right) \land \left( \sum_{k=-1}^{1} (P J+2, k+2 \tilde{p}_{n+1}^k) \right)
\]

\[
= \sum_{J=-1}^{1} \sum_{i=-1}^{1} \sum_{k=-1}^{1} \tilde{P} J+2, i+2 P J+2, k+2 (d \tilde{x}_{n+1}^i \land d \tilde{p}_{n+1}^k)
\]

\[
= \sum_{i=-1}^{1} d \tilde{x}_{n+1}^i \land d \tilde{p}_{n+1}^i = \sum_{J=-1}^{1} d \tilde{x}_{n+1}^J \land d \tilde{p}_{n+1}^J,
\]

Figure 4: The unconditional errors against \( h \) (the slope of the dotted line is two).

Figure 5: The unconditional errors against CPU time.
where \( P^H P = I \) is used here. Similarly, one has \( \sum_{j=-1}^{1} dx_n^J \wedge dp_n^J = \sum_{j=-1}^{1} d\tilde{x}_n^J \wedge d\tilde{p}_n^J \). Thus we only need to prove
\[
\sum_{j=-1}^{1} d\tilde{x}_n^J \wedge d\tilde{p}_n^J, \quad \text{i.e.}
\sum_{j=-1}^{1} d\tilde{x}_n^J \wedge d\tilde{p}_n^J = \frac{1}{2} \sum_{j=-1}^{1} d\tilde{x}_n^J \wedge d(\tilde{\Omega}^J i\tilde{x}_n^J) + \frac{1}{2} \sum_{j=-1}^{1} d\tilde{v}_n^J \wedge d(\tilde{\Omega}^J i\tilde{v}_n^J).
\]

### Symplecticity of the transformed methods.

In this part, we will prove that the result (15) is true if the following conditions are satisfied
\[
\begin{align*}
\gamma_j(K) - K\beta_j(K) &= d_j I, \quad d_j \in \mathbb{C}, \\
\gamma_j(K)[\bar{\varphi}_1(K) - c_j \bar{\varphi}_1(c_j K)] &= \beta_j(K)[e^{-K} + K\bar{\varphi}_1(K) - c_j K\bar{\varphi}_1(c_j K)], \\
\beta_i(K)\gamma_j(K) - \frac{1}{2} K\dot{\beta}_i(K)\beta_j(K) - \alpha_{ij}(K)[\gamma_j(K) - K\beta_j(K)] &
= \beta_j(K)\gamma_i(K) + \frac{1}{2} K\dot{\beta}_j(K)\beta_i(K) - \alpha_{ij}(K)[\gamma_i(K) + K\beta_i(K)],
\end{align*}
\]

where \( i, j = 1, 2, \ldots, s \), and \( K = h\tilde{\Omega} \). Here \( \bar{\varphi}_1 \) denotes the conjugate of \( \varphi_1 \) and the same notation is used for other functions.

According to the definition of differential 2-form (see (11)), it can be proved that \( d\tilde{x}_n^J \wedge d\tilde{v}_n^J = d\tilde{x}_n^J \wedge d\tilde{v}_n^J \) and \( d\tilde{x}_n^J \wedge d\tilde{x}_n^J \in i\mathbb{R} \). In the light of the scheme (14), it is obtained that
\[
\begin{align*}
d\tilde{x}_{n+1}^J \wedge d\tilde{v}_{n+1}^J &- \frac{1}{2} d\tilde{x}_{n+1}^J \wedge d(\tilde{\Omega}^J i\tilde{x}_{n+1}^J) = e^{K^J} d\tilde{x}_n^J \wedge d\tilde{v}_n^J + h \sum_{j=1}^{s} \gamma_j(K^J) d\tilde{x}_n^J \wedge d\tilde{F}_j^J \\
&+ he^{K^J} \bar{\varphi}_1(K^J) d\tilde{v}_n^J \wedge d\tilde{v}_n^J + h^2 \bar{\varphi}_1(K^J) d\tilde{v}_n^J \wedge d\tilde{F}_j^J + h^2 \sum_{j=1}^{s} \beta_j(K^J) e^{K^J} d\tilde{F}_i^J \wedge d\tilde{v}_n^J \\
&+ h^2 \sum_{j=1}^{s} \sum_{j=1}^{s} \beta_j(K^J) \gamma_j(K^J) d\tilde{F}_i^J \wedge d\tilde{F}_j^J + \frac{1}{2} d\tilde{\Omega}^J \wedge d(\tilde{\Omega}^J i\tilde{x}_n^J)
\end{align*}
\]

(17)
According to the fact that any exterior product $\wedge$ appearing here is real, the result of (17) can be simplified as
\begin{align*}
  d\tilde{x}_{n+1}^J \wedge d\tilde{v}_{n+1}^J - \frac{1}{2} d\tilde{x}_{n+1}^J \wedge d(\tilde{\Omega}^J i\tilde{x}_{n+1}^J) &= d\tilde{x}_n^J \wedge d\tilde{v}_n^J - \frac{1}{2} d\tilde{x}_n^J \wedge d(\tilde{\Omega}^J i\tilde{x}_n^J) \\
  + h \sum_{j=1}^s [\gamma_j(K^J) - K^J \beta_j(K^J)] d\tilde{x}_n^J \wedge d\tilde{F}_j^J &+ \frac{1}{2} h^2 \tilde{\Omega}^J i\tilde{\varphi}_1(K^J) [\varphi_1(K^J)] d\tilde{v}_n^J \wedge d\tilde{v}_n^J \\
  + h^2 \sum_{j=1}^s [\tilde{\varphi}_1(K^J) \gamma_j(K^J) - \beta_j(K^J)e^{-K^J} - h\tilde{\Omega}^J i\tilde{\varphi}_1(K^J) \beta_j(K^J)] d\tilde{v}_n^J \wedge d\tilde{F}_j^J \\
  + h^3 \sum_{i,j=1}^s [\tilde{\beta}_i(K^J) \gamma_j(K^J) - \frac{1}{2} h\tilde{\Omega}^J i\tilde{\beta}_i(K^J) \beta_j(K^J)] d\tilde{F}_i^J \wedge d\tilde{F}_j^J,
\end{align*}
where the fact that $e^{K^J} - h\tilde{\Omega}^J i\varphi_1(K^J) = I$ is used here.

On the other hand, from the first formula of (14), it follows that
\begin{align*}
  d\tilde{x}_n^J = d\tilde{X}_i^J - c_i h \varphi_1(c_i K^J) d\tilde{v}_n^J - h^2 \sum_{j=1}^s \alpha_{ij}(K^J) d\tilde{F}_j^J, \quad i = 1, 2, \ldots, s.
\end{align*}
Then we get
\begin{align*}
  d\tilde{x}_n^J \wedge d\tilde{F}_j^J = d\tilde{X}_i^J \wedge d\tilde{F}_j^J - c_i h \varphi_1(c_i K^J) d\tilde{v}_n^J \wedge d\tilde{F}_j^J - h^2 \sum_{i=1}^s \alpha_{ji}(K^J) d\tilde{F}_i^J \wedge d\tilde{F}_j^J, \quad j = 1, 2, \ldots, s.
\end{align*}
Inserting this into (18) and summing over all $J$ yields
\begin{align*}
  \sum_{J=-s}^s d\tilde{x}_{n+1}^J \wedge d\tilde{v}_{n+1}^J - \frac{1}{2} \sum_{J=-s}^s d\tilde{x}_{n+1}^J \wedge d(\tilde{\Omega}^J i\tilde{x}_{n+1}^J) &= \sum_{J=-s}^s d\tilde{x}_n^J \wedge d\tilde{v}_n^J - \frac{1}{2} \sum_{J=-s}^s d\tilde{x}_n^J \wedge d(\tilde{\Omega}^J i\tilde{x}_n^J) \\
  + h \sum_{J=-s}^s \sum_{J=-s}^s [\gamma_j(K^J) - K^J \beta_j(K^J)] d\tilde{X}_j^J \wedge d\tilde{F}_j^J \\
  + h \sum_{J=-s}^s \left[ e^{K^J} \tilde{\varphi}_1(K^J) - \frac{1}{2} K^J \tilde{\varphi}_1(K^J) [\varphi_1(K^J)] d\tilde{v}_n^J \wedge d\tilde{v}_n^J ight] \right) \\
  + h^2 \sum_{J=-s}^s \sum_{J=-s}^s \left[ \tilde{\varphi}_1(K^J) \gamma_j(K^J) - \beta_j(K^J)e^{-K^J} - K^J \varphi_1(K^J) \beta_j(K^J) \right] d\tilde{v}_n^J \wedge d\tilde{F}_j^J \\
  + h^3 \sum_{i,j=1}^s \sum_{J=-s}^s \left[ \tilde{\beta}_i(K^J) \gamma_j(K^J) - \frac{1}{2} h\tilde{\Omega}^J i\tilde{\beta}_i(K^J) \beta_j(K^J) \right] d\tilde{F}_i^J \wedge d\tilde{F}_j^J,
\end{align*}
\(\diamond\) Prove that (16a) = 0.
Based on the first condition of (16), \( \tilde{F}(\tilde{x}) = -\nabla_x U(P\tilde{x}) \) and (18), it can be checked that \( d\tilde{X}_j^f \wedge d\tilde{F}_j^f = dX_j^f \wedge dF_j^f \). Thus, one has

\[
\sum_{j=-1}^{1} |\gamma_j(K^f) - K^f J(\beta_j(K^f))| d\tilde{X}_j^f \wedge d\tilde{F}_j^f = d_j \sum_{j=-1}^{1} d\tilde{X}_j^f \wedge d\tilde{F}_j^f - d_j \sum_{j=-1}^{1} dX_j^f \wedge dX_j^f = -d_j \sum_{j=-1}^{1} (\frac{\partial F_j^f(X_j)}{\partial x_j}) dX_j^f \wedge dX_j^f = 0.
\]

\( \Diamond \) Prove that (19b) = 0.

According to the property of \( \tilde{v}_n \), we have

\[
d\tilde{v}_n^{-1} \wedge d\tilde{v}_n^{-1} = -d\tilde{v}_n^{1} \wedge d\tilde{v}_n^{1}, \quad d\tilde{v}_n^{0} \wedge d\tilde{v}_n^{0} = 0,
\]

and

\[
e^{K_1} \tilde{\varphi}_1(K_1) - \frac{1}{2}K_1 \tilde{\varphi}_1(K_1) \varphi_1(K_1) = e^{K_1-1} \tilde{\varphi}_1(K_1) - \frac{1}{2}K_1^{-1} \tilde{\varphi}_1(K_1) \varphi_1(K_1) = 0.
\]

Therefore, it is arrived that

\[
\sum_{j=-1}^{1} [e^{K_1} \tilde{\varphi}_1(K_1)^f - \frac{1}{2}K_1 \tilde{\varphi}_1(K_1) \varphi_1(K_1)] d\tilde{v}_n^f \wedge d\tilde{v}_n^f = 0.
\]

\( \Diamond \) Prove that (19e) - (19f) = 0.

In the light of the second and third formulae of (16), the last two terms (19e) - (19f) vanish. Based on the above results, we obtain (17). Then, it can be checked easily that the coefficients of M1-M4 satisfy (10). Therefore, all the methods are symplectic.

**Extension of the proof to other \( d \).**

For a general \( d \geq 2 \), since \( B \) is skew-symmetric, there exists a unitary matrix \( P \) and a diagonal matrix \( \Lambda \) such that \( \tilde{B} = P \Lambda P^H \), where

\[
\Lambda = \begin{cases} 
\text{diag}(-\tilde{w}_i, \ldots, -\tilde{w}_i, 0, \tilde{w}_i, \ldots, \tilde{w}_i), & d = 2l + 1, \\
\text{diag}(-\tilde{w}_i, \ldots, -\tilde{w}_i, \tilde{w}_i, \ldots, \tilde{w}_i), & d = 2l.
\end{cases}
\]

(20)

For both cases, the above proof can be extended without any difficulty.

### 5 Proof of long-time energy conservation (Theorem 3.3)

In this section, we will show the long time near-conservation of energy along M2 algorithm. We first derive modulated Fourier expansion with sufficient many terms for M2. Then one almost-invariant of the expansion is studied and based on which the long-time near conservation is confirmed. The proof of other methods can be given by modifying the operators \( L(hD), L(hD) \) and following the way given blew.

Using symmetry, the algorithm M2 can be expressed in the two-step form

\[
\begin{align*}
x_{n+1} - 2x_n + x_{n-1} &= h(\varphi_1(h\Omega) - \varphi_1(-h\Omega))v_n + \frac{h}{2}h^2(\varphi_1(h\Omega) + \varphi_1(-h\Omega))F_n, \\
x_{n+1} - x_{n-1} &= h(\varphi_1(h\Omega) + \varphi_1(-h\Omega))v_n + \frac{h}{2}h^2(\varphi_1(h\Omega) - \varphi_1(-h\Omega))F_n,
\end{align*}
\]

(21)
with \( F_n := F(x_n) \), which yields that

\[
\alpha(h\Omega)\frac{x_{n+1} - 2x_n + x_{n-1}}{h^2} = \beta(h\Omega)\frac{x_{n+1} - x_{n-1}}{2h} + \gamma(h\Omega)F_n,
\]

where

\[
\alpha(\xi) = \frac{\xi}{\varphi_1(\xi) - \varphi_1(-\xi)}, \quad \beta(\xi) = \frac{2}{\varphi_1(\xi) + \varphi_1(-\xi)}, \quad \gamma(\xi) = \frac{2\varphi_1(\xi)\varphi_1(-\xi)}{\varphi_1^2(\xi) - \varphi_1^2(-\xi)}.
\]

For the transformed system \((10)\), it becomes

\[
\tilde{\alpha}(h\tilde{\Omega})\frac{x_{n+1} - 2x_n + x_{n-1}}{h^2} = \tilde{\beta}(h\tilde{\Omega})i\tilde{\Omega}\frac{x_{n+1} - x_{n-1}}{2h} + \tilde{\gamma}(h\tilde{\Omega})\tilde{F}_n,
\]

where the coefficient functions are given by \( \tilde{\alpha}(\xi) = \frac{1}{\text{sinc}(\frac{\xi}{h})}, \quad \tilde{\beta}(\xi) = \frac{1}{\text{sinc}(\xi)}, \quad \tilde{\gamma}(\xi) = \xi \csc(\xi) \) with \( \text{sinc}(\xi) = \sin(\xi)/\xi \).

Define the operators

\[
\mathcal{L}(hD) = \frac{1}{2h \text{sinc}(h\Omega)}(e^{hD} - e^{-hD}), \quad \hat{\mathcal{L}}(hD) = \tilde{\alpha}(h\tilde{\Omega})\frac{hD - 2 + e^{-hD}}{h^2} - \tilde{\beta}(h\tilde{\Omega})i\tilde{\Omega}\frac{hD - e^{-hD}}{2h},
\]

where \( D \) is the differential operator. The Taylor expansions of the operator \( \mathcal{L}(hD) \) are

\[
\mathcal{L}(hD) = \tilde{\Omega} \csc(h\tilde{\Omega})(hD) + \frac{1}{6} \tilde{\Omega} \csc(h\tilde{\Omega})(hD)^3 + \cdots,
\]

\[
\mathcal{L}(hD + i\omega\tilde{\omega}) = \text{diag} \left( h\omega, \frac{\sin(h\omega)}{h}, \omega \right) + \text{diag} \left( \omega \cot(h\omega), \frac{\cos(h\omega)}{h}, \omega \cot(h\omega) \right)(hD) + \cdots,
\]

\[
\mathcal{L}(hD - i\omega\tilde{\omega}) = -\text{diag} \left( h\omega, \frac{\sin(h\omega)}{h}, \omega \right) + \text{diag} \left( \omega \cot(h\omega), \frac{\cos(h\omega)}{h}, \omega \cot(h\omega) \right)(hD) + \cdots,
\]

\[
\mathcal{L}(hD + k\omega\tilde{\omega}) = i\sin(kh\omega)\tilde{\Omega} \csc(h\tilde{\Omega}) + \cos(kh\omega)\tilde{\Omega} \csc(h\tilde{\Omega}) + \cdots, \quad \text{where } |k| > 1.
\]

The operator \( \hat{\mathcal{L}}(hD) \) can be expressed in its Taylor expansion as

\[
\hat{\mathcal{L}}(hD) = -\tilde{\Omega}^2 \csc(h\tilde{\Omega})(ihD) - \frac{1}{4} \tilde{\Omega}^2 \csc^2 \left( \frac{h\tilde{\Omega}}{2} \right)(ihD)^2 + \cdots,
\]

\[
\hat{\mathcal{L}}(hD + i\omega\tilde{\omega}) = \text{diag} \left( -2\omega^2, \frac{2(\cos(h\omega) - 1)}{h^2}, 0 \right)
\]

\[
+ \text{diag} \left( \omega^2(2\cot(h\omega) + \csc(h\omega)), \frac{2\sin(h\omega)}{h^2}, \omega^2 \csc(h\tilde{\Omega}) \right)(ihD) + \cdots,
\]

\[
\hat{\mathcal{L}}(hD - i\omega\tilde{\omega}) = \text{diag} \left( 0, \frac{2(\cos(h\omega) - 1)}{h^2}, -2\omega^2 \right)
\]

\[
- \text{diag} \left( \omega^2 \csc(h\tilde{\Omega}), \frac{2\sin(h\omega)}{h^2}, \omega^2(2\cot(h\omega) + \csc(h\omega)) \right)(ihD) + \cdots,
\]

\[
\hat{\mathcal{L}}(hD + k\omega\tilde{\omega}) = 2\sin \left( \frac{h\tilde{\Omega}}{2} \right) \tilde{\Omega}^2 \csc \left( \frac{h\tilde{\Omega}}{2} \right) \csc(h\tilde{\Omega}) \sin \left( \frac{h\tilde{\Omega}}{2} - k\omega \right)
\]

\[
- \sin \left( \frac{h\tilde{\Omega}}{2} \right) \tilde{\Omega}^2 \csc(h\tilde{\Omega})(ihD) + \cdots, \quad \text{where } |k| > 1.
\]

**Modulated Fourier expansion.**
We first present the modulated Fourier expansion of the numerical result \( \tilde{x}_n \) and \( \tilde{v}_n \) for solving the transformed system \((10)\).
We will look for smooth coefficient functions \( \tilde{\zeta}_k \) and \( \tilde{\eta}_k \) such that the functions
\[
\tilde{x}_k(t) = \sum_{|k|<N} e^{ik\omega t} \tilde{\zeta}_k(t) + \tilde{R}_{hN}(t), \quad \tilde{v}_k(t) = \sum_{|k|<N} e^{ik\omega t} \tilde{\eta}_k(t) + \tilde{S}_{hN}(t)
\]
yield a small defect \( \tilde{R}, \tilde{S} \) when they are inserted into the numerical scheme (22).

- Construction of the coefficients functions.

Inserting the first expansion of (23) into the two-step form (22), expanding the nonlinear function into its Taylor series and comparing the coefficients of \( e^{ik\omega t} \), we obtain
\[
\tilde{L}(hD)\tilde{\zeta}_0 = \gamma(h\Omega) \left( \tilde{F}(\tilde{\zeta}_0) + \sum_{s(\alpha)=0} \frac{1}{m!} \tilde{F}^{(m)}(\tilde{\zeta}_0)(\tilde{\zeta}_0)^\alpha \right),
\]
\[
\tilde{L}(hD + ihk\omega)\tilde{\zeta}_k = \gamma(h\Omega) \sum_{s(\alpha)=k} \frac{1}{m!} \tilde{F}^{(m)}(\tilde{\zeta}_0)(\tilde{\zeta}_0)^\alpha, \quad |k| > 0,
\]
where the sum ranges over \( m \geq 0 \), \( s(\alpha) = \sum_{j=1}^{m} \alpha_j \) with \( \alpha = (\alpha_1, \ldots, \alpha_m) \) and \( 0 < |\alpha_i| < N \), and \( (\tilde{\zeta})^\alpha \)
is an abbreviation for \( \left( \tilde{\zeta}_{\alpha_1}, \ldots, \tilde{\zeta}_{\alpha_m} \right) \). This formula gives the modulation system for the coefficients \( \tilde{\zeta}_k \) of the modulated Fourier expansion. Choosing the dominating terms and considering the Taylor expansion of \( \tilde{L} \) given above, the following ansatz of \( \tilde{\zeta}_k \) can be obtained:
\[
\tilde{\zeta}_0 = \begin{cases} 0, & \text{for } |k| > 0, \\ \frac{\hbar^2}{81 \sin^2(\frac{\hbar}{2} h\omega)} (G^{10}(\cdot) + \cdots), & \text{for } |k| \leq 1, \end{cases}
\]
\[
\tilde{\eta}_0 = \begin{cases} 0, & \text{for } |k| > 0, \\ \frac{\hbar^2}{81 \sin^2(\frac{\hbar}{2} h\omega)} (G^{10}(\cdot) + \cdots), & \text{for } |k| \leq 1, \end{cases}
\]
where the dots stand for power series in \( \sqrt{\hbar} \) and \( A(h\omega) = 2 \sin^2(\frac{\hbar}{2} h\omega) \). In this paper we truncate the ansatz after the \( O(h^{N+1}) \) terms. On the basis of the second formula of (21), one has
\[
\tilde{v}_n = \frac{1}{2 \hbar \sin(\Omega)} (\tilde{x}_{n+1} - \tilde{x}_{n-1}) - \frac{1}{2} \hbar^2 \frac{\phi_1(i\Omega) - \phi_0(-i\Omega)}{\hbar \sin(\Omega)} \tilde{F}(\tilde{x}_n) + \frac{1}{2 \hbar \sin(\Omega)} \tilde{F}(\tilde{x}_n),
\]
(25)
Inserting (23) into (25), expanding the nonlinear function into its Taylor series and comparing the coefficients of \( e^{ik\omega t} \), one arrives
\[
\tilde{\eta}_0 = \tilde{\eta}_0 = L(hD)\tilde{\zeta}_0 - \frac{1}{2} \hbar \tan\left(\frac{\hbar}{2} \Omega\right) \left( \tilde{F}(\tilde{\zeta}_0) + \sum_{s(\alpha)=0} \frac{1}{m!} \tilde{F}^{(m)}(\tilde{\zeta}_0)(\tilde{\zeta}_0)^\alpha \right),
\]
\[
\tilde{\eta}_k = \tilde{\eta}_k = L(hD + ihk\omega)\tilde{\zeta}_k - \frac{1}{2} \hbar \tan\left(\frac{\hbar}{2} \Omega\right) \sum_{s(\alpha)=k} \frac{1}{m!} \tilde{F}^{(m)}(\tilde{\zeta}_0)(\tilde{\zeta}_0)^\alpha, \quad |k| > 0.
\]
This formula gives the modulation system for the coefficients \( \tilde{\eta}_k \) of the modulated Fourier expansion by the Taylor expansion of \( \tilde{L} \) and by choosing the dominating terms.
Initial values. According to the conditions \( \tilde{x}_h(0) = \tilde{x}_0 \) and \( \tilde{v}_h(0) = \tilde{v}_0 \), we have
\[
\begin{align*}
\tilde{x}_0^0 &= \tilde{c}_0^0(0) + O(\tilde{\omega}^{-1}), \quad \tilde{x}_0^{+1} = \tilde{c}_0^{+1}(0) + O(\tilde{\omega}^{-1}), \\
\tilde{v}_0^0 &= \tilde{\gamma}_0^0(0) + O(\tilde{\omega}^{-1}), \quad \tilde{v}_0^{+1} = \tilde{\zeta}_0^{+1}(0) + O(\tilde{\omega}^{-1}), \\
\tilde{v}_1^0 &= \tilde{\gamma}_1^0(0) + \tilde{\eta}_1^0(0) + O(\tilde{\omega}^{-1}), \quad \tilde{v}_1^{+1} = \tilde{\zeta}_1^{+1}(0) + i\tilde{\omega}\tilde{\zeta}_1^{+1}(0) + O(\tilde{\omega}^{-1}), \\
\tilde{v}_0^{-1} &= \tilde{\eta}_0^{-1}(0) + \tilde{\eta}_0^{-1}(0) + O(\tilde{\omega}^{-1}) = \tilde{\zeta}_0^{-1}(0) - i\tilde{\omega}\tilde{\zeta}_0^{-1}(0) + O(\tilde{\omega}^{-1}).
\end{align*}
\]
(26)

Thus the initial values \( \tilde{c}_0^0(0) = O(1) \) and \( \tilde{c}_0^0(0) = O(1) \) can be derived by considering the first and third formulae. According to the second equation of (26), one gets the initial value \( \tilde{c}_0^{+1}(0) = O(1) \).

It follows from the fourth formula that \( \tilde{c}_1^{+1}(0) = \frac{1}{12}(\tilde{v}_0^{+1} - \tilde{c}_0^{+1}(0) + O(h)) = O(\tilde{\omega}^{-1}) \), and likewise one has \( \tilde{c}_1^{-1}(0) = O(\tilde{\omega}^{-1}) \).

Bounds of the coefficient functions. With the ansatz (24), we achieve the bounds
\[
\tilde{\zeta}_0^{\pm 1} = O(h), \quad \tilde{\zeta}_0^0 = O(1), \quad \tilde{\zeta}_1 = O(h), \quad \tilde{\zeta}_1^{-1} = O(h),
\]
\[
\tilde{\zeta}_0^{-1} = O(h^2), \quad \tilde{\zeta}_1^0 = O(h^2), \quad \tilde{\zeta}_1^{-1} = O(h^2).
\]

According to the initial values stated above, the bounds
\[
\tilde{c}_0^{+1} = O(1), \quad \tilde{c}_0^0 = O(1), \quad \tilde{c}_1 = O(h), \quad \tilde{c}_1^{-1} = O(h),
\]
are obtained. Moreover, we have the following results for coefficient functions \( \tilde{\eta} \)
\[
\begin{align*}
\tilde{\eta}_0^0 &= \tilde{\zeta}_0^0 + O(h), \\
\tilde{\eta}_0^{+1} &= \tilde{\zeta}_0^{+1} + O(h), \quad \tilde{\eta}_0^{-1} = \frac{1}{\sin(h\tilde{\omega})}\tilde{\zeta}_0^{+1} + O(h), \\
\tilde{\eta}_1^{+1} &= i\tilde{\omega}\tilde{c}_1^{+1} + O(h), \quad \tilde{\eta}_1^{-1} = i\tilde{\omega}\tilde{c}_1^{-1} + O(h), \quad \tilde{\eta}_1^{-1} = -i\tilde{\omega}\tilde{c}_1^{-1} + O(h).
\end{align*}
\]
(27)

A further result is true
\[
\tilde{\zeta}_k = O(h^{|k|+1}), \quad \tilde{\eta}_k = O(h^{|k|}) \quad \text{for } |k| > 1.
\]

Defect. Define
\[
\begin{align*}
\delta_1(t+h) &= \tilde{x}_h(t+h) - \tilde{x}_h(t) - h\varphi_1(i\tilde{\omega})\tilde{v}_h(t) - \frac{1}{2}h^2\varphi_1(i\tilde{\omega})\tilde{F}(\tilde{x}_h(t)), \\
\delta_2(t+h) &= \tilde{v}_h(t+h) - e^{ih\tilde{\Omega}}\tilde{v}_h(t) - \frac{1}{2}h\varphi_0(ih\tilde{\omega})\tilde{F}(\tilde{x}_h(t)) - \frac{1}{2}h\tilde{F}(\tilde{x}_h(t+h))
\end{align*}
\]
for \( t = nh \). Considering the two-step formulation, it is clear that \( \delta_1(t+h) + \delta_1(t-h) = O(h^4) \).

According to the choice for the initial values, we obtain \( \delta_1(0) = O(h^{N+2}) \). Therefore, one has \( \delta_1(t) = O(h^{N+2}) + O(\tilde{t}h^{N+1}) \). Based on this result and (24), we have \( \delta_2 = O(h^N) \). Then let \( \tilde{R}_n = \tilde{x}_n - \tilde{x}_h(t) \) and \( \tilde{S}_n = \tilde{v}_n - \tilde{v}_h(t) \). With the scheme of M2, the error recursion is obtained as follows:
\[
\begin{pmatrix}
\tilde{R}_{n+1} \\
\tilde{S}_{n+1}
\end{pmatrix} = \begin{pmatrix}
I & h\varphi_1(i\tilde{\omega}) \\
0 & e^{ih\tilde{\Omega}}
\end{pmatrix}
\begin{pmatrix}
\tilde{R}_n \\
\tilde{S}_n
\end{pmatrix} + \frac{1}{2}h \begin{pmatrix}
h\varphi_1\Gamma_n\tilde{R}_n \\
\varphi_0\Gamma_n\tilde{R}_n + \Gamma_n+1\tilde{R}_{n+1}
\end{pmatrix} + \begin{pmatrix}
\delta_1 \\
\delta_2
\end{pmatrix},
\]
15
where $\Gamma_n := \int_0^1 \tilde{F}_x(x_n + \tau \tilde{R}_n) d\tau$. Solving this recursion and the application of a discrete Gronwall inequality gives

$$\tilde{R}_{h,N}(t) = O(t^2 h^N), \quad \tilde{S}_{h,N}(t) = O(t^2 h^{N-1}).$$

Using the relationships shown in [13], the numerical solution of M2 admits the following modulated Fourier expansion

$$x_n = \sum_{|k|<N} e^{ik\omega t} \zeta_k(t) + O(t^2 h^N), \quad v_n = \sum_{|k|<N} e^{ik\omega t} \eta_k(t) + O(t^2 h^{N-1}),$$

where $\zeta_k = P\tilde{\zeta}_k$ and $\eta_k = P\tilde{\eta}_k$. Moreover, we have $\zeta_{-k} = \overline{\zeta_k}$ and $\eta_{-k} = \overline{\eta_k}$. 

**An almost-invariant.**

Denote

$$\vec{\zeta} = (\tilde{\zeta}_{-N+1}, \cdots, \tilde{\zeta}_1, \tilde{\zeta}_0, \tilde{\zeta}_1, \cdots, \tilde{\zeta}_N).$$

An almost-invariant of the modulated Fourier expansion is given as follows. According to the above analysis, it is deduced that

$$\tilde{\gamma}^{-1}(h\tilde{\Omega})\mathcal{L}(hD)\tilde{x}_h = \tilde{F}(\tilde{x}_h) + O(h^N),$$

where we use the denotations $\tilde{x}_h = \sum_{|k|<N} \tilde{x}_{h,k}$ with $\tilde{x}_{h,k} = e^{ik\omega t} \tilde{\zeta}_k$. Multiplication of this result with $P$ yields

$$P\tilde{\gamma}^{-1}(h\tilde{\Omega})\mathcal{L}(hD)P^H\tilde{x}_h = P\tilde{F}(\tilde{x}_h) + O(h^N),$$

where $x_h = \sum_{|k|<N} x_{h,k}$ with $x_{h,k} = e^{ik\omega t} \zeta_k$. Rewrite the equation in terms of $x_{h,k}$ and then one has

$$P\tilde{\gamma}^{-1}(h\tilde{\Omega})\mathcal{L}(hD)P^H x_{h,k} = -\nabla_{x_{h,k}} \mathcal{U}(\vec{x}) + O(h^N),$$

where $\mathcal{U}(\vec{x})$ is defined as

$$\mathcal{U}(\vec{x}) = U(x_{h,0}) + \sum_{s(\alpha)=0} \frac{1}{m!} U^{(m)}(x_{h,0})(x_h)$$

with $\vec{x} = (x_{h,-N+1}, \cdots, x_{h,-1}, x_{h,0}, x_{h,1}, \cdots, x_{h,N-1})$. Multiplying this equation with $(\tilde{x}_{h,-k})^T$ and summing up yields

$$\sum_{|k|<N} (\tilde{x}_{h,-k})^T P\tilde{\gamma}^{-1}(h\tilde{\Omega})\mathcal{L}(hD)P^H x_{h,k} + \frac{dx}{dt} \mathcal{U}(\vec{x}) = O(h^N).$$
Denoting \( \hat{\zeta} = (\zeta_{-N+1}, \cdots, \zeta_{-1}, \zeta_0, \zeta_1, \cdots, \zeta_{N-1}) \) and switching to the quantities \( \zeta^k \), we obtain

\[
O(h^N) = \sum_{|k|<N} (\zeta_k - i k \tilde{\omega} \zeta_k) P \gamma^{-1}(h \tilde{\Omega}) \hat{L}(hD + ihk \tilde{\omega}) P^H \zeta_k + \frac{d}{dt} U(\tilde{\zeta})
\]

\[
= \sum_{|k|<N} (\hat{\zeta}_k - i k \tilde{\omega} \hat{\zeta}_k) P \gamma^{-1}(h \tilde{\Omega}) \hat{L}(hD + ihk \tilde{\omega}) P^H \hat{\zeta}_k + \frac{d}{dt} U(\hat{\zeta})
\]

\[
= \sum_{|k|<N} (\hat{\zeta}_k - i k \tilde{\omega} \hat{\zeta}_k) P \gamma^{-1}(h \tilde{\Omega}) \hat{L}(hD + ihk \tilde{\omega}) P^H \hat{\zeta}_k + \frac{d}{dt} U(\hat{\zeta})
\]

\[
= \sum_{|k|<N} (\hat{\zeta}_k - i k \tilde{\omega} \hat{\zeta}_k) \tilde{\gamma}^{-1}(h \tilde{\Omega}) \hat{L}(hD + ihk \tilde{\omega}) \hat{\zeta}_k + \frac{d}{dt} U(\hat{\zeta}).
\]

(28)

In what follows, we show that the right-hand side of (28) is the total derivative of an expression that depends only on \( \zeta_k, \bar{\eta}_k \) and deriviates thereof. Consider \( k = 0 \) and then it follows that

\[
\hat{L}(hD) \hat{\zeta}_0 = ihM_1 \hat{\zeta}_0 + h^2 M_2 \bar{\zeta}_0 + ih^3 M_3 \bar{\zeta}_0 + \cdots,
\]

where \( M_k \in \mathbb{R}^{3 \times 3} \) for \( k = 1, 2, \ldots \).

By the formulae given on p. 508 of [11], we know that \( \text{Re}(\bar{\zeta}_0)^T \hat{L}(hD) \hat{\zeta}_0 \) is a total derivative. For \( k \neq 0 \), in the light of

\[
\hat{L}(hD + ihk \tilde{\omega}) \bar{\zeta}_k = N_0 \bar{\zeta}_k + ihN_1 \bar{\zeta}_k + h^2 N_2 \bar{\zeta}_k + ih^3 N_3 \bar{\zeta}_k + \cdots,
\]

where \( N_k \in \mathbb{R}^{3 \times 3} \) for \( k = 0, 1, \ldots \), it is easy to check that \( \text{Re}(\bar{\zeta}_k)^T \gamma^{-1}(h \tilde{\Omega}) \hat{L}(hD + ihk \tilde{\omega}) \bar{\zeta}_k \) and \( \text{Re}(i k \tilde{\omega} \bar{\zeta}_k)^T \gamma^{-1}(h \tilde{\Omega}) \hat{L}(hD + ihk \tilde{\omega}) \bar{\zeta}_k \) are both total derivatives. Therefore, there exists a function \( \mathcal{E} \) such that \( \frac{d}{dt} \mathcal{E}[\hat{\zeta}](t) = O(h^N) \). By an integration, it is arrived that

\[
\mathcal{E}[\hat{\zeta}](t) = \mathcal{E}[\hat{\zeta}](0) + O(th^N).
\]

(29)

According to the previous analysis, the construction of \( \mathcal{E} \) is derived as follows

\[
\mathcal{E}[\hat{\zeta}] = \frac{1}{2} \frac{\bar{\zeta}_0}{\varphi_1(ih \Omega) \varphi_1(-ih \Omega) \varphi_1(ih \Omega)} \left[ \begin{array}{c} \bar{\zeta}_0 \end{array} \right] \left[ \begin{array}{c} 2 \text{sinc}(\frac{4}{h} \bar{\omega}) \\ 2 \text{sinc}^2(\frac{4}{h} \bar{\omega}) \\ \frac{1}{2} \frac{1}{h} \tilde{\omega} \varphi_1(ih \Omega) \varphi_1(-ih \Omega) \varphi_1(ih \Omega) \left( |\bar{\zeta}_1| + |\bar{\zeta}^{-1}_1| \right)^2 \right] + U(\tilde{\zeta}) + O(h^2)
\]

\[
= \frac{1}{2} \frac{\bar{\zeta}_0^2}{2 \tilde{\omega}^2(\tilde{\zeta}_1^2 + |\tilde{\zeta}^{-1}_1|^2)} + U(P^H \zeta_0^0) + O(h).
\]

• Long-time near-conservation.

Considering the result of \( \mathcal{E} \) and the relationship (27) between \( \hat{\zeta} \) and \( \bar{\eta} \), we obtain

\[
\mathcal{E}[\tilde{\zeta}] = \frac{1}{2} \frac{|\tilde{\zeta}_0|}{2 \tilde{\omega}^2(\tilde{\zeta}_1^2 + |\tilde{\zeta}^{-1}_1|^2)} + U(P^H \zeta_0^0) + O(h)
\]

\[
= \frac{1}{2} \left| \tilde{\eta}_0 \right|^2 + \frac{1}{2} \left( |\tilde{\eta}_1|^2 + |\tilde{\eta}^{-1}_1|^2 \right) + U(P^H \zeta_0^0) + O(h).
\]

(30)
We are now in a position to show the long-time conservations of M2.

In terms of the bounds of the coefficient functions, one arrives at

\[
E(x_n, v_n) = \tilde{E}(\tilde{x}_n, \tilde{v}_n) = \frac{1}{2} \left( |\tilde{\omega}_0|^2 + |\tilde{\omega}_1|^2 + |\tilde{\omega}_{-1}|^2 \right) + U(P^H \tilde{\omega}) + O(h).
\] (31)

A comparison between (30) and (31) gives

\[
\mathcal{E}_\varepsilon(t) = E(x_n, v_n) + O(h).
\]

Based on (29) and this result, the statement (7) is easily obtained by following the way presented in Chap. XIII of [11].

**Extension of the proof to other d.**

According to the scheme (20) of Λ, the operators \(L(hD)\) and \(\dot{\Lambda}(hD)\) as well as their properties can be changed accordingly. The modulated Fourier expansions are modified as

\[
\tilde{x}_h(t) = \sum_{k \in \mathcal{N}^*} e^{i(k \cdot \hat{\Omega}) t} \tilde{x}_k(t) + \tilde{R}_{h, N}(t), \quad \tilde{v}_h(t) = \sum_{k \in \mathcal{N}^*} e^{i(k \cdot \hat{\Omega}) t} \tilde{v}_k(t) + \tilde{S}_{h, N}(t)
\]

where \(k = (k_1, \ldots, k_l)\), \(\hat{\Omega} = (\hat{\omega}_1, \ldots, \hat{\omega}_l)\), \(k \cdot \hat{\Omega} = k_1 \hat{\omega}_1 + \cdots + k_l \hat{\omega}_l\). The set \(\mathcal{N}^*\) is defined as follows.

For the resonance module \(M = \{ k \in \mathbb{Z}^l : k \cdot \hat{\Omega} = 0 \}\), we let \(K\) be a set of representatives of the equivalence classes in \(\mathbb{Z}^l \setminus M\) which are chosen such that for each \(k \in K\) the sum \(|k|\) is minimal in the equivalence class \(|k| = k + M\), and that with \(k \in K\), also \(-k \in K\). We denote, for the positive integer \(N\), \(\mathcal{N} = \{ k \in K : |k| \leq N \}\), \(\mathcal{N}^* = \mathcal{N} \setminus \{(0, \ldots, 0)\}\). Then the almost-invariant can be modified accordingly and the long time near conservation can be proved.

**6 Proof of conditional and unconditional convergence (Theorem 3.5)**

In this section, we discuss the convergence of the algorithms. The proof will be given for M5 and it can be adapted to other methods easily.

In order to establish the unconditional convergence [86], the strategy developed in [8, 22] will be used in the proof. This means that the time re-scaling \(t \to t \varepsilon\) is considered and the convergent analysis will be given for the following long-time problem

\[
\dot{x} = \varepsilon v, \quad \dot{v} = \hat{B} v + \varepsilon F(x), \quad t \in [0, \frac{T}{\varepsilon}], \quad x(0) = x_0, \quad v(0) = v_0.
\] (32)

The solution of this system satisfies \(\|x\|_{L^\infty(0, T/\varepsilon)} + \|v\|_{L^\infty(0, T/\varepsilon)} \lesssim 1\) and for solving [86], the method M5 becomes

\[
x_{n+1} = x_n + \varepsilon \varphi_1(h\hat{B}) v_n + \frac{h^2 \varepsilon^2}{2} \varphi_2(h\hat{B}) \int_0^1 F(\rho x_n + (1 - \rho)x_{n+1}) d\rho, \quad 0 \leq n < \frac{T}{\varepsilon},
\]

\[
v_{n+1} = \varepsilon h\hat{B} v_n + h \varepsilon \varphi_1(h\hat{B}) \int_0^1 F(\rho x_n + (1 - \rho)x_{n+1}) d\rho.
\] (33)

**Local truncation errors.**
Based on (33), the local truncation errors \( \xi_n^u \) and \( \xi_n^v \) for \( 0 \leq n < T/\varepsilon \) are defined as

\[
x(t_n + h) = x(t_n) + h \varepsilon \varphi_1(h \tilde{B}) v(t_n) + \frac{h^2 \varepsilon^2}{2} \varphi_2(h \tilde{B}) \int_0^1 F(\rho x(t_n) + (1 - \rho)x(t_n + h)) d\rho + \xi_n^x,
\]

\[
v(t_n + h) = e^{h \tilde{B}} v(t_n) + h \varepsilon \varphi_1(h \tilde{B}) \int_0^1 F(\rho x(t_n) + (1 - \rho)x(t_n + h)) d\rho + \xi_n^v.
\]

By this result and the variation-of-constants formula of (32), we compute

\[
v(t_{n+1}) - v_{n+1} = \varepsilon h \int_0^1 e^{(1-\tau)h \tilde{B}} F(x(t_n + h \tau)) d\tau - \varepsilon h \varphi_1(h \tilde{B}) \int_0^1 F(x(t_n) + \sigma(x(t_{n+1}) - x(t_n))) d\sigma
\]

\[
= \varepsilon \int_0^1 e^{(1-\tau)h \tilde{B}} \sum_{j=0}^1 \frac{h^j \tau^j}{j!} \hat{F}^{(j)}(t_n) d\tau + O(\varepsilon^3)
\]

\[
- \varepsilon h \varphi_1(h \tilde{B}) \int_0^1 [F(x(t_n)) + \sigma \partial F(x(t_n)) (x(t_{n+1}) - x(t_n))] d\sigma
\]

\[
= \varepsilon \int_0^1 \sum_{j=0}^1 h^{j+1} \varphi_{j+1}(h \tilde{B}) \hat{F}^{(j)}(t_n) - \varepsilon^2 h^2 \varphi_1(h \tilde{B}) \int_0^1 \partial F(x(t_n)) (x(t_{n+1}) - x(t_n)) d\sigma + O(\varepsilon^3)
\]

\[
= \varepsilon h^2 \varphi_2(h \tilde{B}) \hat{F}^{(1)}(t_n) - \frac{1}{2} \varepsilon^2 h^2 \varphi_1^2(h \tilde{B}) \frac{\partial F}{\partial x}(x(t_n)) v(t_n) + O(\varepsilon^3),
\]

where \( \hat{F}(\xi) = F(x(\xi)) \) and \( \hat{F}^{(j)} \) denotes the \( j \)th derivative of \( \hat{F} \) with respect to \( t \). By this definition, it follows that

\[
\hat{F}^{(1)}(t_n) = \frac{\partial F}{\partial x}(x(t_n)) \frac{dx}{dt}(t_n) = \frac{\partial F}{\partial x}(x(t_n)) \varepsilon v(t_n).
\]

Consequently, the local error becomes

\[
\xi_n^v = v(t_{n+1}) - v_{n+1} = \varepsilon^2 h^2 \left( \varphi_2(h \tilde{B}) - \frac{1}{2} \varphi_1^2(h \tilde{B}) \right) \frac{\partial F}{\partial x}(x(t_n)) v(t_n) + O(\varepsilon^3) = O(\varepsilon^3). \tag{35}
\]

Similarly, we obtain

\[
\xi_n^x = O(\varepsilon^2 h^3). \tag{36}
\]

• Conditional convergence.

In this part, we will first prove the following boundedness of M5: there exists a generic constant \( h_0 > 0 \) independent of \( \varepsilon \) and \( n \), such that for \( 0 < h \leq h_0 \),

\[
|x_n| \leq \|x\|_{L^\infty(0,T/\varepsilon)} + 1, \quad |v_n| \leq \|v\|_{L^\infty(0,T/\varepsilon)} + 1, \quad 0 \leq n \leq T/\varepsilon. \tag{37}
\]

For \( n = 0 \), (37) is obviously true. Then we assume (37) is true up to some \( 0 \leq m < T/\varepsilon \), and we shall show that (37) holds for \( m + 1 \).

For \( n \leq m \), subtracting (34) from the scheme (33) leads to

\[
e_n^{v_{n+1}} = e_n^v + h \varepsilon \varphi_1(h \tilde{B}) e_n^v + \eta_n^v + \xi_n^x, \quad e_n^{v_{n+1}} = e^{h \tilde{B}} e_n^v + \eta_n^v + \xi_n^x, \quad 0 \leq n \leq m. \tag{38}
\]
where we use the following notations
\[
\eta_n^x = \frac{h^2 \epsilon^2}{2} \varphi_2(h \tilde{B}) \int_0^1 \left[ E \left( \rho x(t_n) + (1 - \rho)x(t_n + h) \right) - E \left( \rho x_n + (1 - \rho)x_{n+1} \right) \right] d\rho, \\
\eta_n^v = h \epsilon \varphi_1(h \tilde{B}) \int_0^1 \left[ E \left( \rho x(t_n) + (1 - \rho)x(t_n + h) \right) - E \left( \rho x_n + (1 - \rho)x_{n+1} \right) \right] d\rho.
\]

From the induction assumption of the boundedness, it follows that
\[
|\eta_n^x| \lesssim h^2 \epsilon^2 \left( |e_x^x| + |e_x^{n+1}| \right), \quad |\eta_n^v| \lesssim h \epsilon \left( |e_v^x| + |e_v^{n+1}| \right), \quad 0 \leq n < m.
\]

Taking the absolute value (euclidean norm) on both sides of (38) and using (39), it is arrived that
\[
|e_{n+1}^x| + |e_{n+1}^v| - |e_n^x| \lesssim h \epsilon \left( |e_n^x| + |e_n^x| + |e_{n+1}^x| \right) + |\xi_n^x| + |\xi_n^v|, \quad 0 \leq n \leq m.
\]
Summing them up for \(0 \leq n \leq m\) gives
\[
|e_{m+1}^x| + |e_{m+1}^v| \lesssim h \epsilon \sum_{n=0}^m \left( |e_n^x| + |e_n^x| + |e_{n+1}^x| \right) + \sum_{n=0}^m \left( |\xi_n^x| + |\xi_n^v| \right).
\]
In the light of the truncation errors in (38) and the fact that \(mh\epsilon \lesssim 1\), one has
\[
|e_{m+1}^x| + |e_{m+1}^v| \lesssim h \epsilon \sum_{n=0}^m \left( |e_n^x| + |e_n^x| + |e_{n+1}^x| \right) + h^2,
\]
and then further by Gronwall’s inequality gets
\[
|e_{m+1}^x| + |e_{m+1}^v| \lesssim h^2, \quad 0 \leq m < T/\epsilon.
\]
This result shows the conditional convergence (38) given in Theorem 3.5. Meanwhile, concerning
\[
|x_{m+1}| \leq |x(t_{m+1})| + |e_{m+1}^x|, \quad |v_{m+1}| \leq |v(t_{m+1})| + |e_{m+1}^v|,
\]
there exists a generic constant \(h_0 > 0\) independent of \(\epsilon\) and \(m\), such that for \(0 < h \leq h_0\), (37) holds for \(m + 1\), which completes the induction.

**Unconditional convergence.**

By the skew-symmetry of \(\tilde{B}\), it is known that the propagator \(e^{t \tilde{B}}\) generates a periodic flow whose single period is denoted by \(T_0 > 0\). Then we divide \(T\) into \(T = T_0 M + t_r\), \(0 \leq t_r < T_0\), where the integer \(M = \left\lfloor \frac{T}{T_0} \right\rfloor = \mathcal{O}(1/\epsilon)\). Without loss generality, it is assumed that \(t_r = 0\) in the following proof. To present the convergence, we introduce the parallel component of \(v\): \(v^\parallel(t) := \frac{\tilde{B}}{||\tilde{B}||} \cdot v(t)\), \(t \geq 0\), and similarly for the numerical velocity as \(v_n^\parallel := \frac{B}{||B||} \cdot v_n\), \(n \geq 0\), where \(B = (\tilde{B}(2,3), \tilde{B}(3,1), \tilde{B}(1,2))^T\).

First of all, we choose \(N_0 > 0\) and the stepsize \(h = T_0/N \leq h_0\) with \(N \geq N_0\) such that the boundedness (37) holds. Using the new notations \(t_n^m = mT_0 + nh\), \(0 \leq m < M\), we denote the numerical solution from M5 at \(t_n^m\) as
\[
x_n^m \approx x(t_n^m), \quad v_n^m \approx v(t_n^m), \quad 0 \leq m < M, \quad 0 \leq n \leq N,
\]

\[20\]
and the error as
\[ e_{n,m}^x = x(t_n^m) - x_n^m, \quad e_{n,m}^v = v(t_n^m) - v_n^m. \]

By these notations, we have that \( e_{0,m+1}^x = e_{N,m}^x \) and \( e_{0,m+1}^v = e_{N,m}^v \). Moreover, the error equation \((38)\) now becomes
\[
\begin{align*}
\epsilon_{n+1,m}^x &= \epsilon_{n,m}^x + h\epsilon \varphi_1(h\tilde{B})\epsilon_{n,m}^v + \eta_{n,m}^x + \xi_{n,m}^x, \\
\epsilon_{n+1,m}^v &= e^{h\tilde{B}}\epsilon_{n,m}^v + \eta_{n,m}^v + \xi_{n,m}^v, \quad 0 \leq n \leq N - 1, \quad 0 \leq m < M.
\end{align*}
\] (40a)

(40b)

It is noted that the notations for the other error terms are updated in the straightforward manner.

According to this error equation, the local error bounds \((35),(36)\) and the estimate \((39)\), we get
\[
\begin{align*}
\frac{1}{\varepsilon} |\epsilon_{j,m}^x| - \frac{1}{\varepsilon} |\epsilon_{j-1,m}^x| &\lesssim h^2 |e_{j,m}^v| + \varepsilon h \left( |\epsilon_{j,m}^x| + |\epsilon_{j-1,m}^x| \right) + h^3, \\
|\epsilon_{j,m}^v| - |\epsilon_{j-1,m}^v| &\lesssim \varepsilon h \left( |\epsilon_{j,m}^x| + |\epsilon_{j-1,m}^x| \right) + h^3, \quad 1 \leq j \leq N, \quad 0 \leq m < M,
\end{align*}
\]

By adding the above two inequalities together and summing up for \( j = 1, \ldots, n \) with any \( 1 \leq n \leq N \), and then by Gronwall’s inequality, it is arrived that
\[
\frac{1}{\varepsilon} |\epsilon_{0,m}^x| + |\epsilon_{n,m}^v| \lesssim \varepsilon h^2 + \frac{1}{\varepsilon} |\epsilon_{0,m}^x| + |\epsilon_{0,0}^v|, \quad 1 \leq n \leq N, \quad 0 \leq m < M.
\] (41)

In what follows, we need to show how the error propagates through each period. For \((40a)\) with some \( 0 \leq m < M \), summing up for \( n = 0, \ldots, N - 1 \) gives
\[
\epsilon_{N,m}^x = \epsilon_{0,m}^x + h\epsilon \varphi_1(h\tilde{B}) \sum_{n=0}^{N-1} \epsilon_{n,m}^v + \sum_{n=0}^{N-1} \left( \eta_{n,m}^x + \xi_{n,m}^x \right).
\] (42)

For the part \( \epsilon_{n,m}^v \) appearing in this formula, based on \((40b)\) we can rewrite it as
\[
\epsilon_{n,m}^v = e^{h\tilde{B}}\epsilon_{n-1,m}^v + \eta_{n-1,m}^v + \xi_{n-1,m}^v, \quad 1 \leq n \leq N, \quad 0 \leq m < M,
\]
which gives that for any \( 1 \leq n \leq N, \quad 0 \leq m < M, \)
\[
\epsilon_{n,m}^v = e^{nh\tilde{B}}\epsilon_{0,m}^v + \sum_{j=0}^{n-1} e^{(n-1-j)h\tilde{B}} \left[ \eta_{j,m}^v + \xi_{j,m}^v \right],
\]
and so
\[
h\epsilon \varphi_1(h\tilde{B}) \sum_{n=0}^{N-1} \epsilon_{n,m}^v = h\epsilon \varphi_1(h\tilde{B}) \sum_{n=0}^{N-1} \sum_{j=0}^{N-1-n} e^{nh\tilde{B}} \epsilon_{0,m}^v + h\epsilon \varphi_1(h\tilde{B}) \sum_{n=0}^{N-1} \sum_{j=0}^{n-1} e^{(n-j)h\tilde{B}} \left[ \eta_{j,m}^v + \xi_{j,m}^v \right].
\]

Inserting the above result into \((42)\) implies
\[
\epsilon_{N,m}^x = \epsilon_{0,m}^x + h\epsilon \varphi_1(h\tilde{B}) \sum_{n=0}^{N-1} e^{nh\tilde{B}} \epsilon_{0,m}^v + \gamma_m, \quad 0 \leq m < M.
\] (43)
where
\[ \gamma^m := \sum_{n=0}^{N-1} \left( \eta_{n,m}^x + \xi_{n,m}^x \right) + h \varepsilon \varphi_1(h \hat{B}) \sum_{n=0}^{N-1} \sum_{j=0}^{n-1} e^{(n-j-1)h \hat{B}} \left[ \eta_{j,m}^v + \xi_{j,m}^v \right]. \]

By (39) and noting \( e \), we use the notation \( \hat{e} \).

Noting the quadrature error of trapezoidal rule again, it follows from (43) that
\[ \sum_{n=0}^{N-1} \sum_{j=0}^{n-1} e^{(n-j-1)h \hat{B}} \left[ \eta_{j,m}^v + \xi_{j,m}^v \right] \lesssim \varepsilon^2 h^2 + \varepsilon^2 h \sum_{n=0}^{N-1} \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right), \]
and therefore \( \gamma^m \) has the following bound
\[ |\gamma^m| \lesssim \varepsilon^2 h^2 + \varepsilon^2 h \sum_{n=0}^{N-1} \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right), \quad 0 \leq m < M. \]

Noting the quadrature error of trapezoidal rule again, it follows from (43) that
\[ \int_0^{T_0} e^{s \hat{B}} ds e_{0,m}^v + \varepsilon^2 h^2 + \varepsilon^2 h \sum_{n=0}^{N-1} \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right). \]

By the Rodrigues’ formula, it is arrived that
\[ e^{s \hat{B}} e_{0,m}^v = \cos(s ||\hat{B}||) e_{0,m}^v + \sin(s ||\hat{B}||) e_{0,m}^v \times \hat{B} + \left( 1 - \cos(s ||\hat{B}||) \right) \left( \hat{B} \cdot e_{0,m}^v \right) \hat{B}, \]
where we use the notation \( \hat{B} = B/||B|| \). From the above result, it follows that \( \int_0^{T_0} e^{s \hat{B}} ds e_{0,m}^v = T_0 \left( \hat{B} \cdot e_{0,m} \right) \hat{B} \).

Thus, (44) reads
\[ \left| e_{N,m}^x \right| - \left| e_{0,m}^x \right| \lesssim \varepsilon \left| \left( \hat{B} \cdot e_{0,m}^v \right) \hat{B} \right| + \varepsilon^2 h^2 + \varepsilon^2 h \sum_{n=0}^{N-1} \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right), \]
\[ \lesssim \varepsilon \left| e_{0,m}^v \right| + \varepsilon^2 h^2 + \varepsilon^2 h \sum_{n=0}^{N-1} \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right), \quad 0 \leq m < M, \]
where \( e_{0,m}^v \) denotes the error \( e_{0,m}^v \) in the parallel direction of \( B \), i.e.
\[ e_{0,m}^v := \left( \hat{B} \cdot e_{0,m}^v \right) \hat{B}, \quad 0 \leq n \leq N, \quad 0 \leq m < M. \]

Then by (41) and noting \( e_{x,m}^x \), we get
\[ \left| e_{0,m+1}^x \right| - \left| e_{0,m}^x \right| \lesssim \varepsilon \left| e_{0,m}^v \right| + \varepsilon^2 \left( |e_{0,m}^x| + |e_{0,m+1}^x| \right) + \varepsilon^2 h^2, \quad 0 \leq m < M. \]

On the other hand, taking inner product on both sides of (40b) with \( \hat{B} \) leads to
\[ \left| e_{n+1,m}^v \right| \leq \hat{B} \cdot \left( \epsilon h \hat{B} e_{n+1,m}^v \right) + \left| \eta_{n,m}^v + \xi_{n,m}^v \right| + \left| \xi_{n,m} \cdot \hat{B} \right| \]
\[ = \left| e_{n,m}^v \right| + \left| \eta_{n,m}^v + \xi_{n,m}^v \right| + \left| \xi_{n,m} \cdot \hat{B} \right|. \]

(46)
Using the results (39) and (35), we induce from (46) that for $0 \leq n \leq N$, $0 \leq m < M$,
\[
|e_{n+1,m}^v - e_{n,m}^v| \lesssim h \varepsilon \left( |e_{n+1,m}^x| + |e_{n,m}^x| \right) + |e_{n,m}^x \dot{B}|. \tag{47}
\]
By the Rodrigues’ formula again as well as (34), it is easy to get $\xi_{n,m}^v \dot{B} = 0$. Therefore, (47) becomes
\[
|e_{n+1,m}^v - e_{n,m}^v| \lesssim h \varepsilon \left( |e_{n+1,m}^x| + |e_{n,m}^x| \right) + \varepsilon h^3, \quad 0 \leq n < N, \quad 0 \leq m < M. \tag{48}
\]
Summing up (48) for $n = 0, \ldots, N - 1$, we obtain
\[
|e_{0,m+1}^v - e_{0,m}^v| \lesssim h \varepsilon \sum_{n=0}^{N-1} \left( |e_{n+1,m}^x| + |e_{n,m}^x| \right) + \varepsilon h^2. \tag{49}
\]
Plugging (41) into the above gives
\[
|e_{0,m+1}^v - e_{0,m}^v| \lesssim \varepsilon \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right) + \varepsilon h^2, \quad 0 \leq m < M. \tag{49}
\]
Finally, combining (49) and (41), we have for $0 \leq m < M$
\[
|\xi_{0,m+1}^v - \xi_{0,m}^v| \lesssim \varepsilon \left( |\xi_{0,m}^v| \right) + \varepsilon h^2,
\]
then by Gronwall’ inequality with noting $e_{0,0}^v = e_{0,0}^c = 0$, we get
\[
|\xi_{0,m}^v| + |\xi_{0,m}^c| \lesssim \varepsilon h^2, \quad 0 \leq m \leq M.
\]
The estimates at the intermediates time grids, i.e. $e_{n,m}^x$ and $e_{n,m}^v$, for $0 < n < N$, are direct results of (48) and (41), and the whole proof is complete for the unconditional convergence (38).

- **Extension of the proof to other $d$.** For the conditional convergence (36), the above analysis holds for any $d > 1$. For the unconditional convergence (38), when $d = 2l + 1$, there exists a vector $\alpha$ such that $\dot{B}\alpha = 0$. Therefore, we have $\xi_{n,m}^v \alpha = 0$. For this case, the formula (44) has the following bound
\[
|\xi_{N,m}^v| \leq \varepsilon |\xi_{0,m}^v| + \varepsilon^2 h^2 + \varepsilon h \sum_{n=0}^{N-1} \left( |e_{n,m}^x| + |e_{n+1,m}^x| \right), \quad 0 \leq m < M,
\]
where $e_{0,m}^v$ is changed into
\[
e_{n,m}^v := (\alpha/|\alpha| \cdot e_{n,m}^v)|\alpha|, \quad 0 \leq n \leq N, \quad 0 \leq m < M.
\]
Then the unconditional convergence (38) can be proved by following the way stated above.

If $d = 2l$, the above proof cannot be applied to derive unconditional convergence. For this case, the modulated Fourier expansions of the numerical solutions and exact solutions should be constructed to obtain an unconditional result. The procedure is similar to that of Section 5 and we do not present it again in this paper for brevity.

**Remark 6.1** We have noticed that the unconditional convergence (38) with $d = 3$ can also be proved by the analysis given in [13] under a requirement on the stepsize $h$ that:
\[
h \text{ and } \varepsilon \text{ are of the same magnitude.} \tag{50}
\]
It is noted that by using the way given in this paper, there is no any restriction on $h$. But for the case of $d = 2l$, we also need (36) to derive the unconditional convergence.
7 Conclusions

Structure-preserving algorithms constitute an interesting and important class of numerical methods. Furthermore, uniformly accurate algorithms of highly oscillatory systems have received a great deal of attention. In this paper, we have formulated and analysed some uniformly accurate structure-preserving algorithms for solving nonlinear Hamiltonian systems with highly oscillatory solution. Two kinds of algorithms with uniform accuracy were given to preserve the symplecticity and energy, respectively. All the theoretical results were supported by a numerical experiment and were proved in detail.

Last but not least, it is noted that all the algorithms and analysis are also suitable to the non-highly oscillatory system \( \mathbf{H} \) with \( \varepsilon = 1 \). Meanwhile, there are some issues brought by this paper which can be researched further. For the system \( \mathbf{H} \) with a matrix \( \mathbf{B}(x) \) depending on \( x \), how to modify the methods and extend the analysis to get second-order and higher order uniformly accurate structure-preserving algorithms? This point will be considered in future. Another issue for future exploration is the extension and application of the methods presented in this paper to the Vlasov equations under strong magnetic field \([3,4]\).

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