Long-time momentum and actions behaviour of energy-preserving methods for semi-linear wave equations via spatial spectral semi-discretisations

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Abstract
It is known that wave equations have physically very important properties which should be respected by numerical schemes in order to predict correctly the solution over a long time period. In this paper, the long-time behaviour of momentum and actions for energy-preserving methods is analysed for semi-linear wave equations. A full discretisation of wave equations is derived and analysed by firstly using a spectral semi-discretisation in space and then by applying the adopted average vector field (AAVF) method in time. This numerical scheme can exactly preserve the energy of the semi-discrete system. The main theme of this paper is to analyse another important physical property of the scheme. It is shown that this scheme yields near conservation of a modified momentum and modified actions over long times. The results are rigorously proved based on the technique of modulated Fourier expansions in two stages. First, a multi-frequency modulated Fourier expansion of the AAVF method is constructed, and then two almost-invariants of the modulation system are derived.

Keywords Semi-linear wave equations · Energy-preserving methods · Multi-frequency modulated Fourier expansion · Momentum and actions conservation

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1 Introduction

This paper is concerned with the long-time behaviour of energy-preserving (EP) methods when applied to the following one-dimensional semi-linear wave equation (see [8, 9, 24])

\[ u_{tt} - u_{xx} + \rho u + g(u) = 0, \quad t > 0, \quad -\pi \leq x \leq \pi, \]

where \( g \) is a non-linear and smooth real function with \( g(0) = g'(0) = 0 \) and \( \rho \) is a real number satisfying \( \rho > 0 \). Similar to the refs. [8, 9, 24], the initial values \( u(\cdot, 0) \) and \( u_t(\cdot, 0) \) for this equation are assumed to be bounded by a small parameter \( \epsilon \), which provides small initial data in appropriate Sobolev norms. Meanwhile, periodic boundary conditions are considered in this paper.

It is noted that several important quantities are conserved by the solution of (1). The total energy

\[ H(u, v) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left( \frac{1}{2} (v^2 + (\partial_x u)^2 + \rho u^2)(x) + U(u(x)) \right) dx \]

is exactly preserved along the solution, where \( v = \partial_t u \) and the potential \( U(u) \) is of the form \( U'(u) = g(u) \). The solution of (1) also conserves the momentum

\[ K(u, v) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \partial_x u(x)v(x)dx = -\sum_{k=-\infty}^{\infty} ij u_{-j} v_j, \]

where \( u_j \) and \( v_j \) are the Fourier coefficients in the series \( u(x) = \sum_{j=-\infty}^{\infty} u_j e^{ijx} \) and \( v(x) = \sum_{j=-\infty}^{\infty} v_j e^{ijx} \), respectively. Moreover, the harmonic actions

\[ I_j(u, v) = \frac{\omega_j}{2} |u_j|^2 + \frac{1}{2\omega_j} |v_j|^2, \quad j \in \mathbb{Z} \]

are conserved for the linear wave equation, where \( \omega_j = \sqrt{\rho + j^2} \) for \( j \in \mathbb{Z} \). For the non-linear case, it has been proved in [1, 9] that for smooth and small initial data and almost all values of \( \rho > 0 \), the actions remain constant up to small deviations over a long time period.

In recent decades, many numerical methods have been developed and researched for solving wave equations (see, e.g., [3–5, 11, 17–19, 28, 35, 39]). In recent years, in the sense of geometric numerical integration, the consideration of qualitative properties in ordinary/partial differential equations has become increasingly important in designing numerical schemes. As one important aspect of the analysis, long-time conservation properties of wave equations and of numerical methods when applied to wave equations have been well studied, and we refer the reader to [8, 9, 13, 14, 24]. All these analyses are achieved by the technique of modulated Fourier expansions, which was developed by Hairer and Lubich in [23] and has been frequently used in the long-term analysis (see, e.g., [7, 22, 25, 31, 34]). On the other hand, as an important kind of methods, energy-preserving (EP) methods have also been the subject of many investigations for wave equations. EP methods can exactly preserve...
the energy of the considered system, and with regard to some examples of this topic, we refer the reader to [2, 6, 27, 29, 30, 32, 38]. Unfortunately, however, it seems that the long-time behaviour of EP methods in other structure-preserving aspects has not been studied for wave equations in the literature, such as the numerical conservation of momentum and actions. This motivates the research of this paper.

The main contribution of this paper is to rigorously analyse the long-time momentum and actions conservations of EP methods for wave equations. To our knowledge, this is the first research that studies the long-time behaviour of EP methods on wave equations by using modulated Fourier expansions. We organise the rest of this paper as follows. A full discretisation of the semi-linear wave equation (1) is formulated in Section 2, which is obtained by using spectral semi-discretisation in space and EP methods in time. The main result of this paper is presented in Section 3 and a numerical experiment is carried out to support the theoretical result. The proof of the main result is given in detail in Section 4, where the modulated Fourier expansion of EP methods is constructed and two almost-invariants of the modulated system are studied. In Section 5, the analysis for the method with a quadrature rule is presented. Some conclusions and further discussions are included in Section 6.

2 Full discretisation

In this section, a full discretisation for solving the semi-linear wave equation (1) is presented. To this end, we first consider a spectral semi-discretisation in space and then use EP methods in time.

2.1 Spectral semi-discretisation in space

We first discretise the wave equation in space by using a spectral semi-discretisation introduced in [8, 24]. Choose equidistant collocation points \( x_k = k\pi/M \) (for \( k = -M, -M + 1, \ldots, M - 1 \)) for the pseudo-spectral semi-discretisation in space and consider the real-valued trigonometric polynomials as an approximation for the solution of (1)

\[
\begin{align*}
    u^M(x, t) &= \sum_{|j| \leq M} q_j(t) e^{ix}, \\
    v^M(x, t) &= \sum_{|j| \leq M} p_j(t) e^{ix},
\end{align*}
\]

(2)

where \( p_j(t) = \frac{d}{dt} q_j(t) \) and the prime indicates that the first and last terms in the summation are taken with the factor 1/2. We collect all the \( q_j \) in a \( 2M \)-periodic coefficient vector \( \mathbf{q}(t) = (q_j(t)) \), which is a solution of the \( 2M \)-dimensional system of oscillatory ODEs

\[
\frac{d^2 \mathbf{q}}{dt^2} + \Omega^2 \mathbf{q} = f(\mathbf{q}),
\]

(3)

where \( f(\mathbf{q}) = -\mathcal{F}_{2M} g(\mathcal{F}_{2M}^{-1} \mathbf{q}) \), \( \Omega \) is diagonal with entries \( \omega_j \) and \( \mathcal{F}_{2M} \) denotes the discrete Fourier transform \( (\mathcal{F}_{2M} w)_j = \frac{1}{2M} \sum_{k=-M}^{M-1} w_k e^{-ij\pi k} \) for \( |j| \leq M \). It is
clear that the system (3) is a finite-dimensional complex Hamiltonian system with the energy

$$H_M(q, p) = \frac{1}{2} \sum_{|j| \leq M} \left( |p_j|^2 + \omega_j^2 |q_j|^2 \right) + V(q), \quad (4)$$

where $V(q) = \frac{1}{2M} \sum_{k=-M}^{M-1} U((j_{2M}^{-1} q)_k)$. The actions (for $|j| \leq M$) and the momentum of (3) are respectively expressed as

$$I_j(q, p) = \omega_j^2 |q_j|^2 + \frac{1}{2\omega_j} |p_j|^2, \quad K(q, p) = -\sum_{|j| \leq M} ijq_j p_j,$$

where the double prime indicates that the first and last terms in the summation are taken with the factor $1/4$. We are interested in real approximation (2) throughout this study, and thus it holds that $q_{-j} = \bar{q}_j$, $p_{-j} = \bar{p}_j$ and $I_{-j} = I_j$.

It is noted that the energy (4) is exactly preserved along the solution of (3). For the momentum and actions in the semi-discretisation, the following results have been proved in [24].

**Theorem 2.1** (See [24].) Under the non-resonance condition (10) and the assumption (7) which are stated in Section 3.1, it holds that

$$\sum_{l=0}^{M} \omega_j^{2l+1} \left| I_l(q(t), p(t)) - I_l(q(0), p(0)) \right| \leq C\epsilon,$$

$$\frac{|K(q(t), p(t)) - K(q(0), p(0))|}{\epsilon^2} \leq C t \epsilon M^{-s+1},$$

where $0 \leq t \leq \epsilon^{-N+1}$ and the constant $C$ is independent of $\epsilon, M, h$ and $t$.

### 2.2 EP methods in time

**Definition 2.2** (See [36, 40].) For efficiently solving the oscillatory system (3), the adopted average vector field (AAVF) method has been developed, which is defined as

\[
\begin{align*}
q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)p_n + h^2\phi_2(V) \int_0^1 f((1 - \sigma)q_n + \sigma q_{n+1})d\sigma, \\
p_{n+1} &= -h\Omega^2\phi_1(V)q_n + \phi_0(V)p_n + h\phi_1(V) \int_0^1 f((1 - \sigma)q_n + \sigma q_{n+1})d\sigma,
\end{align*}
\]

where $h$ is the stepsize, and

$$\phi_l(V) := \sum_{k=0}^{\infty} \frac{(-1)^k V^k}{(2k + l)!}, \quad l = 0, 1, 2$$

are matrix-valued functions of $V = h^2 \Omega^2$. 

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It follows from (6) that
\[ \phi_0(V) = \cos(h\Omega), \quad \phi_1(V) = \sin(h\Omega)(h\Omega)^{-1}, \quad \phi_2(V) = (I - \cos(h\Omega))(h\Omega)^{-2}. \]
We note that this method (5) reduces to the well-known average vector field (AVF) method when \( V = 0 \). The following properties of the AAVF method have been shown in [36, 40].

**Proposition 2.3** (See [36, 40].) The AAVF method is symmetric and exactly preserves the energy (4), which means that
\[ H_M(q_{n+1}, p_{n+1}) = H_M(q_n, p_n) \quad \text{for} \quad n = 0, 1, \ldots. \]

Clearly, the energy-preserving AAVF method does not exclude the symmetry structure, and as is known, preserving the energy and symmetry of the systems simultaneously at the discrete level is important for geometry integrators.

### 3 Main result and numerical experiment

In this paper, we take the following notations, which have been used in [8]. For sequences of integers \( k = (k_l)_l=0^M, \quad \omega = (\omega_l)_l=0^M \), and a real \( \sigma \), denote
\[ |k| = (|k_l|)_l=0^\infty, \quad \|k\| = \sum_{l=0}^M |k_l|, \quad k \cdot \omega = \sum_{l=0}^M k_l\omega_l, \quad \omega^\sigma[k] = \prod_{l=0}^M \omega_l^{|k_l|}. \]
Denote by \( \langle j \rangle \) the unit coordinate vector \((0, \ldots, 0, 1, 0, \ldots, 0)^T\) with the only entry 1 at the \( |j| \)-th position. For \( s \in \mathbb{R}^+ \), the Sobolev space of \( 2M \)-periodic sequences \( q = (q_j) \) endowed with the weighted norm \( \|q\|_s = \left( \sum_{|j| \leq M} \omega_j^{2s} |q_j|^2 \right)^{1/2} \) is denoted by \( H^s \). Moreover, we set \( [[k]] = \begin{cases} (\|k\| + 1)/2, & k \neq 0, \\ 3/2, & k = 0. \end{cases} \)

In what follows, we first present the main result of this paper and then carry out some numerical experiments to show the numerical performance and support the theoretical result.

#### 3.1 Main result

Before presenting the main result of this paper, the following assumptions are needed (see [8]).

**Assumption 3.1** • It is assumed that the initial values of (3) are bounded by
\[ \left( \|q(0)\|_{s+1}^2 + \|p(0)\|_s^2 \right)^{1/2} \leq \epsilon \quad (7) \]
with a small parameter \( \epsilon > 0 \).
The non-resonance condition is considered for a given stepsize $h$:

$$
\left| \sin \left( \frac{h}{2} (\omega_j - k \cdot \omega) \right) \cdot \sin \left( \frac{h}{2} (\omega_j + k \cdot \omega) \right) \right| \geq \epsilon^{1/2} h^2 (\omega_j + |k \cdot \omega|). \tag{8}
$$

If this is violated, we define a set of near-resonant indices

$$
\mathcal{R}_{\epsilon,h} = \{(j,k) : |j| \leq M, \|k\| \leq 2N, k \neq \pm (j), \text{not satisfying (8)}\}, \tag{9}
$$

where $N \geq 1$ is the truncation number of the expansion (15) which will be presented in the next section. We make the following assumption for this set. Suppose that there exist $\sigma > 0$ and a constant $C_0$ such that

$$
\sup_{(j,k) \in \mathcal{R}_{\epsilon,h}} \frac{\omega_j^\sigma}{\omega_j^\sigma |k|^2} e^{\|k\|/2} \leq C_0 \epsilon^N. \tag{10}
$$

We require the following numerical non-resonance condition

$$
|\sin(h\omega_j)| \geq h\epsilon^{1/2} \text{ for } |j| \leq M. \tag{11}
$$

For a positive constant $c > 0$, consider another non-resonance condition

$$
|\sin \left( \frac{h}{2} (\omega_j - k \cdot \omega) \right) \cdot \sin \left( \frac{h}{2} (\omega_j + k \cdot \omega) \right)| \geq c \epsilon^2 |2\phi_2(h^2 \omega_j^2)|
$$

for $(j,k)$ of the form $j = j_1 + j_2$ and $k = \pm (j_1) \pm (j_2)$, \tag{12}

which leads to improved conservation estimates.

We are now in a position to present the main result of this paper.

**Theorem 3.2 (Main result of this paper.)** Define the following modified momentum and actions, respectively

$$
\hat{I}_j(q, p) = \frac{\cos \left( \frac{1}{2} h\omega_j \right)}{\text{sinc} \left( \frac{1}{2} h\omega_j \right)} I_j(q, p), \quad \hat{K}(q, p) = - \sum_{|j| \leq M} i_j \frac{\cos \left( \frac{1}{2} h\omega_j \right)}{\text{sinc} \left( \frac{1}{2} h\omega_j \right)} q_{-j} p_j.
$$

The stepsize $h$ is chosen such that

$$
\left| \frac{\cos \left( \frac{1}{2} h\omega_j \right)}{\text{sinc} \left( \frac{1}{2} h\omega_j \right)} \right| \leq C_1 \text{ for } |j| \leq M. \tag{13}
$$

Suppose that the conditions of Assumptions 3.1 are true with $s \geq \sigma + 1$. Then for the AAVF method (5) and $0 \leq t = nh \leq \epsilon^{-N+1}$, the following near-conservation estimates of the modified momentum and actions

$$
\sum_{l=0}^{M-2s+1} \omega_l^2 \left| \hat{I}_l(q_n, p_n) - \hat{I}_l(q_0, p_0) \right| \leq C \epsilon,
$$

$$
\left| \hat{K}(q_n, p_n) - \hat{K}(q_0, p_0) \right| \leq C (\epsilon^2 + M^{-s} + \epsilon t M^{-s+1}).
$$
hold with a constant $C$ which depends on $s, N, C_0$ and $C_1$, but not on $\epsilon, M, h$ and the time $t$. If (12) is not satisfied, then the bound $Ce$ is weakened to $C\epsilon^{1/2}$.

The proof of this theorem will be presented in detail in Section 4 by using the technique of multi-frequency modulated Fourier expansions. It is noted that the above result for the AAVF method with the integral is still true for the AAVF method with some quadrature rule and it will be proved briefly in Section 5.

We have noticed that the authors in [8] analysed the long-time behaviour of a symmetric and symplectic trigonometric integrator for solving wave equations. It was shown in [8] that this integrator has a near-conservation of energy, momentum, and actions in numerical discretisations, which is advantageous with respect to other methods. It is noted that the method studied in [8] cannot preserve the energy (4) exactly. However, it follows from Proposition 2.3 and Theorem 3.2 that the AAVF method not only preserves the energy (4) exactly but also has a near-conservation of modified momentum and actions over long times.

**Remark 3.3** It can be concluded from this theorem that the AAVF method has a near-conservation of a modified momentum and modified actions over long terms. It is noted that we have tried to prove the long-time conservations for natural discretizations. However, after the whole procedure of the proof using modulated Fourier expansion, it turns out that there are artificial coefficients $\cos(h\omega_j)/\sin(h\omega_j/2)$ turn up at each term of the summation of the natural discretisation. Therefore, we only obtain the conservations of the modified momentum and modified actions. Similar situation has also happened frequently in some other publications. For example, the authors in [22] proved long-time conservations of modified energy and modified action for the Störmer-Verlet method and in [21], the conservations of modified energy and modified magnetic moment were shown for a variational integrator. In both the publications, long-time conservations for natural invariants are not obtained.

We also note that although the result cannot be obtained for the momentum $K$ and actions $I_j$, $K$ and $I_j$ are no longer exactly conserved quantities in the semi-discretisation, which is seen from Theorem 2.1. Moreover, it will be shown in the next subsection that in comparison with the near-conservation of $K$ and $I_j$, the modified momentum and modified actions are preserved rather well by AAVF method. This soundly supports the result of Theorem 3.2.

### 3.2 Numerical experiment

We now carry out two numerical experiments to show the numerical behaviour of the AAVF method. It is noted that for implicit methods, fixed-point iteration is used in practical computation. We set $10^{-16}$ as the error tolerance and 100 as the maximum number of each fixed-point iteration.

**Problem 1** The semi-linear wave equation (1) with $\rho = 0.5$ and $g(u) = -u^2$ is considered (see [8]) and its initial conditions are given by $u(x, 0) = 0.1(x - 1)^2(x + 1)^2$, $\partial_t u(x, 0) = 0.01(x - 1)(x + 1)^2$ for $-\pi \leq x \leq \pi$. We consider the spatial...
discretisation with the dimension $2M = 2^{71}$ and consider applying midpoint rule to the integral appearing in the AAVF formula (5), which yields

$$
\begin{align*}
q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)p_n + h^2\phi_2(V)f((q_n + q_{n+1})/2), \\
p_{n+1} &= -h\Omega^2\phi_1(V)q_n + \phi_0(V)p_n + h\phi_1(V)f((q_n + q_{n+1})/2).
\end{align*}
$$

(14)

It can be checked that the assumption (7) holds for $s = 2$ with $\epsilon \approx 0.1$. This problem is solved with the stepsize $h = 0.05$ on $[0,10000]$ and the relative errors of momentum/modified momentum and actions/modified actions against $t$ are shown in Fig. 1. Here, we use the following notations in the figures: $\text{errK} = |K(q_n,p_n) - K(q_0,p_0)|/|K(q_0,p_0)|$, $\text{errMK} = |\hat{K}(q_n,p_n) - \hat{K}(q_0,p_0)|/|\hat{K}(q_0,p_0)|$ and $\text{errI} = \sum_{l=0}^{M} \omega_l^5 |I_l(q_n,p_n) - I_l(q_0,p_0)|/\sum_{l=0}^{M} \omega_l^5 |I_l(q_0,p_0)|$, $\text{errMI} = \sum_{l=0}^{M} \omega_l^5 |\hat{I}_l(q_n,p_n) - \hat{I}_l(q_0,p_0)|/\sum_{l=0}^{M} \omega_l^5 |\hat{I}_l(q_0,p_0)|$. It follows from the results that the modified momentum and modified actions are better conserved than the momentum and actions, which supports the results given in Theorem 3.2.

Moreover, in order to show the efficiency of the AAVF method in comparison with some other methods, we consider the classical Störmer-Verlet formula (denoted by SV), the Gautschi’s method of order two (denoted by GM1s2) given in [23]...
and the two-stage diagonally implicit symplectic Runge-Kutta method of order three (denoted by RK2s3) presented in [10]. For Gautschi’s method, its coefficient functions are chosen as $\phi(\xi) = 1$ and $\psi(\xi) = (\sin(\xi)/\xi)^2$. The long-time behaviour of this method has been shown in [23] and the non-resonance conditions given in [8] are satisfied for this method. We first solve the system on $[0, 10]$ with $h = 0.2/2^j$ for $j = 2, 3, 4, 5$ and the errors $GE = (\|q_n - q\|_3^2 + \|p_n - p\|_2^2)^{1/2}$ measured at final time against the CPU time are presented in Fig. 2(i). Then, the problem is integrated on $[0, t_{\text{end}}]$ with $h = 0.01$ and $t_{\text{end}} = 10^j$ for $j = 0, 1, 2, 3$. The errors of the semi-discrete energy conservation are presented in Fig. 2(ii).

**Problem 2** Consider the semi-linear Klein-Gordon equation
\[
\begin{align*}
\frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} &= bu^3 - au, \quad -L \leq x \leq L, \quad 0 \leq t \leq T, \\
u(x, 0) &= \sqrt{2a/b} \text{sech}(\lambda x), \quad u_t(x, 0) = c\lambda \sqrt{2a/b} \text{sech}(\lambda x) \tanh(\lambda x)
\end{align*}
\]
with $\lambda = \sqrt{\frac{a}{a^2 - c^2}}$ and $a, b, a^2 - c^2 > 0$. The exact solution is given by $u(x, t) = \sqrt{\frac{2a}{b}} \text{sech}(\lambda(x - ct))$. We choose the parameters $a = 1$, $b = 0.01$, $c = 0.25$ and $L = \pi$, and then this problem fits the form (1).

The spatial discretisation with the dimension $2M = 2^j$ is also considered for this problem and it can be checked that the assumption (7) is true for $s = 1$ with $\epsilon \approx 0.015$. We solve this problem on $[0, 10000]$ with $h = 0.05$ and present the relative errors of momentum/modified momentum and actions/modified actions against $t$ in Fig. 3. Moreover, we apply our method as well as the methods SV, GM1s2 and RK2s3 to the system in $[0, 100]$ with $h = 0.2/2^j$ for $j = 0, 1, 2, 3$. The errors measured at final time against the CPU time are given in Fig. 4(i). Finally, we solve the problem on $[0, t_{\text{end}}]$ with $h = 0.01$ and $t_{\text{end}} = 10^j$ for $j = 0, 1, 2, 3$, and present the errors of the semi-discrete energy conservation in Fig. 4(ii). It is noted that for this problem,
the conservations of modified momentum and modified actions seem to be similarly to those on the natural discretisations of momentum and actions. The reason is that for some problems, it can be checked that the modified momentum and modified actions are very closed to the natural ones of the considered system. Besides, according to Fig. 4, it is more than expected that the Gautschi method behaves at least as well

**Fig. 3** The logarithm of the errors against $t$

**Fig. 4** Left: the logarithm of the errors against the logarithm of CPU time. Right: the logarithm of the energy errors against the logarithm of time
as AAVF since both methods behave similarly with respect to the conservation of invariants, but the Gautschi method is explicit and AAVF is implicit.

4 The proof of the main result

In this section, the result of Theorem 3.2 is proved. Since the proof is long, we first present the outline of the proof and then show the key points one by one.

4.1 The outline of the proof

The proof relies on a careful research of a modulated Fourier expansion of the AAVF method (5). Assume that the conditions of Theorem 3.2 are true. For the numerical solution \((q_n, p_n)\) given by (5), we will construct the following truncated multi-frequency modulated Fourier expansion (with \(N\) from (9))

\[
\tilde{q}(t) = \sum_{\|k\| \leq 2N} e^{i(k \cdot \omega)t} \zeta^k(\epsilon t), \quad \tilde{p}(t) = \sum_{\|k\| \leq 2N} e^{i(k \cdot \omega)t} \eta^k(\epsilon t),
\]

where \(t = nh\) and \(\zeta_{j}^{-k} = \bar{\zeta}_{\bar{k}}, \eta_{j}^{-k} = \bar{\eta}_{\bar{k}}\). For this modulated Fourier expansion, the following key points will be considered one by one in the rest of this section.

- In Section 4.2, formal modulation equations for the modulation functions are derived.
- In Section 4.3, we consider an iterative construction of the functions using reverse Picard iteration.
- We then work with a more convenient rescaling and study the estimation of non-linear terms in Section 4.4.
- Abstract reformulation of the iteration is presented in Section 4.5.
- In Section 4.6, we control the size of the numerical solution by studying the bounds of modulation functions.
- In Section 4.7, the bound of the defect is estimated.
- We study the difference between the numerical solution and its modulated Fourier expansion in Section 4.8.
- In Section 4.9, we show two invariants of the modulation system and establish their relationship with the modified momentum and modified actions.
- Finally, the previous results that are valid only on a short time interval are extended to a long time interval in Section 4.10.

It is noted that the above procedure is a standard approach to studying the long-time behaviour of numerical methods of Hamiltonian partial differential equations by using modulated Fourier expansions (see, e.g., [8, 9, 13, 14, 24]). Although the proof presented here closely follows these previous publications, there are novel modifications adapted to the AAVF method in each part. The differences in the analysis arise due to the implicitness of the AAVF method and the integral appearing in the method.
Throughout the proof, denote by $C$, a generic constant which is independent of $\epsilon, M, h$ and $t = nh$. The following lemma is given in [9] which will be needed in the analysis of this paper.

**Lemma 4.1** (See [9].) For $s > 1/2$, one has \( \sum_{|k| \leq K} \omega^{-2s|k|} \leq C_{K,s} \leq \infty \). For $s > 1/2$ and $m \geq 2$, it is true that

\[
\sup_{|k| \leq K} \sum_{k^1 + \cdots + k^m = k} \omega^{-2s(|k^1| + \cdots + |k^m|)} \leq C_{m,K,s} < \infty,
\]

where the sum is taken over \((k^1, \ldots, k^m)\) satisfying \(|k^m| \leq K\). For $s \geq 1$, it is further true that \( \sup_{|k| \leq K} \frac{\omega^{-2s(|k^m|)}}{\omega^{-2s|k^1|}} \leq C_{K,s} < \infty \).

### 4.2 Modulation equations

In order to derive modulation equations of the modulated functions, we need to define five operators by

\[
L^1_k := e^{i(k \omega)h} e^{e h D} - 2 \cos(h \Omega) + e^{-i(k \omega)h} e^{-e h D},
\]

\[
L^2_k := e^{\frac{1}{2}i(k \omega)h} e^{\frac{1}{2} e h D} + e^{-\frac{1}{2}i(k \omega)h} e^{-\frac{1}{2} e h D},
\]

\[
L^3_k := (e^{i(k \omega)h} e^{e h D} - 1)(e^{-i(k \omega)h} e^{-e h D} + 1)^{-1},
\]

\[
L^4_k(\sigma) := (1 - \sigma)e^{-\frac{1}{2}i(k \omega)h} e^{-\frac{1}{2} e D} + \sigma e^{\frac{1}{2}i(k \omega)h} e^{\frac{1}{2} e D},
\]

\[
L^k := (L^4_k)^{-1} = L^k,
\]

where $D$ is the differential operator (see [25]). For these operators, the following results are important in the analysis.

**Proposition 4.2** The operator $L^k$ can be expressed in Taylor expansions as follows:

\[
L^{(j)}(hD)\alpha_j^{(j)}(\epsilon t) = \pm 2i e h s_j(\epsilon t)\alpha_j^{(j)}(\epsilon t) + \frac{1}{2} i e^2 h^2 \sec(\frac{1}{2} h \omega_j)\alpha_j^{(j)}(\epsilon t) + \cdots,
\]

\[
L^k(hD)\alpha_j^k(\epsilon t) = 2 \frac{S(j) + k S(j) - k}{c_k} \alpha_j^k(\epsilon t) + i e h \frac{s_k(1 + c(j) + k c(j) - k)}{c_k^2} \alpha_j^k(\epsilon t) + \cdots,
\]

(16)

for $|j| > 0$ and $k \neq \pm(j)$, where $s_k = \sin(h \frac{1}{2}(k \cdot \omega))$ and $c_k = \cos(h \frac{1}{2}(k \cdot \omega))$. The Taylor expansions of $L^k_3$ are given by

\[
L^k_3\alpha_j^k(\epsilon t) = i \tan(\frac{1}{2} h (k \cdot \omega)) \alpha_j^k(\epsilon t) + \frac{h e}{1 + c_{2k}} \alpha_j^k(\epsilon t) + \cdots,
\]

for $|j| > 0$ and $|k| \leq 2N$. Moreover, for the operator $L^k_4(\sigma)$ with $|k| \leq 2N$, we have

\[
L^k_4(\frac{1}{2}) = \cos \left( \frac{h (k \cdot \omega)}{2} \right) + \frac{1}{2} \sin \left( \frac{h (k \cdot \omega)}{2} \right)(i e D) + \cdots.
\]
Proposition 4.3 (Modulation equations.) The formal modulation equations of modulated functions $\xi^k$ are given by

$$L^\pm j \xi^j = -h^2 \phi_2(h^2 \omega_j^2) \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} \sum'_{k^1 + \cdots + k^m = \pm j, j_1 + \cdots + j_m \equiv j \mod 2M} \int_0^1 \left[ (\xi^1_{j_1} \cdots \xi^m_{j_m})(t\epsilon, \sigma) \right] d\sigma,$$

$$L^k \xi^j = -h^2 \phi_2(h^2 \omega_j^2) \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} \sum'_{k^1 + \cdots + k^m = k, j_1 + \cdots + j_m \equiv j \mod 2M} \int_0^1 \left[ (\xi^1_{j_1} \cdots \xi^m_{j_m})(t\epsilon, \sigma) \right] d\sigma, \quad \text{for } k \neq \pm j,$$

(17)

where $L^k$ is defined by (16) and

$$\xi^k(\epsilon t, \sigma) = L^k_4(\sigma) \xi^k(\epsilon t).$$

The modulation equations of $\eta^k$ are determined by

$$\eta^\pm j = \pm i\omega_j \xi^\pm j + O(h\epsilon), \quad \eta^k = \frac{\tan(\frac{1}{2} h(k \cdot \omega))}{\tan(\frac{1}{2} h\omega_j)} i\omega_j \xi^k + O(h\epsilon)$$

(18)

for $k \neq \pm j$.

Proof. Proof of (17).

In the light of the symmetry of the AAVF method and the following property

$$\int_0^1 f((1 - \sigma)q_n + \sigma q_{n-1}) d\sigma = \int_0^1 f((1 - \sigma)q_{n-1} + \sigma q_n) d\sigma,$$

one obtains

$$q_{n+1} - 2 \cos(h\Omega) q_n + q_{n-1}$$

$$= h^2 \phi_2(V) \left[ \int_0^1 f((1 - \sigma)q_n + \sigma q_{n+1}) d\sigma + \int_0^1 f((1 - \sigma)q_{n-1} + \sigma q_n) d\sigma \right].$$

(19)

We look for a modulated Fourier expansion of the form

$$\tilde{q}_h(t + \frac{h}{2}, \sigma) = \sum_{\|k\| \leq 2N} e^{i(k \cdot \omega)(t + \frac{h}{2})} \xi^k \left( \epsilon(t + \frac{h}{2}), \sigma \right).$$
for the term \((1 - \sigma)\mathbf{q}_n + \sigma \mathbf{q}_{n+1}\). Then, it is obtained that
\[
\tilde{\xi}^k\left(\epsilon(t + \frac{h}{2}), \sigma\right) = \left((1 - \sigma)e^{\frac{1}{2}i(k \cdot \omega)h}e^{-\frac{1}{2}\epsilon D} + \sigma e^{\frac{1}{2}i(k \cdot \omega)h}e^{\frac{1}{2}\epsilon D}\right)\xi^k\left(\epsilon(t + \frac{h}{2})\right)
\]
\[
= L_4^k(\sigma)\xi^k\left(\epsilon(t + \frac{h}{2})\right).
\] (20)

In the same way, for \((1 - \sigma)\mathbf{q}_{n-1} + \sigma \mathbf{q}_n\), we have the following modulated Fourier expansion
\[
\tilde{\mathbf{q}}_h(t - \frac{h}{2}, \sigma) = \sum_{\|\mathbf{k}\| \leq 2N} e^{i(k \cdot \omega)(t - \frac{h}{2})}\tilde{\xi}^k\left(\epsilon(t - \frac{h}{2}), \sigma\right)
\]
with
\[
\tilde{\xi}^k\left(\epsilon(t - \frac{h}{2}), \sigma\right) = L_4^k(\sigma)\xi^k(\epsilon(t - \frac{h}{2})�).
\] (21)

Inserting the modulated Fourier expansions (15), (20), and (21) into (19) yields
\[
\tilde{\mathbf{q}}(t + h) - 2 \cos(h\Omega)\tilde{\mathbf{q}}(t) + \tilde{\mathbf{q}}(t - h) = h^2\phi_2(V)\left[\int_0^1 f\left(\tilde{\mathbf{q}}_h(t + \frac{h}{2}, \sigma)\right)d\sigma + \int_0^1 f\left(\tilde{\mathbf{q}}_h(t - \frac{h}{2}, \sigma)\right)d\sigma\right],
\]
which can be rewritten as
\[
(e^{\frac{1}{2}hD} + e^{-\frac{1}{2}hD})^{-1}(e^{hD} - 2 \cos(h\Omega) + e^{-hD})\tilde{\mathbf{q}}(t) = h^2\phi_2(V)\int_0^1 f\left(\tilde{\mathbf{q}}_h(t, \sigma)\right)d\sigma.
\] (22)

In what follows, we rewrite this equation by using the same way introduced in [24]. We start with making the following notation. For a \(2\pi\)-periodic function \(w(x)\), denote by \((\hat{Q}w)(x)\) the trigonometric interpolation polynomial to \(w(x)\) in the points \(x_k\). If \(w(x)\) is of the form \(w(x) = \sum_{j=-\infty}^{\infty} w_j e^{ijx}\), then one has that
\[(\hat{Q}w)(x) = \sum_{|j| \leq M} \left(\sum_{l=-\infty}^{\infty} w_{j+2Ml} e^{ijx}\right)\]
by considering \(x_k = \frac{k\pi}{M}\). For a \(2M\)-periodic coefficient sequence, \(\mathbf{q} = (q_j)\), \((P\mathbf{q})(x)\) is referred to the trigonometric polynomial with coefficients \(q_j\), i.e., \((P\mathbf{q})(x) = \sum_{|j| \leq M} q_j e^{ijx}\). By using these new denotations, (22) becomes
\[
(e^{\frac{1}{2}hD} + e^{-\frac{1}{2}hD})^{-1}(e^{hD} - 2 \cos(h\Omega) + e^{-hD})P\mathbf{q}(t) = h^2\phi_2(V)\int_0^1 \hat{Q}g\left(P\tilde{\mathbf{q}}_h(t, \sigma)\right)d\sigma.
\] (23)
Taylor expansion of the non-linearity $Qg$ at 0 is given by
\begin{equation}
Qg(P\tilde{q}_h(t, \sigma)) = \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} Q(P\tilde{q}_h(t, \sigma))^m
\end{equation}
\begin{equation}
= \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} \left( \sum_{|j_1| \leq M} \sum_{l=-\infty}^{\infty} \sum' \sum \mid k \mid \leq 2N e^{i(k^1 \cdot \omega)t} \xi_{j_1}^1 \xi_{j_1+2Ml}(\tau, \sigma) e^{ij_1x} \right)
\end{equation}
\begin{equation}
\cdots \left( \sum_{|j_m| \leq M} \sum_{l=-\infty}^{\infty} \sum' \sum \mid k \mid \leq 2N e^{i(k^m \cdot \omega)t} \xi_{j_m}^m \xi_{j_m+2Ml}(\tau, \sigma) e^{ij_mx} \right)
\end{equation}
\begin{equation}
= \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} \left( \sum_{|j| \leq M} \sum_{j_1, \ldots, j_m} \mid k \mid \leq 2N \mid k^1 \mid \leq 2N \ldots \mid k^m \mid \leq 2N e^{i(k^1 + \cdots + k^m \cdot \omega)t} \right)
\end{equation}
\begin{equation}
\cdot e^{i(k^1 + \cdots + k^m \cdot \omega)t} e^{ijx},
\end{equation}
where $\tau = h\epsilon$ and the prime on the sum indicates that a factor $1/2$ is included in the appearance of $\xi_{j_i}^1$ with $j_i = \pm M$. Inserting this into (23), considering the $j$th Fourier coefficient and comparing the coefficients of $e^{i(k^1 \cdot \omega)t}$, we obtain (17).

On the other hand, it needs to derive the initial values for $\xi_{j}^{\pm(j)}$ appearing in (17). By considering $\tilde{q}(0) = q(0)$, one has
\begin{equation}
\xi_{j}^{(j)}(0) + \xi_{j}^{-(j)}(0) = q_j(0) - \sum_{k \neq \pm(j)} \xi_{j}^k(0).
\end{equation}
Moreover, it follows from $\tilde{p}(0) = p(0)$ that $\eta_{j}^{(j)}(0) + \eta_{j}^{-(j)}(0) = p_j(0) - \sum_{k \neq \pm(j)} \eta_{j}^k(0)$, which yields
\begin{equation}
i\omega_j (\xi_{j}^{(j)}(0) - \xi_{j}^{-(j)}(0)) = p_j(0) - \sum_{k \neq \pm(j)} \eta_{j}^k(0)
\end{equation}
\begin{equation}
= p_j(0) - \sum_{k \neq \pm(j)} \frac{\tan(\frac{1}{2}h(k^1 \cdot \omega))}{\tan(\frac{1}{2}h\omega_j)} \tan(\frac{1}{2}h\omega_j) e^{i\omega_j \xi_{j}^k(0) + O(h\epsilon)}.
\end{equation}
The formulae (24) and (25) determine the initial values for $\xi_{j}^{\pm(j)}$.

**Proof of (18).**

For the modulation equations of $\eta^k$, it follows from (5) that
\begin{equation}
q_{n+1} - q_n = \Omega^{-1} \tan(\frac{1}{2}h\Omega)(p_{n+1} + p_n).
\end{equation}
By the definition of $L_3$, this relation can be expressed as
\begin{equation}
L_3^k \xi^k = \Omega^{-1} \tan(\frac{1}{2}h\Omega) \eta^k.
\end{equation}
\footnote{It is noted that $g(0) = g'(0) = 0$ is used here.}
In terms of the Taylor series of $L^k_3$, the relationship between $\eta^k$ and $\zeta^k$ can be established by (18).

### 4.3 Reverse Picard iteration

Following [8, 24], the reverse Picard iteration of the functions $\zeta^k$ is considered here such that after $4N$ iteration steps, the defects in (17), (24) and (25) are of magnitude $O(\epsilon N^2)$ in the $H^s$ norm.

Denote by $[\cdot]^{(n)}$ the $n$th iterate. For $k = \pm \langle j \rangle$ and according to (17), we consider the iteration procedure as follows:

$$
\pm 2i s(j) h e^{\left[\zeta^{\pm(j)}_j(n+1)\right]} = \left[-h^2 \phi_2(h^2 \omega^2_j) \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} \sum_{k^1, \ldots, k^m = k} \int_0^1 \left[(s_{k_1} \xi \cdots \xi_{k_m})(t, \sigma) - \left(\frac{1}{2} \epsilon^2 h^2 \sec \left(\frac{1}{2} h \omega_j \zeta^{\pm(j)}_j \right) + \cdots\right)\right]^{(n)} \right],
$$

(27)

For $k \neq \pm \langle j \rangle$ and $j$ satisfying the non-resonant (8), the iteration procedure is of the form

$$
2 \frac{s(j) + k^2(j) - k}{c_k} [\zeta^k]^{(n+1)} = \left[-h^2 \phi_2(h^2 \omega^2_j) \sum_{m \geq 2} \frac{g^{(m)}(0)}{m!} \sum_{k^1, \ldots, k^m = k} \int_0^1 \left[(s_{k_1} \xi \cdots \xi_{k_m})(t, \sigma) - \left(\epsilon h s_{k_1} + \cdots\right)\right]^{(n)} \right],
$$

(28)

where we let $\zeta^k = 0$ for $k \neq \pm \langle j \rangle$ in the near-resonant set $\mathcal{R}_{\epsilon, h}$. For the initial values (24) and (25), the iteration procedure reads

$$
\left[\zeta^j_j(0) + \zeta^{-j}_j(0)\right]^{(n+1)} = \left[q_j(0) - \sum_{k \neq \pm \langle j \rangle} \zeta^k_j(0)\right]^{(n)},
$$

$$
i \omega_j \left[\zeta^j_j(0) - \zeta^{-j}_j(0)\right]^{(n+1)} = \left[p_j(0) - \sum_{k \neq \pm \langle j \rangle} \frac{\tan(\frac{1}{2} h (k \cdot \omega))}{\tan(\frac{1}{2} h \omega_j)} \frac{\iota \omega_j \zeta^k_j(0) + O(\epsilon h)}{c_k} \right]^{(n)},
$$

(29)

In these iterations, it is assumed that $\|k\| \leq K := 2N$ and $\|k^i\| \leq K$ for $i = 1, \ldots, m$. There is an initial value problem of first-order ODEs for $\zeta^\pm_j$ (for $|j| \leq M$) and algebraic equations for $\zeta^k_j$ with $k \neq \pm \langle j \rangle$ at each iteration step. The starting iterates ($n = 0$) are chosen as $\zeta^k_j(\tau) = 0$ for $k \neq \pm \langle j \rangle$, and $\zeta^\pm_j(\tau) = \zeta^\pm_j(0)$, where $\zeta^\pm_j(0)$ are determined by (29).
4.4 Rescaling and estimation of the non-linear terms

Similarly to Sect. 3.5 of [9] and Sect. 6.3 of [8], in what follows, we consider a more convenient rescaling

\[ c_{\zeta_j}^k = \frac{\omega^{|k|}}{\epsilon[|k|]} \zeta_j^k, \quad c_{\zeta}^k = \left( c_{\zeta_j}^k \right)_{|j| \leq M} = \frac{\omega^{|k|}}{\epsilon[|k|]} \zeta^k \]

in the space \( H^s = (H^s)^C = \{ c_{\zeta} = (c_{\zeta_j}^k)_{k \in \mathcal{K}} : c_{\zeta_j}^k \in H^s \} \). The norm of this space is defined as \( \| |c_{\zeta_j}| \|^2 = \sum_{k \in \mathcal{K}} \| c_{\zeta_j}^k \|^2 \), where the set \( \mathcal{K} = \{ k = (k_l)_{l=0}^M \text{ with integers } k_l : \| k \| \leq K \} \) with \( K = 2N \). Likewise, we use the notation \( c_{\xi}^k \in H^s \) with the same meaning.

In order to express the non-linearity of (17) in these rescaled variables, define the non-linear function \( f = (f_j^k) \) by

\[ f_j^k(c_{\xi}(\tau)) = \frac{\omega^{|k|}}{\epsilon[|k|]} \sum_{m=2}^N \frac{N}{m!} \sum_{k_1 + \cdots + k_m = k} \frac{\epsilon[|k_1|+\cdots+|k_m|]}{\epsilon^{|k_1|+\cdots+|k_m|}} \sum_{j_1 + \cdots + j_m = j \mod 2M} \int_0^1 (c_{\xi_j}^{k_1} \cdots c_{\xi_j}^{k_m})(\tau, \sigma)d\sigma. \]

Regarding this function, we have the following bounds, which can be proved by using the similar arguments in [8, 9].

**Proposition 4.4** *(Estimation of the non-linear terms.)* It is true that

\[ \sum_{k \in \mathcal{K}} \| f_j^k(c_{\xi}) \|^2_s \leq C \epsilon P(\| |c_{\tilde{\xi}}| \|^2_s), \quad \sum_{|j| \leq M} \| f_{\pm(j)}^k(c_{\xi}) \|^2_s \leq C \epsilon^3 P_1(\| |c_{\tilde{\xi}}| \|^2_s), \] (30)

where \( c_{\tilde{\xi}}(\tau) := \sup_{0 \leq \sigma \leq 1} \{ c_{\xi}(\tau, \sigma) \} \) and \( P \) and \( P_1 \) are polynomials with coefficients bounded independently of \( \epsilon, h, \) and \( M \).

In a similar way, we consider different rescaling

\[ \hat{c}_{\zeta_j}^k = \frac{\omega^{s[|k|]}}{\epsilon[|k|]} \zeta_j^k, \quad \hat{c}_{\zeta}^k = \left( \hat{c}_{\zeta_j}^k \right)_{|j| \leq M} = \frac{\omega^{s[|k|]}}{\epsilon[|k|]} \zeta^k \]

in \( H^1 = (H^1)^C \) with norm \( \| |\hat{c}_{\zeta}| \|^2_1 = \sum_{|k| \leq K} \| \hat{c}_{\zeta_j}^k \|^2_1 \), where \( \hat{f}_j^k \) is defined as \( f_j^k \) but with \( \omega^{|k|} \) replaced by \( \omega^{s[|k|]} \). We use similar notations \( \hat{c}_{\xi}^k \in H^1 \) and also get similar bounds

\[ \sum_{k \in \mathcal{K}} \| \hat{f}_j^k(\hat{c}_{\xi}) \|^2_1 \leq C \epsilon \hat{P}(\| |\hat{c}_{\tilde{\xi}}| \|^2_1), \quad \sum_{|j| \leq M} \| \hat{f}_{\pm(j)}^k(\hat{c}_{\xi}) \|^2_1 \leq C \epsilon^3 \hat{P}_1(\| |\hat{c}_{\tilde{\xi}}| \|^2_1) \]

with other functions \( \hat{P} \) and \( \hat{P}_1 \).
4.5 Reformulation of the reverse Picard iteration

In this subsection, in the light of the two cases: $k = \pm \langle j \rangle$ and $k \neq \pm \langle j \rangle$, we split $c\zeta$ into two parts as follows:

\[
\begin{align*}
\alpha_k^j = c_k^j & \quad \text{if } k = \pm \langle j \rangle, \quad \text{and } 0 \text{ else}, \\
\beta_k^j = c_k^j & \quad \text{if } (8) \text{ is satisfied, } \quad \text{and } 0 \text{ else}. 
\end{align*}
\]

(32)

We remark that for $a\zeta = (a_k^j) \in H^s$ and $b\zeta = (b_k^j) \in H^s$, one has $a\zeta + b\zeta = c\zeta$ and $|||a\zeta|||^2_s + |||b\zeta|||^2_s = |||c\zeta|||^2_s$. The same denotation and property are used for $c\xi$.

We try to rewrite the iterations (27) and (28) in an abstract form

\[
\begin{align*}
\alpha_k^j(n+1) = \Omega^{-1} F(a_k^{(n)}, b_k^{(n)}) - Aa_k^{(n)}, \\
\beta_k^j(n+1) = \Omega^{-1} \Psi G(a_k^{(n)}, b_k^{(n)}) - Bb_k^{(n)}, 
\end{align*}
\]

(33)

where

\[
(\Omega x)_k^j = (\omega_j + |k \cdot \omega|)x_k^j, \quad (\Psi x)_k^j = 2\phi_2(h^2 \omega_j^2) \cos\left(\frac{1}{2} h(k \cdot \omega)\right)x_k^j,
\]

and the operators $A$, $B$ are respectively defined as

\[
\begin{align*}
(Aa_k^j)_{\pm\langle j \rangle}^k &= \frac{1}{\pm 2i s(j)} \left(\frac{1}{2} e^2 h^2 \sec\left(\frac{1}{2} h\omega_j\right) a_{\pm\langle j \rangle}^k + \cdots \right), \\
(Bb_k^j)_k^j &= \frac{c_k^j}{2 s(j) + k s(j) - k} \left(ie^h s_k^j(1 + c(j) + k c(j) - k) b_{\pm\langle j \rangle}^k + \cdots \right)
\end{align*}
\]

for $(j, k)$ satisfying (8).

The functions $F = (F_k^j)$ and $G = (G_k^j)$ are given respectively by

\[
F_{\pm\langle j \rangle}^j(a\zeta, b\zeta) = \frac{1}{\mp ie} \frac{2\phi_2(h^2 \omega_j^2)}{\sin\left(\frac{1}{2} h\omega_j\right)} f_{\pm\langle j \rangle}^j(c\zeta), \quad G_{k}^j(a\zeta, b\zeta) = -\frac{h^2(\omega_j + |k \cdot \omega|)}{4 s(j) + k s(j) - k} f_{k}^j(c\zeta)
\]

for $(j, k)$ satisfying (8).

**Proposition 4.5** The operators $A$ and $B$ are bounded by

\[
|||(Aa\zeta)(\tau)|||_s \leq C \sum_{l=2}^{N} h^{l-2} e^{l-3/2} \left\| d^{l} (a\zeta)(\tau) \right\|_s, \\
|||(Bb\zeta)(\tau)|||_s \leq C e^{1/2} |||(b\zeta)(\tau)|||_s + C \sum_{l=2}^{N} h^{l-2} e^{l-1/2} \left\| d^{l} (b\zeta)(\tau) \right\|_s.
\]

Moreover, we have

\[
|||F|||_s \leq C e^{1/2}, \quad |||G|||_s \leq C, \quad ||||\Psi^{-1} \Omega^{-1} F|||_s \leq C.
\]
Proof Since
\[
\left| \frac{1}{\pm 2i s(j) \epsilon} \frac{1}{2} \epsilon^2 h^2 \sec \left( \frac{1}{2} h \omega_j \right) \right| = \left| \frac{1}{2} \epsilon h \epsilon \sin(h \omega_j) \right| \leq \frac{1}{2} \epsilon^{1/2},
\]
the bound of \( A \) is obtained. We then compute
\[
\left| \frac{c_k}{s(j) \pm k} \frac{i \epsilon h}{s_k(1 + c(j) + k c(j) - k)} \right| \leq \left| \frac{\epsilon h}{\epsilon h^2 (\omega_j + |k \cdot \omega|)} \frac{s_k(1 + c(j) + k c(j) - k)}{c_k} \right| \leq \left| \frac{\epsilon h}{\epsilon \sin(h \epsilon)} \sin(h \omega_j) \right| \leq \frac{1}{2} \epsilon^{1/2},
\]
where we used \( |s_k| \leq \frac{h}{2} |k \cdot \omega| \). Thus, the bound of \( B \) is yielded.

From
\[
\left| \frac{2 \phi_2(h^2 \omega_j^2)}{\sin(h \omega_j)} \right| = \left| \sin \left( \frac{1}{2} h \omega_j \right) \right| \leq 1 \text{ and (30)}, \]
it follows that \(|\| F \|_s \leq C \epsilon^{1/2}\).

By considering (8) and (30), one gets \(|\| G \|_s \leq C\). Moreover, according to (11), we have
\[
|\| \Psi - \Omega^{-1} F \|_s^2 = \sum_{k \in K} \sum_{|j| \leq M} \left( \Psi^{-1} \Omega^{-1} F \right)_j^k \leq \sum_{k \in K} \sum_{|j| \leq M} \left( \frac{h}{2 \epsilon} \right)^2 \left| f_j^{\pm(j)} \right|^2 \leq C \sum_{k \in K} \sum_{|j| \leq M} \left( \frac{1}{\epsilon^{3/2}} \right)^2 \left| f_j^{\pm(j)} \right|^2 = \frac{C}{\epsilon^3} |\| f^{\pm(j)} \|_s^2 \leq C,
\]
which implies \(|\| \Psi - \Omega^{-1} F \|_s \leq C\). \qed

For the initial value condition (29), it can be rewritten as
\[
a_j^{(n+1)}(0) = v + P b_j^{(n)}(0) + Q b_j^{(n)}(0), \quad (34)
\]
where \( v_j^{\pm(j)} = \frac{\omega_j}{\epsilon} \left( \frac{1}{2} q_j(0) \mp \frac{i}{2 \omega_j} p_j(0) \right) \) and the operators \( P \) and \( Q \) are defined by
\[
(P b_j)^{\pm(j)}(0) = -\frac{1}{2} \frac{\omega_j}{\epsilon} \sum_{k \neq \pm(j)} \frac{e_k(k)}{\omega_k} b_j^k(0),
\]
\[
(Q b_j)^{\pm(j)}(0) = \frac{1}{2 \omega_j} \frac{\omega_j}{\epsilon} \sum_{k \neq \pm(j)} \frac{e_k(k)}{\omega_k} b_j^k(0).
\]
From (7), it can be verified that $v$ is bounded in $H^s$. For the bounds of the operators $P$ and $Q$, we have

$$
\|\|P \xi \|\|^2_s = \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega_j^{2s} \left| \frac{1}{2} \frac{\omega_j}{\epsilon} \sum_{k \neq \pm (j)} \frac{e^{[k]}}{\omega |k|} b\xi_k(0) \right|^2
\leq \frac{1}{4 \epsilon^2} \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega_j^{2s+2} \left( \sum_{k \neq \pm (j)} \frac{e^{2[k]}}{\omega^2 |k|} \right) \left( \sum_{k \neq \pm (j)} b\xi_k(0)^2 \right)
\leq \frac{1}{4} \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega_j^{2s+2} \left( \sum_{k \neq \pm (j)} \omega^{-2[k]} \right) \left( \sum_{k \neq \pm (j)} b\xi_k(0)^2 \right)
\leq C \|\|Q \Omega \xi(0)\|\|^2_s \leq C \|\|b\xi(0)\|\|^2_s + 1. \tag{35}
$$

and likewise it is true that

$$
\|\|Q b \xi(0)\|\|^2_s \leq C \|\|b \eta(0)\|\|^2_s.
$$

Thence, the bounds $\|\|P \xi(0)\|\|_s \leq C$ and $\|\|Q \xi(0)\|\|_s \leq C$ are obtained. The starting iterates of (34) are chosen as $a\xi (0)(\tau) = v$ and $b\xi (0)(\tau) = 0$.

### 4.6 Bounds of the coefficient functions

**Proposition 4.6 (Bounds of the modulation functions.)** The modulation functions $\xi_k$ of (15) are bounded by

$$
\sum_{|k| \leq 2N} \left| \frac{\omega^{|k|}}{\epsilon^{[k]}} \right| \left\| \xi_k(\epsilon t) \right\|^2_s \leq C \tag{35}
$$

and the same bound holds for any fixed number of derivatives of $\xi_k$ with respect to the slow time $\tau = \epsilon t$.

**Proof** On the basis of the above analysis and by induction, it is easy to prove that the iterates $a\xi^{(n)}$, $b\xi^{(n)}$ and their derivatives with respect to $\tau$ are bounded in $H^s$ for $0 \leq \tau \leq 1$ and $n \leq 4N$. These bounds show that $c\xi^{(n)} = a\xi^{(n)} + b\xi^{(n)}$ is bounded in $H^s$, and then the bound (35) is obtained.

**Proposition 4.7 (Bounds of the expansion.)** The expansion (15) is bounded by

$$
\|\hat{q}(t)\|_{s+1} + \|\hat{p}(t)\|_s \leq C \epsilon \quad for \quad 0 \leq t \leq \epsilon^{-1}. \tag{36}
$$

For $|j| \leq M$, it further holds that

$$
\hat{q}_j(t) = \xi^{(j)}_j(\epsilon t)e^{i\omega j t} + \xi^{(-j)}_j(\epsilon t)e^{-i\omega j t} + r_j \quad with \quad \|r\|_{s+1} \leq C \epsilon^2. \tag{37}
$$

If the condition (12) fails to be satisfied, then the bound is $\|r\|_{s+1} \leq C \epsilon^{3/2}$. 

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Proof More precisely, the following bounds for the \((4N)\)th iterates can be obtained
\[
\|\|a\zeta(0)\|\|_s \leq C, \quad |||\Omega a\zeta(\tau)\|\|_s \leq C\epsilon^{1/2},
\]
where \(C\) depends on \(N\), but not on \(\epsilon, h, M\). It follows from these results (38) that
\[
|||a\zeta|||_s + 1 = |||\Omega a\zeta|||_s \leq C\epsilon^{1/2},
\]
\[
|||b\zeta|||_s + 1 = \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega^{j + 2} \left| b\zeta_j \right|^2 = \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega^{j + 2} \left| \frac{\omega_j}{(\omega_j + |k \cdot \omega|)} \right|^2 \left| (\omega_j + |k \cdot \omega|) b\zeta_j \right|^2
\]
\[
\leq |||\Omega b\zeta(\tau)|||_s \leq C.
\]

Hence, we have
\[
|||c\zeta(\tau) - a\zeta(0)|||_s + 1 = |||a\zeta(\tau) + b\zeta(\tau) - a\zeta(0)|||_s + 1 \leq |||a\zeta|||_s + 1 + |||b\zeta|||_s + 1 \leq C.
\]

Then, according to the fact that \(\zeta_j^{(k)} = \frac{e^{[|k|]} \left( c\zeta_j^{(k)}(0) + a\zeta_j^{(k)}(0) \right)}{\omega_j} \), it is yielded that
\[
|||\hat{\zeta}|||_s + 1 = \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega^{j + 2} \left| \frac{\omega_j}{\omega_j} \right|^2 \left| e^{[|k|]} \left( c\zeta_j^{(k)}(0) + a\zeta_j^{(k)}(0) \right) \right|^2
\]
\[
\leq 2\epsilon^2 \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega^{j + 2} \left( \sum_{|k| \leq 2N} e^{[|k|]} \left| c\zeta_j^{(k)} - a\zeta_j^{(k)}(0) \right| \right)^2
\]
\[
\leq 4\epsilon^2 |||a\zeta(0)|||_s^2 + 2 \sum_{k \in \mathcal{K}} \sum_{|j| \leq M} \omega^{j + 2} \left( \sum_{|k| \leq 2N} e^{2[|k|]} \left| c\zeta_j^{(k)} - a\zeta_j^{(k)}(0) \right| \right)^2
\]
\[
\leq 4\epsilon^2 |||a\zeta(0)|||_s^2 + 2C_{K,1}\epsilon^2 |||c\zeta - a\zeta(0)|||_s + 1 \leq C\epsilon^2.
\]

By (26) and similar analysis, it can be proved that \(|||\hat{\pi}|||_s \leq C\epsilon\). Thus, the bound (36) is true.

It then follows from (30) and (33) that
\[
\left( \sum_{|k| = 1} \left\| \Omega b\zeta^k \right\|^2 \right)^{1/2} \leq C\epsilon
\]
for \(b\zeta = (b\zeta)^{(4N)}\). Moreover, in terms of (12), it is obtained that
\[
\sum_{|j| \leq M} \sum_{j_1 + j_2 = j} \sum_{k = \pm(j_1) \pm (j_2)} \omega^{j + (s - 1)} \left| b\zeta_j^k \right|^2 \leq C\epsilon.
\]

These bounds as well as (38) lead to (37).

For the alternative scaling (31), one can obtain the same bounds
\[
|||a\zeta(0)|||_1 \leq C, \quad |||\Omega a\zeta(\tau)|||_1 \leq C\epsilon^{1/2}, \quad |||\psi^{-1}\Omega b\zeta(\tau)|||_1 \leq C\epsilon. \quad (39)
\]
The following bound is also true for this scaling:

\[
\left( \sum_{\|k\| = 1} \left\{ (\Psi^{-1} \Omega \hat{b} \zeta)^k \right\}_1^2 \right)^{1/2} \leq C\epsilon. \tag{40}
\]

### 4.7 Defects

We express the defect in (5) as another form

\[
\delta_j(t) = \tilde{q}_j(t + h) - 2 \cos(h\omega_j) \tilde{q}_j(t) + \tilde{q}_j(t - h)
\]

\[
- \left[ \int_0^1 f_j((1 - \sigma)\tilde{q}_h(t) + \sigma \tilde{q}_h(t + h))d\sigma + \int_0^1 f_j((1 - \sigma)\tilde{q}_h(t - h) + \sigma \tilde{q}_h(t))d\sigma \right],
\]

where \(\tilde{q}_j\) is determined in (15) with \(\zeta_k^j = (\zeta_k^j)^{(4N)}\) obtained after \(4N\) iterations of the procedure in Section 4.3. This defect can also be rewritten as

\[
\delta_j(t) = \sum_{\|k\| \leq NK} d_k^k(\epsilon t)e^{i(k \cdot \omega)t} + R(t),
\]

where

\[
d_k^k = \frac{1}{h^2\phi_2(h^2\omega_j^2)} \tilde{L}_j^k \xi_k^j + \sum_{m=2}^N \frac{g^{(m)}(0)}{m!} \sum_{k_1 + \cdots + k_m = k} \sum_{j_1 + \cdots + j_m \equiv j \mod 2M} \sum_{i=1}^{\epsilon N}
\]

\[
\int_0^1 \left[ (\tilde{\xi}_{j_1}^1 \cdot \cdots \cdot \tilde{\xi}_{j_m}^m)(t\epsilon, \sigma) \right]d\sigma.
\]

It is noted that here we consider \(\|k\| \leq NK\) for \(d_k^k\), and it is assumed that \(\zeta_j^k = \eta_j^k = 0\) for \(\|k\| > K := 2N\). The truncation of the operator \(\tilde{L}_j^k\) after the \(\epsilon N\) term is denoted by \(\tilde{L}_j^k\). The remainder terms of the Taylor expansion of \(f\) after \(N\) terms are contained in \(R\). By the bound (36) and the estimates (38), it is true that \(\|R\|_{s+1} \leq C\epsilon^{N+1}\).

Using Cauchy-Schwarz inequality and Lemma 4.1, we obtain

\[
\left\| \sum_{\|k\| \leq NK} d_k^k(\epsilon t)e^{i(k \cdot \omega)t} \right\|_s^2 = \sum_{|j| \leq M} \sum_{\|k\| \leq NK} d_j^k e^{i(k \cdot \omega)t}
\]

\[
\leq \sum_{|j| \leq M} \omega_j^{2s} \sum_{\|k\| \leq NK} \omega^{-2|k|} \leq C_{NK,1} \sum_{\|k\| \leq NK} \|\omega^{|k|}d_k^k(\epsilon t)\|_s^2.
\]
The right-hand side of this result can be estimated as follows.

**Proposition 4.8 (Bounds of the defects.)** It is obtained that  
\[
\sum_{|k| \leq N/K} \left\| \omega^k \cdot d^k(\epsilon t) \right\|^2_s \leq C \epsilon^{2(N+1)}.
\]

**Proof** We will prove this result for three cases: truncated, near-resonant and non-resonant modes.

- **Truncated and near-resonant modes.** The result for these two cases can be obtained by using the similar analysis given in Sect. 6.8 of [8].

- **Non-resonant mode.** For the non-resonant mode (\(|k| > K\) and \((j, k)\) satisfies (8)), we reformulate the defect in the scaled variables of Section 4.4 as  
\[
\omega^k \cdot d^k_j = \epsilon |k| \left( \frac{1}{h^2 \phi_2(h^2 \omega_j^2)} \hat{L}_j c_j^k + f_j^k(c_j^k) \right).
\]

Splitting them into \(k = \pm(j)\) and \(k \neq \pm(j)\) yields  
\[
\omega_j \cdot d_j^{\pm(j)} = \epsilon \left( \pm i \epsilon \omega_j \left( \sin(c(h \omega_j^2)/2) \right) (a_j^{\pm(j)} + (Aa_j^{\pm(j)}) + j^{\pm(j)}(c_j^k)),
\omega^k \cdot d^k_j = \epsilon |k| \left( \frac{2\epsilon h_j^k \omega_j^2 - \frac{k}{h_j^2 \phi_2(h^2 \omega_j^2)} \hat{L}_j c_j^k + f_j^k(c_j^k) \right).
\]

It is noted that the functions here are actually the 4Nth iterates of the iteration in Section 4.3. By expressing \(f_j^{\pm(j)}\) and \(f_j^k\) in terms of \(F, G\) and inserting them from (33) into this defect, it is arrived at that  
\[
\omega_j \cdot d_j^{\pm(j)} = 2 \omega_j a_j^{\pm(j)} \left( [a_j^{\pm(j)}]_{(4N)} - [a_j^{\pm(j)}]_{(4N+1)} \right), \quad \alpha_j^{\pm(j)} = \pm i \epsilon^2 \left( \sin(c(h \omega_j^2)/2) \right) \frac{h_j^2 \phi_2(h^2 \omega_j^2)}{2} ^2.
\]

Looking closer at these expressions, we consider new variables given as  
\[
\tilde{a}_j^{\pm(j)} = \alpha_j^{\pm(j)} a_j^{\pm(j)}, \quad \tilde{b}_j^k = \beta_j^k b_j^k
\]

and rewrite the iteration (33) in these variables as  
\[
\hat{\alpha}_j^{(n+1)} = \Omega^{-1} \tilde{F}(\tilde{a}_j^{(n)}, \tilde{b}_j^{(n)}) - A \hat{\alpha}_j^{(n)},
\hat{\beta}_j^{(n+1)} = \tilde{G}(\tilde{a}_j^{(n)}, \tilde{b}_j^{(n)}) - B \tilde{b}_j^{(n)}.
\]

Here, the transformed functions are defined by  
\[
\tilde{F}_j^{\pm(j)}(\tilde{a}_j, \tilde{b}_j) = \alpha_j^{\pm(j)} F_j^{\pm(j)}(\alpha^{-1} \tilde{a}_j, \beta^{-1} \tilde{b}_j) = -\epsilon f_j^{\pm(j)}(\alpha^{-1} \tilde{a}_j + \beta^{-1} \tilde{b}_j),
\tilde{G}_j^k(\tilde{a}_j, \tilde{b}_j) = \beta_j^k \left( \Psi \Omega^{-1} G_j^k(\alpha^{-1} \tilde{a}_j, \beta^{-1} \tilde{b}_j) = -\epsilon |k| f_j^k(\alpha^{-1} \tilde{a}_j + \beta^{-1} \tilde{b}_j).
\]

In the iteration for the initial values, one has  
\[
\hat{\alpha}_j^{(n)}(0) = \alpha v + \tilde{P} \hat{b}_j^{(n)}(0) + \tilde{Q} \hat{b}_j^{(n)}(0),
\]

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where $\tilde{P} = \alpha P \beta^{-1}$, $\tilde{Q} = \alpha Q \beta^{-1}$. For the bound of $\tilde{P}$, we have
\[
\||| \tilde{P} \tilde{b} \tilde{\zeta}(0) |||^2 \\
\leq \sum_{k \in K} \sum'_{|j| \leq M} \omega^2 j \left| e^{2\text{sinc}(h\omega j/2)} \frac{1}{2} \sum_{k \neq \pm(j)} h^2 c_k \phi_2(h^2 \omega_j^2) \frac{\epsilon}{\epsilon(2s_{(j)+k}s_{(j)}-k)} \frac{\omega^-|k|}{\omega} \tilde{b} \tilde{\zeta}_j^k(0) \right|^2
\leq \sum_{k \in K} \sum'_{|j| \leq M} \omega^2 j \left( \sum_{k \neq \pm(j)} \frac{\omega}{|s(j)+k|} \omega^-|k| \tilde{b} \tilde{\zeta}_j^k(0) \right)^2
\leq \sum_{k \in K} \sum'_{|j| \leq M} \frac{\epsilon}{64} \left( \sum_{k \neq \pm(j)} \omega^-2|k| \sum_{k \neq \pm(j)} (\tilde{b} \tilde{\zeta}_j^k(0))^2 \right) \leq C \epsilon \||| \tilde{b} \tilde{\zeta}(0) |||^2.
\]

Similarly, the following result can be derived:
\[
\||| \tilde{Q} \tilde{b} \tilde{\zeta}(0) |||^2 \leq C \epsilon \||| \tilde{b} \tilde{\zeta}(0) |||^2.
\]

It can be verified that in an $H^s$-neighbourhood of 0 where the bounds (38) hold, the partial derivatives of $\tilde{F}$ with respect to $\tilde{a} \zeta$ and $\tilde{b} \zeta$ are bounded by $O(\epsilon^{1/2})$. Meanwhile, the partial derivative of $\tilde{G}$ with respect to $\tilde{b} \tilde{\zeta}$ is bounded by $O(\epsilon^{1/2})$ but that of $\tilde{G}$ with respect to $\tilde{a} \tilde{\zeta}$ is only $O(1)$. In fact, these results are the same as those described in Sect. 6.9 of [8]. Likewise, we obtain
\[
\||| \Omega(\tilde{a} \tilde{\zeta}^{(4N+1)} - \tilde{a} \tilde{\zeta}^{(4N)}) ||| \leq C \epsilon^{N+2},
\]
\[
\||| \tilde{b} \tilde{\zeta}^{(4N+1)} - \tilde{b} \tilde{\zeta}^{(4N)} ||| \leq C \epsilon^{N+2},
\]
\[
\||| \tilde{a} \tilde{\zeta}(0)^{(4N+1)} - \tilde{a} \tilde{\zeta}(0)^{(4N)} ||| \leq C \epsilon^{N+2}.
\]

Thus, it is yielded for $\tau \leq 1$ and $(j, k) \in R_{\epsilon, h}$ that
\[
\left( \sum_{||k|| \leq K} \omega^{|k|} d^k(\tau) \right)^2 \leq C \epsilon^{N+1}.
\tag{43}
\]

With (43), the defect (41) has the bound $\||| \delta(t) ||| \leq C \epsilon^{N+1}$ for $t \leq \epsilon^{-1}$. For the defect in the initial conditions (24) and (25), it holds that
\[
\| q(0) - \tilde{q}(0) \|_{s+1} + \| p(0) - \tilde{p}(0) \|_s \leq C \epsilon^{N+1}.
\]

With the alternative scaling (31), the following result is derived
\[
\left( \sum_{||k|| \leq K} \omega^{|k|} d^k(\tau) \right)^2 \leq C \epsilon^{N+1}.
\tag{44}
\]
4.8 Remainders

**Proposition 4.9 (Remainders.)** For the difference of the numerical solution and its modulated Fourier expansion, we have

\[
\|q_n - \tilde{q}(t)\|_{s+1} + \|p_n - \tilde{p}(t)\|_{s} \leq C\epsilon^N \quad \text{for} \quad 0 \leq t = nh \leq \epsilon^{-1}. \quad (45)
\]

**Proof** With the notations \( \Delta q_n = \tilde{q}(tn) - q_n, \Delta p_n = \tilde{p}(tn) - p_n, \) one gets

\[
\left( \frac{\Delta q_{n+1}}{\Omega - 1} \right) = \left( \begin{array}{cc}
\cos(h\Omega) & \sin(h\Omega) \\
-\sin(h\Omega) & \cos(h\Omega)
\end{array} \right) \left( \frac{\Delta q_n}{\Omega - 1} \right) + h \left( \frac{h\Omega \phi_2(V) \Omega^{-1}(\Delta f + \delta)}{\phi_1(V) \Omega^{-1}(\Delta f + \delta)} \right),
\]

where

\[
\Delta f = \int_0^1 \left( f((1 - \sigma)q_n + \sigma q_{n+1}) - f((1 - \sigma)\tilde{q}(tn) + \sigma \tilde{q}(tn + h)) \right) d\sigma.
\]

Using the Lipschitz bound given in Sect. 4.2 of [24] and Sect. 6.10 of [8], we have

\[
\|\Omega^{-1} \Delta f\|_{s+1} = \|\Delta f\|_s \leq \epsilon(\|\Delta q_n\|_s + \|\Delta q_{n+1}\|_s).
\]

Moreover, it is clear that \( \|\Omega^{-1} \delta(t)\|_{s+1} = \|\delta(t)\|_s \leq C\epsilon^{N+1}. \) Therefore, we obtain

\[
\left\| \left( \frac{\Delta q_{n+1}}{\Omega - 1} \right) \right\|_{s+1} \leq \left\| \left( \frac{\Delta q_n}{\Omega - 1} \right) \right\|_{s+1} + h \left( C\epsilon \|\Delta q_n\|_s + C\epsilon \|\Delta q_{n+1}\|_s + C\epsilon^{N+1} \right),
\]

which implies \( \|\Delta q_n\|_{s+1} + \|\Omega^{-1} \Delta p_n\|_{s+1} \leq C(1 + t_n)\epsilon^{N+1} \) for \( t_n \leq \epsilon^{-1}. \) This proves \( (45). \)

4.9 Almost invariants

According to the above analysis, we can rewrite the defect formula \( (42) \) as

\[
\frac{1}{h^2 \phi_2(h^2\omega_j^2)} F_j \xi_j k^j + \nabla_{-j}^k \mathcal{U}(\xi(t)) = d_j^k,
\]

where \( \nabla_{-j}^k \mathcal{U}(y) \) is the partial derivative with respect to \( y_{-j}^k \) of the extended potential (see, e.g., [8, 24])

\[
\mathcal{U}(\xi(t, \sigma)) = \sum_{l=-N}^N \mathcal{U}_l(\xi(t, \sigma)),
\]

\[
\mathcal{U}_l(\xi(t, \sigma)) = \sum_{m=2}^N \frac{U^{(m+1)}(0)}{(m+1)!} \sum_{k^1+\cdots+k^{m+1}=0}^l \sum_{j_1,\ldots,j_{m+1}=2}^l \int_0^1 \left( \xi_{j_1}^{k_1} \cdots \xi_{j_{m+1}}^{k_{m+1}} \right)(t, \sigma) d\sigma.
\]

Following [8], define \( S_\mu(\theta)y = (e^{i(k\mu_\theta)j}y_j)_{|j|\leq M, \|k\|\leq K} \) and \( T(\theta)y = (\xi^{j\theta}y_j)_{|j|\leq M, \|k\|\leq K}, \) where \( \mu = (\mu_\theta)_{t\geq 0} \) is an arbitrary real sequence for \( \theta \in \mathbb{R}. \)
Accoding to the results given in [8], we obtain \( \mathcal{U}(S_{\mu}(\theta)y) = \mathcal{U}(y) \) and \( \mathcal{U}_0(T(\theta)y) = \mathcal{U}_0(y) \) for \( \theta \in \mathbb{R} \). Therefore,

\[
0 = \frac{d}{d\theta} \bigg|_{\theta=0} \mathcal{U}(S_{\mu}(\theta)\xi(t, \sigma)), \quad 0 = \frac{d}{d\theta} \bigg|_{\theta=0} \mathcal{U}_0(T(\theta)\xi(t, \sigma)).
\]

(47)

**Proposition 4.10 (Two almost-invariants.)** There exist two functions \( \mathcal{J}_l[\xi, \eta](\tau) \) and \( \mathcal{K}[\xi, \eta](\tau) \) such that

\[
\sum_{l=1}^{M} \omega_l^{2s+1} \left| \frac{d}{d\tau} \mathcal{J}_l[\xi, \eta](\tau) \right| \leq C\epsilon^{N+1},
\]

\[
\left| \frac{d}{d\tau} \mathcal{K}[\xi, \eta](\tau) \right| \leq C(\epsilon^{N+1} + \epsilon^2 M^{-s+1})
\]

for \( \tau \leq 1 \). Moreover, it is true that

\[
\mathcal{J}_l[\xi, \eta](\epsilon t_n) = \hat{J}_l(q_n, p_n) + \gamma_l(t_n)\epsilon^3,
\]

\[
\mathcal{K}[\xi, \eta](\epsilon t_n) = \hat{K}(q_n, p_n) + \mathcal{O}(\epsilon^3) + \mathcal{O}(\epsilon^2 M^{-s}),
\]

where

\[
\hat{J}_l = \hat{I}_l + \hat{I}_{-l} = 2\hat{I}_l \quad \text{for} \quad 0 < l < M, \quad \hat{J}_0 = \hat{I}_0, \quad \hat{J}_M = \hat{I}_M.
\]

Here, all the constants are independent of \( \epsilon, M, h, \) and \( n \), and \( \sum_{l=0}^{M} \omega_l^{2s+1} \gamma_l(t_n) \leq C \) for \( t_n \leq \epsilon^{-1} \).

**Proof** • **Proof of (48).**

It follows from the first formula of (47) that

\[
0 = \frac{d}{d\theta} \bigg|_{\theta=0} \mathcal{U}(S_{\mu}(\theta)\xi(t, \sigma)) = \sum_{\|k\| \leq K} \sum_{|j| \leq M} i(k \cdot \mu)\xi_{-j}^{-k}(t, \sigma) \nabla_{-j}^{-k} \mathcal{U}(\xi(t, \sigma))
\]

\[
= \sum_{\|k\| \leq K} \sum_{|j| \leq M} i(k \cdot \mu)L_4^{-k}(\sigma)\xi_{-j}^{-k}\left( \frac{1}{h^2\phi_2(h^2\omega_j^2)} \tilde{f}_j^k \xi_j^k - d_j^k \right).
\]

Since the right-hand side is independent of \( \sigma \), we choose \( \sigma = 1/2 \) in the following analysis. With the above formula, we have

\[
\sum_{\|k\| \leq K} \sum_{|j| \leq M} i(k \cdot \mu)L_4^{-k}(\frac{1}{2})\xi_{-j}^{-k}\left( \frac{1}{h^2\phi_2(h^2\omega_j^2)} \tilde{f}_j^k \xi_j^k \right) = \sum_{\|k\| \leq K} \sum_{|j| \leq M} i(k \cdot \mu)L_4^{-k}(\frac{1}{2})\xi_{-j}^{-k}d_j^k.
\]

(50)

By the expansions of \( L_4^{-k}(\frac{1}{2}) \) and \( \tilde{f}_j^k \) and the “magic formulas” on p. 508 of [25], it is known that the left-hand side of (50) is a total derivative of function \( \epsilon \mathcal{J}_\mu[\xi, \eta](\tau) \).
which depends on $\xi(\tau)$, $\eta(\tau)$ and their up to $(N - 1)$th order derivatives. This means that (50) is identical to

$$-\epsilon \frac{d}{d\tau} J_\mu[\xi, \eta](\tau) = \sum_{|k| \leq K} \sum_{|j| \leq M} \frac{i}{\epsilon} (k \cdot \mu) L_4^{-k} \left( \frac{1}{2} \right) \zeta_{-j} d_j.$$

Consider the special case of $\mu = \langle l \rangle$ in what follows. By letting $z^k_j = L_4^k(1/2)\xi_j^k$ and the property of $L_4^k(1/2)$, it is easy to know that the bounds of $z^k_j$ and $\xi_j^k$ are of the same magnitude. Splitting $d = ad + bd$ into two parts: the diagonal ($k = \pm(j)$) and non-diagonal ($k \neq \pm(j)$), it is clear that

$$\left| \|ad\|_s^2 + \|\omega^{[k]}bd\|_s^2 \right| = \sum_{|k| \leq K} \|\omega^{[k]}d^k\|_0^2 \leq C e^{2N + 2},$$

where (44) is used. According to Lemma 3 of [9] and the fact that $z_j^k = \frac{\epsilon}{\omega_j^k} z_j^k + \frac{\epsilon}{\omega_j^k} \hat{a} z_j^k$ and $||\hat{a} z_j^k||_1 \leq C$, $||\Omega \hat{b} z_j^k||_1 \leq C$ from (39), one arrives at

$$\sum_{l=1}^{M} \omega_l^{2s+1} \frac{d}{d\tau} J_l[\xi, \eta](\tau) \leq \frac{1}{\epsilon} \sum_{l=1}^{M} \omega_l^{2s+1} \sum_{|k| \leq K} \sum_{j=-\infty}^{\infty} \left| \zeta_j^k d_j^k \right|$$

$$\leq \frac{1}{\epsilon} \left( \sum_{|k| \leq K} \|\omega^{[k]}bd\|_s^2 \right)^{1/2} \left( \sum_{|k| \leq K} \left( \sum_{|l| \leq K} \|\omega^{[l]}(1 + |k \cdot \omega|) \|\hat{a} \zeta_j^k\|_0^2 \right)^{1/2} \right).$$

The first statement of (48) is proved.

With the second formula of (47) and in a similar way, one gets

$$\sum_{|k| \leq K} \sum_{|j| \leq M} \frac{i}{\epsilon} (k \cdot \mu) L_4^{-k} \left( \frac{1}{2} \right) \zeta_{-j} \frac{1}{h^2 \phi_2(h^2 \omega_j^k)} \tilde{L}_j^k.$$

$$= \sum_{|k| \leq K} \sum_{|j| \leq M} \frac{i}{\epsilon} (k \cdot \mu) L_4^{-k} \left( \frac{1}{2} \right) \zeta_{-j} \left( d_j^k - \sum_{l \neq 0} \nabla_{-j}^k (U_l(\xi(t, \sigma))) \right).$$

(51)

A careful observation shows that the left-hand side of (51) can be written as a total derivative of function $\epsilon \hat{K}[\xi, \eta](\tau)$, which yields

$$-\epsilon \frac{d}{d\tau} \hat{K}[\xi, \eta](\tau) = \sum_{|k| \leq K} \sum_{|j| \leq M} \frac{i}{\epsilon} (k \cdot \mu) L_4^{-k} \left( \frac{1}{2} \right) \zeta_{-j} \left( d_j^k - \sum_{l \neq 0} \nabla_{-j}^k (U_l(\xi(t, \sigma))) \right).$$

(52)
For the first expression in the right-hand side of this formula, it follows from the Cauchy–Schwarz inequality and the bound \( |j| \leq \omega_j \) that

\[
\left| \sum_{\|k\| \leq K} \sum'_{|j| \leq K} i j z_{-j}^{-k} d_j^k \right| \leq \left( \sum_{\|k\| \leq K} \sum'_{|j| \leq K} \omega_j^2 \left| z_j^k \right|^2 \right)^{1/2} \left( \sum_{\|k\| \leq K} \sum'_{|j| \leq K} \left| d_j^k \right|^2 \right)^{1/2} \leq C \varepsilon
\]

\[
\leq C \varepsilon \left( \sum_{\|k\| \leq K} \sum'_{|j| \leq K} \frac{\omega_j^2}{\varepsilon} \frac{\varepsilon}{[|k|]} \left| z_j^k \right|^2 \right)^{1/2} \left( \sum_{\|k\| \leq K} \sum'_{|j| \leq K} \left| d_j^k \right|^2 \right)^{1/2} \leq C \varepsilon^{N + 2}.
\]

The remaining expression of (52) contains the form of

\[
\sum_{\|k\| \leq K} \sum'_{|j| \leq K} i j z_j^{-k} \nabla_j^{-k} U_{ij}(\xi(t, \sigma))
\]

\[
= \sum_{m=2}^{N} \frac{U^{(m+1)}(0)}{m!} \sum_{k_1 + \ldots + k_{m+1} = k} \sum' z_{j_1}^{k_1} \ldots z_{j_m}^{k_m} i j_{m+1} z_{j_{m+1}}^{k_{m+1}},
\]

which is the 2\(M\)th Fourier coefficient of the function (see [24])

\[
w(x) := \sum_{m=2}^{N} \frac{U^{(m+1)}(0)}{m!} \sum_{k_1 + \ldots + k_{m+1} = k} \mathcal{P}_z^{k_1}(x) \ldots \mathcal{P}_z^{k_m}(x) \cdot \frac{d}{dx} \mathcal{P}_z x^{k_{m+1}}(x).
\]

As shown in the proof of Theorem 5.2 of [24], it can be confirmed that \( \|w\|_{L^1} \leq C \varepsilon^3 \), and the 2\(M\)th Fourier coefficient of \( w \) is bounded by \( C \varepsilon^3 \omega_j^{2 + 1} \leq C \varepsilon^3 (2M)^{-s+1} \). In this way, the second statement of (48) is obtained by (52).

**Proof of (49).**

In what follows, only the second statement of (49) is proved since the first one can be obtained in a similar way.

By the scheme of AAVF method, it is obtained that

\[
2h \text{sinc}(h \Omega) \tilde{p}(t) = \tilde{q}(t + h) - \tilde{q}(t - h) + \mathcal{O}(h^2),
\]

which gives \( \tilde{p}_j(t) = i \omega_j (\eta_j^{(j)}(\varepsilon t) e^{i \omega_j t} - \eta_j^{-(j)}(\varepsilon t) e^{-i \omega_j t}) + \mathcal{O}(h^2 \varepsilon^2) + \mathcal{O}(h^3 \varepsilon^2) \). Therefore, it is true that \( \tilde{\zeta}_j^{(j)} = \frac{1}{2} (\tilde{q}_j + \frac{1}{i \omega_j} \tilde{p}_j) + \mathcal{O}(\varepsilon^2) \) and \( \tilde{\zeta}_j^{-(j)} = \frac{1}{2} (\tilde{q}_j - \frac{1}{i \omega_j} \tilde{p}_j) + \mathcal{O}(\varepsilon^2) \). With these results, the construction of \( K \) is given below:

\[
K[\xi, \eta](\tau) = \sum_{|j| \leq M} j \frac{4 e h \sin(\frac{1}{2} h \omega_j) \cos(\frac{1}{2} h \omega_j)}{2 h^2 \phi_2(h^2 \omega_j^2)} \left( |\zeta_j^{(j)}|^2 - |\zeta_j^{-(j)}|^2 \right) + \mathcal{O}(\varepsilon^3)
\]

\[
= \sum_{|j| \leq M} j \omega_j \frac{\cos(\frac{1}{2} h \omega_j)}{\text{sinc}(\frac{1}{2} h \omega_j)} \left( |\zeta_j^{(j)}|^2 - |\zeta_j^{-(j)}|^2 \right) + \mathcal{O}(\varepsilon^3)
\]
Long-time behaviour of energy-preserving methods for wave equations

\[
\sum_{|j| \leq M} \frac{j \omega_j}{4} \cos \left( \frac{1}{2} h \omega_j \right) \left( |\tilde{q}_j + \frac{1}{i \omega_j} \tilde{p}_j|^2 - |\tilde{q}_j - \frac{1}{i \omega_j} \tilde{p}_j|^2 \right) + O(\epsilon^3)
\]

\[
\frac{1}{4} \left( \frac{j \omega_j}{\sin(\frac{1}{2} h \omega_j)} \right) \frac{1}{i \omega_j} \tilde{q}_j - \frac{1}{i \omega_j} \tilde{p}_j + O(\epsilon^3)
\]

\[
= \tilde{K}(\tilde{q}, \tilde{p}) + O(\epsilon^3) + O(\epsilon^2 M^{-s}) = \tilde{K}(q_n, p_n) + O(\epsilon^3) + O(\epsilon^2 M^{-s}),
\]

where the results (45) and (37) are used.

4.10 From short to long time intervals

It is noted that with the analysis presented in this paper, the statement of Theorem 3.2 can be proved by patching together many intervals of length \(\epsilon^{-1}\) in the same way as that used in [8, 9].

5 Analysis for the AAVF method with a quadrature rule

It is noted that the above analysis is done for the AAVF method with the integral appearing in (5), which usually cannot be solved exactly and a quadrature rule is needed. For this case, we will show that the main result for the AAVF method with the integral is still true for the AAVF method with some quadrature rule.

As example, let us consider the following AAVF method with the midpoint rule

\[
\begin{aligned}
q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)p_n + h^2\phi_2(V)f((q_n + q_{n+1})/2), \\
p_{n+1} &= -h\Omega^2\phi_1(V)q_n + \phi_0(V)p_n + h\phi_1(V)f((q_n + q_{n+1})/2).
\end{aligned}
\]

(53)

For this method, the main result given in Theorem 3.2 is still true. The proof follows the same way given in previous sections but with some modifications for the operator and the non-linearity. In what follows, we just present the main differences and omit the details for brevity.

- Modifications for Section 4.2.
  Since the term \(\int_0^1 f((1 - \sigma)q_n + \sigma q_{n+1})d\sigma\) is replaced by \(f((q_n + q_{n+1})/2)\), the function \(\xi_k^j(\epsilon(t + \frac{h}{2}), \sigma)\) should be changed to \(\xi^k(\epsilon(t + \frac{h}{2}), 1/2)\) and the operator \(L_4^k(\sigma)\) is replaced by \(L_4^k(1/2)\). Then, all the analysis and results in Section 4.2 still hold for (53).

- Modifications for Section 4.3.
  For this part, we only need to change \(\int_0^1 [\xi_1^k \cdots \xi_m^k](t\epsilon, \sigma) d\sigma\) to \(\xi_1^k \cdots \xi_m^k(t\epsilon, 1/2)\).

- Modifications for Section 4.4.
  One part of the function \(f_k^j(c\xi(\tau))\) here is \(c\xi_1^k \cdots \xi_m^k(\tau, 1/2)\) instead of \(\int_0^1 (c\xi_1^k \cdots \xi_m^k)(\tau, \sigma) d\sigma\) and then the property of \(f_k^j(c\xi(\tau))\) given in Proposition 4.4 is still true.

- Modifications for Section 4.7.
Since the defect expressed by (41) needs to be modified according to the scheme (53), the term \( \int_0^1 \left[ (\xi_{j1}^{k_1} \cdots \xi_{jm}^{k_m}) (t \epsilon, \sigma) \right] d\sigma \) appearing in (42) should be replaced by \( (\xi_{j1}^{k_1} \cdots \xi_{jm}^{k_m}) (t \epsilon, 1/2) \). For this situation, we still obtain the same bounds of the defects as before.

– Modifications for Section 4.8.

Here, only the expression of \( \Delta f \) should be modified in the light of (53).

– Modifications for Section 4.9.

A new function \( U_l(\xi) = \sum_{m=2}^{N} \frac{U^{(m+1)}(0)}{(m+1)!} \sum_{k_1+\cdots+k_{m+1}=0}^{M} \sum_{j_1+\cdots+j_{m+1}=2M} (\xi_{j1}^{k_1} \cdots \xi_{jm+1}^{k_{m+1}})(t, 1/2) \) will be used here instead of the previous one.

As the last part of this section, we note that since the AAVF method with the integral is only of order two, the long-time momentum and action behaviour do not change for (53). For the AAVF method with other quadrature rules, the main result can also be obtained by following the same way.

6 Conclusions

In this paper, we have shown the long-time behaviour of the AAVF method when applied to semi-linear wave equations via spatial spectral semi-discretisations. This method can exactly preserve the energy in the semi-discretisation and has a near-conservation of modified actions and modified momentum over long terms. The main result is proved by developing modulated Fourier expansion of the AAVF method and showing two almost-invariants of the modulation system.

The main result of this paper explains rigorously the good long-time behaviour of EP methods in the numerical treatment of semi-linear wave equations. The analysis for multi-dimensional wave equations will be considered. It is also noted that long-term analysis of many different methods except EP methods has been given recently for Schrödinger equations and the reader is referred to \([7, 12, 15, 16]\). Our another work will be devoted to the long-term analysis of energy-preserving methods for solving Schrödinger equations. We are hopeful of obtaining near-conservation of actions, momentum and density as well as exact-conservation of energy for some EP methods when applied to Schrödinger equations.

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