LARGE-STEPSIZE INTEGRATORS WITH OPTIMAL UNIFORM ACCURACY AND LONG TIME CONSERVATION FOR HIGHLY OSCILLATORY SECOND-ORDER DIFFERENTIAL EQUATIONS

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ABSTRACT. In this paper, we are concerned with large-stepsize highly accurate integrators for highly oscillatory second-order differential equations \( \ddot{q}(t) + \frac{1}{\varepsilon^2} A q(t) = \frac{1}{\varepsilon^2} F(q(t)) \) with large initial data, a scaling parameter \( 0 < \varepsilon \ll 1 \) and \( m = 0, 1 \). The highly oscillatory property of this model problem corresponds to the parameter \( \varepsilon \). We propose and analyze a novel class of highly accurate integrators which is based on some formulation approaches to the problem, Fourier pseudo-spectral method and exponential integrators. Two practical integrators up to order four are constructed by using the proposed symmetric property and stiff order conditions of implicit exponential integrators. The convergence of the obtained integrators is rigorously studied, and it is shown that the accuracy is improved to be \( \mathcal{O}(\varepsilon^{-r} r^h h^r) \) in the absolute position error for the time stepsize \( h \) and the order \( r \) of the integrator. The near energy conservation over long times is established for the multi-stage integrators by using modulated Fourier expansions. These theoretical results are achievable even if large stepsizes are utilized in the schemes. Numerical results on the Duffing equation and a nonlinear relativistic Klein–Gordon equation show that the proposed integrators with large stepsizes have optimal uniformly high accuracy, excellent long time energy conservation and competitive efficiency.

KEYWORDS: Large-stepsize integrators, Highly oscillatory problem, Highly accurate methods, Long time energy conservation, modulated Fourier expansion

AMS Subject Classification: 65L05, 65P10, 65L20, 65L70.

1. Introduction

A large amount of dynamics can be described by the following highly oscillatory second-order differential equations

\[
\ddot{q}(t) + \frac{1}{\varepsilon^2} A q(t) = \frac{1}{\varepsilon^2} F(q(t)), \quad q(0) = \psi_1, \quad \dot{q}(0) = \frac{\psi_2}{\varepsilon}, \quad t \in [0, T],
\]

where \( q(t) : \mathbb{R} \to X \) represents the position living in a finite dimensional space or some functional (Hilbert) space \( X \), \( A \) is a positive definite operator on \( X \), \( 0 < \varepsilon \ll 1 \) is a dimensionless parameter, \( \psi_1 \) and \( \psi_2 \) are initial values independent of \( \varepsilon \), and \( F(q(t)) \) is a given nonlinear function. In this paper, we consider two cases of \( m: m = 0 \) or \( 1 \), which correspond to different kinds of problems arising in practical applications. Clearly, the solution of (1.1) becomes highly oscillatory when large frequencies are involved in the equation, which corresponds to the parameter \( 0 < \varepsilon \ll 1 \). Its computation represents major challenges because of this high oscillation.

This model often arises in a variety of fields such as applied mathematics, quantum physics, classical mechanics, engineering, chemistry, molecular biology and so on. For the system (1.1) with \( m = 0 \), some classical examples could be the Duffing equation, Fermi-Pasta-Ulam problem, Hénon-Heiles model, and molecular dynamics [7, 22, 26, 32, 34]. When \( m = 1 \), a well-known example is the nonlinear relativistic Klein–Gordon (NRKG) equation (11) [1, 4, 5, 10, 33]

\[
\partial_t u(x,t)u(x,t) + \frac{1}{i\varepsilon}(1 - \varepsilon \Delta) u(x,t) = \frac{1}{\varepsilon^2} \lambda |u(x,t)|^p u(x,t), \quad x \in \Omega^d, \quad t > 0, \\
\partial_t u(x,0) = \phi(x), \quad u_t(x,0) = \frac{i}{\varepsilon} \gamma(x),
\]

where \( \Omega = (-L, L), \) is time, \( x \in \Omega^d \) is the spatial coordinate, \( u(x, t) \) is a complex-valued scalar field, \( 0 < \varepsilon \ll 1 \) is a dimensionless parameter inversely proportional to the speed of light, \( \lambda \in \mathbb{R} \) is a given dimensionless parameter (positive and negative for defocusing and focusing self-interaction, respectively), and \( \phi \) and \( \gamma \) are given complex-valued \( \varepsilon \)-independent initial data. It is clear that the NRKG equation (1.2) fits the scheme (1.1) with \( m = 1 \).
If we further assume that $A$ is symmetric and $F(q) = -\nabla U(q)$ with a smooth potential $U$, the model \((1.1)\) is a Hamiltonian system with the following Hamiltonian function \([17]\):

$$H(q, p) = \frac{1}{2} \langle p, p \rangle_Y + \frac{1}{2\varepsilon} \langle q, Aq \rangle_X + \frac{1}{\varepsilon m} U(q),$$

where $p := \dot{q} : \mathbb{R} \to Y$ and $\langle \cdot, \cdot \rangle_X$ or $Y$ denotes the inner product on $X$ or $Y$. This energy is conserved along the exact solution of \((1.1)\). It is noted that the scales of $\psi_1, \psi_2$ will lead to different properties of the system. In this paper, we consider the following scale of $\psi_1, \psi_2$:

$$\text{large initial data: } \psi_1 = O(1), \quad \psi_2 = O(1) \rightarrow \text{energy unbounded system} \quad (1.1). \quad (1.3)$$

Although this type of system can be transformed into energy bounded case by using a scaling to the variables, the large initial data case has more essential differences such as the stronger oscillation feature and this makes the construction and analysis of numerical methods be more difficult and challenging \([43]\). We should note that all the methods and analysis presented in this paper are applicable to energy bounded system \((1.1)\) where a small $\psi_2$ is chosen as $\psi_2 = O(\varepsilon)$.

The time integration of such equation \((1.1)\) is a basic algorithmic task and it has been received much attention in recent decades. Due to the high oscillations, the traditional methods such as symplectic/symmetric Runge–Kutta–Nyström (RKN) methods \([18, 35]\) or energy-preserving Runge-Kutta methods \([6, 37]\) often result in convergence problems. In order to get more competitive methods, Gaußschi-type trigonometric integrators were developed in \([29]\) and different kinds of trigonometric integrators were formulated and studied in \([19, 20, 24, 25, 38, 32]\). However, for these integrators, they at most have uniform second order accuracy in the absolute position error w.r.t. $\varepsilon$ and only have uniform first order accuracy in velocity error \([24]\) for $m = 0$. As a result, it is challenging to get trigonometric integrators with uniform higher-order accuracy.

Recently, some new methods with uniform accuracy (w.r.t $\varepsilon$) for highly oscillatory systems have been proposed and analysed such as two-scale formulation methods \([10, 11]\), uniformly accurate exponential-type integrators \([5]\), nested Picard iterative integrators \([9]\), multiscale time integrators \([2, 3, 4, 5, 9, 10, 11, 12, 13, 14, 33, 41]\) and uniformly accurate methods with averaging \([13, 14]\). In \([4]\), various uniformly accurate (UA) methods have been compared systematically for solving the NRKG equation \((1.2)\). Recently, time-splitting methods were proved to have improved uniform error bounds for solving nonlinear Klein–Gordon equation with weak nonlinearity \([1]\). Most of these uniformly accurate methods can be applied to the system \((1.1)\) and they have excellent uniform accuracy in both position and velocity. Unfortunately, most of them do not have good long time conservation behaviour when applied to conservative systems. More precisely, if a UA method is considered as the approximation of \((1.1)\), the numerical energy error will increase as time evolves. In a recent work \([13]\), the UA method named as pullback method is shown to hold the long time conservation by the numerical results but without rigorous analysis. In a more recent work \([11]\), the authors succeed in making the two-scale method with near conservation laws for first-order systems. However, only one-stage type methods of order two are presented there and the equation \((1.1)\) does not share the form of the system considered in \([41]\), which means that the analysis of \((1.1)\) is no longer applicable for the system \((1.1)\) of this paper. Moreover, the second-order differential equation \((1.1)\) has its special structure which will be neglected if we rewrite it as a general highly oscillatory first-order differential equation $\dot{u}(t) = \frac{1}{\varepsilon} Ku(t) + g(u(t))$. Therefore, it is necessary and meaningful to design and analyze UA methods with uniform high order and good long time energy conservation for solving the second-order system \((1.1)\). It is worth pointing out that the integrators derived in this paper will be shown to have long time conservation and better accuracy than uniform accuracy when $m = 0$ in \((1.1)\), which is $O(\varepsilon^r h^r)$ for the time stepsize $h$ and the order $r$ of the integrator. This optimal uniformly high accuracy is different from the existing UA methods \([2, 3, 4, 5, 9, 10, 11, 12, 13, 14, 33, 41]\) and seems surprising at the first glance of \((1.1)\) due to the $O(1/\varepsilon^2)$ commutator.

In this paper we are interested in using numerical integrators with time stepsize $h$ that are much larger than the $\varepsilon$ of the system to obtain optimal uniform accuracy and good long-time energy conservation when solving \((1.1)\). To obtain the integrators with optimal uniform accuracy, we take advantage of two-scale formulation approach, spectral semi-discretisation and exponential
integrators with more than one stage. However, this brings some challenges and difficulties in the achievement and analysis of long time energy conservation. a) The two-scale formulation approach results in a new system which has a completely different linear part and nonlinear function in comparison with the original problem (1.1). This brings more difficulties in the proof of energy conservation of the original problem (1.1). b) Long term analysis of high-order splitting integrators for Schrödinger equations was discussed in [21] and it was shown that these high-order integrators have the same long-time behaviour as the low-order splitting, which is somewhat unreasonable for high order methods. One open question that whether high-order methods behave better than low-order methods was proposed in [21]. To achieve high order optimal uniform accuracy and good long time behaviour, two-stage and three-stage exponential integrators are chosen in this paper. Unfortunately, however, for a method with more than one stage applied to highly oscillatory systems, long time analysis has not been done for any method so far. As pointed out in [15], there is the technical difficulty coming from the identification of invariants in the corresponding modulation system. Thus, it remains a challenge to study long time behaviour for a method with more than one stage. c) The third challenge comes from the diversity of (1.1) considered in this paper. Large initial data case (1.3) usually leads to large bounds of the coefficient functions in the modulated Fourier expansion, which prevents the derivation of the long time conservation.

To overcome these difficulties and make the analysis go smoothly, a novel approach to the design of integrators is established. The main contributions of this paper are as follows.

a) We consider three transformations of the original system and use symmetric exponential integrators which satisfy the derived stiff order conditions. The transformations of the system and stiff order conditions proposed in this paper can keep the optimal uniform accuracy, and the symmetry yields good long time energy conservation. It will be shown that these both important properties can be hold for the integrators used with large time stepsizes, which is very effective and efficient in scientific computing over long times.

b) Compared with the existing UA methods, the accuracy of our \( r \)-th order integrators is improved to be \( O(\varepsilon^r h^r) \) for solving (1.1) with \( m = 0 \) and as \( \varepsilon \) decreases, the integrators are more accurate. This optimal uniformly high accuracy is very competitive in the numerical computation of highly oscillatory systems where \( \varepsilon \ll 1 \).

c) Moreover, we should note that we managed to derive the long-time energy conservation for the two-stage and three-stage methods applied to the large initial value system (1.3), which is different form the existing long term analysis work [15, 16, 17, 23, 25, 27, 29, 41], where only one-stage type methods and small initial value are both necessary. The long time analysis presented in this paper provides an extension of the powerful technique named as modulated Fourier expansion [15, 17, 23, 25, 27] to multi-stage methods and with such extension it is believed that more numerical methods with complicated scheme can be studied.

The rest of this paper is organized as follows. In Section 2, we firstly present the formulation process of the integrators, and then we construct two practical integrators by using the proposed symmetry and stiff order conditions. The main results concerning the optimal uniformly high accuracy and near energy conservation are given in Section 3 and some applications to the Duffing equation and nonlinear relativistic Klein–Gordon equation are made to show these two properties. The optimal uniformly high accuracy is proved in Section 4 and the long-time analysis of energy conservation is drawn in Section 5. The last section includes the conclusions of this paper.

2. Formulation of the numerical integrators

2.1. The construction process of integrators. In the formulation of the numerical scheme, we first make some transformations of the system and then consider the numerical integration. There are in all three steps in the process and we present them one by one.

Step 1. Three transformations of the system. Firstly, since the operator \( A \) is symmetric and positive definite, there exist a unitary operator \( P \) and an invertible diagonal operator \( \Lambda \) such that \( A = P \Lambda^2 P^\dagger \). Then letting \( y = P^\dagger q \) transforms the original system (1.1) into

\[
\ddot{y}(t) + \frac{1}{\varepsilon} \Lambda^2 y(t) = f(y(t)), \quad y(0) = P^\dagger \psi_1, \quad \dot{y}(0) = P^\dagger \dot{\psi}_1, \quad t \in [0, T], \tag{2.1}
\]
where \( f(y) = -\nabla_y U(Py) \). This is still a conservative system and its energy is given by

\[
H_1(y, \dot{y}) = \frac{1}{2} (\dot{y}, \dot{y})_Y + \frac{1}{2\varepsilon^2} (y, \Lambda^2 y)_X + \frac{1}{\varepsilon^m} U(Py).
\]

By using a scaling to the variables \( \dot{\mathbf{q}} = y(t) \) and \( \mathbf{p}(t) = \varepsilon \dot{y}(t) \), a new system is obtained immediately

\[
\dot{\mathbf{q}}(t) = \frac{1}{\varepsilon} \mathbf{p}(t), \quad \dot{\mathbf{p}}(t) = -\Lambda^2 \mathbf{q} + \frac{1}{\varepsilon^{m-1}} f(\mathbf{q}(t)), \quad \mathbf{q}(0) = P^H \psi_1, \quad \mathbf{p}(0) = P^H \psi_2.
\]

(2.2)

It can be verified that the solution of this system conserves the following energy

\[
\mathbf{H}(\mathbf{q}, \mathbf{p}) := \frac{1}{2\varepsilon^2} (\mathbf{p}, \mathbf{p})_Y + \frac{1}{2\varepsilon^2} (\mathbf{q}, \Lambda^2 \mathbf{q})_X + \frac{1}{\varepsilon^m} U(P\dot{\mathbf{q}}).
\]

Then letting

\[
\dot{\mathbf{q}}(t) = \cos(t\Lambda/\varepsilon)x(t) + \Lambda^{-1}\sin(t\Lambda/\varepsilon)v(t), \quad \mathbf{p}(t) = -\Lambda \sin(t\Lambda/\varepsilon)x(t) + \cos(t\Lambda/\varepsilon)v(t),
\]

we obtain

\[
\dot{x}(t) = -\varepsilon^{1-m} \Lambda^{-1} \sin(t\Lambda/\varepsilon)f\left(\cos(t\Lambda/\varepsilon)x(t) + \Lambda^{-1} \sin(t\Lambda/\varepsilon)v(t)\right), \quad x(0) = P^H \psi_1,
\]

\[
\dot{v}(t) = \varepsilon^{1-m} \cos(t\Lambda/\varepsilon)f\left(\cos(t\Lambda/\varepsilon)x(t) + \Lambda^{-1} \sin(t\Lambda/\varepsilon)v(t)\right), \quad v(0) = P^H \psi_2.
\]

(2.3)

**Remark 2.1.** Without loss of generality, it is assumed in this paper that the propagators \( \sin(t\Lambda/\varepsilon) \) and \( \cos(t\Lambda/\varepsilon) \) are \( 2\pi \)-periodic. If this is not true, the equation (2.1) can be transformed into this case by decomposing a leading part from \( \Lambda \). More precisely, with the help of the asymptotical expansion \( \Pi \) or the Diophantine approximation \( \Pi \), the \( \Lambda \) can be reformulated as \( \Lambda = \Lambda_0 + \mathcal{O}(\varepsilon) \) with a new \( \Lambda_0 \) whose eigenvalues are integer-multiples of a mono-frequency. Then the equation (2.1) becomes

\[
\dot{\mathbf{q}}(t) + \frac{1}{\varepsilon^2} \Lambda_0^2 g(t) = \bar{f}(y(t)) := \frac{1}{\varepsilon^m} f(y(t)) + \frac{\Lambda_0^2 - \Lambda^2}{\varepsilon^2} g(t),
\]

and both the numerical scheme and analysis of this paper are applicable to this new system.

**Step 2. Two-scale formulation.** By isolating the fast time variable \( t/\varepsilon \) as another variable \( \tau \) and denoting \( X(t, t/\varepsilon) = x(t), \ V(t, t/\varepsilon) = v(t) \), the two-scale pattern of (2.3) can be formulated as follows:

\[
\partial_t X(t, \tau) + \frac{1}{\varepsilon} \partial_\tau X(t, \tau) = -\varepsilon^{1-m} \Lambda^{-1} \sin(\tau \Lambda) F(\cos(\tau \Lambda) X(t, \tau) + \Lambda^{-1} \sin(\tau \Lambda) V(t, \tau)),
\]

\[
\partial_t V(t, \tau) + \frac{1}{\varepsilon} \partial_\tau V(t, \tau) = \varepsilon^{1-m} \cos(\tau \Lambda) F(\cos(\tau \Lambda) X(t, \tau) + \Lambda^{-1} \sin(\tau \Lambda) V(t, \tau)), \quad t > 0, \ \tau \in \mathbb{T},
\]

(2.4)

where \( X(t, \tau) \) and \( V(t, \tau) \) are the unknowns which are periodic in \( \tau \) on the torus \( \mathbb{T} = (0, 2\pi) \). It is noted that this new variable \( \tau \) offers a free degree for designing the initial dates \( X(0, \tau) \) and \( V(0, \tau) \). This two-scale equation (2.4) with a modified initial data is analysed in [10] [14] to construct uniformly accurate methods. We here use the strategy from [10] [14] to obtain the fourth-order initial data for (2.4), which is presented briefly as follows.

For some periodic \( v(\cdot) \) on \( \mathbb{T} \), we introduce the notations

\[
L := \partial_\tau, \quad \Pi v := \frac{1}{2\pi} \int_0^{2\pi} v(\tau) d\tau, \quad A := L^{-1}(I - \Pi).
\]

It is obvious that

\[
L^{-1} v = (I - \Pi) \int_0^{\tau} v(\theta) d\theta, \quad L\Pi = 0, \quad \Pi^2 = \Pi,
\]

\[
\Pi L v = \frac{1}{2\pi} \int_0^{2\pi} \partial_\tau v d\tau = \frac{1}{2\pi} (v(2\pi) - v(0)) = 0,
\]

\[
\Pi A = \Pi L^{-1}(I - \Pi) = \Pi(I - \Pi) \int_0^{\tau} v(\theta) d\theta (I - \Pi) = 0,
\]

\[
LA = I - \Pi, \quad LA^2 = (I - \Pi)A = A - \Pi A = A.
\]

(2.5)
Let \( U(t, \tau) = [X(t, \tau); V(t, \tau)] \) and
\[
\begin{bmatrix}
-\varepsilon^{-1-m} \Lambda^{-1} \sin(\tau \Lambda) F(\cos(\tau \Lambda) X(t, \tau) + \Lambda^{-1} \sin(\tau \Lambda) V(t, \tau)) \\
\varepsilon^{-1-m} \sin(\tau \Lambda) F(\cos(\tau \Lambda) X(t, \tau) + \Lambda^{-1} \sin(\tau \Lambda) V(t, \tau))
\end{bmatrix} := \varepsilon^{-1-m} g_\tau(U(t, \tau)).
\]
Based on the Chapman-Enskog expansion \(^{(13\ 14)}\), the solution \( U(t, \tau) \) can be formulated as
\[
U(t, \tau) = \hat{U}(t) + \kappa(t, \tau) \quad \text{with} \quad \hat{U}(t) = \Pi U(t, \tau), \quad \Pi \kappa(t, \tau) = 0.
\]
From the fact \( \partial_t U(t, \tau) + \frac{1}{\varepsilon} \partial_\tau U(t, \tau) = f_\tau(U(t, \tau)) \), it follows that
\[
\dot{U}(t) = \Pi f_\tau(\hat{U}(t) + \kappa(t, \tau)).
\]
Then the correction \( \kappa \) satisfies the differential equation
\[
\partial_t \kappa(t, \tau) + \frac{1}{\varepsilon} \partial_\kappa(t, \tau) = (I - \Pi) f_\tau(\dot{U}(t) + \kappa(t, \tau)),
\]
which can be reformulated as
\[
\kappa(t, \tau) = \varepsilon A f_\tau(\hat{U}(t) + \kappa(t, \tau)) - \varepsilon L^{-1}(\partial_t \kappa(t, \tau)). \tag{2.6}
\]
We seek an expansion in powers of \( \varepsilon \) for the compositor \( \kappa \):
\[
\kappa(t, \tau) = \varepsilon \kappa_1(t, \hat{U}(t)) + \varepsilon^2 \kappa_2(t, \hat{U}(t)) + \varepsilon^3 \kappa_3(t, \hat{U}(t)) + \mathcal{O}(\varepsilon^4). \tag{2.7}
\]
Inserting (2.7) into (2.6) and using the Taylor series of \( f_\tau \) at \( \hat{U} \) yield (we omit \( \hat{U}(t) \) for conciseness)
\[
\begin{align*}
\varepsilon \kappa_1 + \varepsilon^2 \kappa_2 + \varepsilon^3 \kappa_3 + \mathcal{O}(\varepsilon^4) &= \varepsilon A f_\tau(\hat{U}) + \varepsilon A \partial_\tau f_\tau(\hat{U})(\varepsilon \kappa_1 + \varepsilon^2 \kappa_2) + \frac{1}{2} \varepsilon A \partial^2_\tau f_\tau(\hat{U})(\varepsilon \kappa_1, \varepsilon \kappa_1) - \varepsilon L^{-1}(\varepsilon \partial_t \kappa_1 + \varepsilon^2 \partial_t \kappa_2) + \mathcal{O}(\varepsilon^4).
\end{align*}
\]
By comparing the coefficients of \( \varepsilon^j \) with \( j = 1, 2, 3 \), one gets
\[
\begin{align*}
\kappa_1 &= A f_\tau(\hat{U}), \\
\kappa_2 &= A \partial_\tau f_\tau(\hat{U}) A f_\tau(\hat{U}) - L^{-1}(\partial_t \kappa_1), \\
\kappa_3 &= A \partial^2_\tau f_\tau(\hat{U}) (\kappa_1, \kappa_1) - L^{-1}(\partial_t \kappa_2). \tag{2.8}
\end{align*}
\]
We further compute
\[
\begin{align*}
\partial_t \kappa_1 &= A \partial_t f_\tau(\hat{U}) = A \partial_\tau f_\tau(\hat{U}) \dot{U} = A \partial_\tau f_\tau(\hat{U}) \Pi f_\tau(\hat{U}), \\
\partial_t \kappa_2 &= A \partial^2_\tau f_\tau(\hat{U})(\Pi f_\tau(\hat{U}), A f_\tau(\hat{U})) + A \partial_\tau f_\tau(\hat{U}) A \partial_\tau f_\tau(\hat{U}) (\Pi f_\tau(\hat{U}), f_\tau(\hat{U})) - A^2 \partial^2_\tau f_\tau(\hat{U})(\Pi f_\tau(\hat{U}), f_\tau(\hat{U})) - A^2 \partial_\tau f_\tau(\hat{U}) (\Pi f_\tau(\hat{U}), f_\tau(\hat{U})) - A^2 \partial_\tau f_\tau(\hat{U}) (\Pi f_\tau(\hat{U}), f_\tau(\hat{U})),
\end{align*}
\]
and then (2.8) becomes
\[
\begin{align*}
\kappa_1(t, \hat{U}) &= A f_\tau(\hat{U}), \\
\kappa_2(t, \hat{U}) &= A \partial_\tau f_\tau(\hat{U}) A f_\tau(\hat{U}) - A^2 \partial_\tau f_\tau(\hat{U}) (\Pi f_\tau(\hat{U}), f_\tau(\hat{U})), \\
\kappa_3(t, \hat{U}) &= A \partial^2_\tau f_\tau(\hat{U})(\Pi f_\tau(\hat{U}), f_\tau(\hat{U})) - A^2 \partial^2_\tau f_\tau(\hat{U})(\Pi f_\tau(\hat{U}), f_\tau(\hat{U})) + A^2 \partial_\tau f_\tau(\hat{U}) (\Pi f_\tau(\hat{U}), f_\tau(\hat{U})), \tag{2.9}
\end{align*}
\]
Here we have used the results \( U = \hat{U} + \mathcal{O}(\varepsilon) \) and \( f_\tau(U) = f_\tau(\hat{U}) + \varepsilon \partial_\tau f_\tau(\hat{U}) \kappa_1 + \mathcal{O}(\varepsilon^2) \), and removed the term \( -\varepsilon A^2 \partial_\tau f_\tau(\hat{U})(\Pi f_\tau(\hat{U}), f_\tau(\hat{U})) \) from \( \kappa_2 \) to \( \kappa_3 \). With these preparations, consider the following initial condition
\[
U_0(\tau) := U^{[0]} + \varepsilon \kappa_1(\tau, U^{[0]}) + \varepsilon^2 \kappa_2(\tau, U^{[0]}) + \varepsilon^3 \kappa_3(\tau, U^{[0]}), \tag{2.10}
\]
where \( U^{[0]} := [P^H \psi_1; P^H \psi_2] \) and \( \kappa_1, \kappa_2, \kappa_3 \) are defined by (2.9). For the two-scale system (2.4) with this initial data, the following estimate of the solution is obtained.
Proposition 2.2. For all $\alpha \in \{0, 1\}$ and $\beta \in \{0, 1, \ldots, 4\}$ and for the function $g_r(U)$, it is assumed that the functional $\partial^\alpha \partial^\beta g_r(U)$ is continuous and locally bounded w.r.t. $\varepsilon$ from $T \times H^s$ to $L(H^s \times \cdots \times H^s, H^{s-2\alpha})$, where $s \geq \sigma > 2\alpha + d$. Moreover, suppose that $U_0^{[0]} \in H^{s+2}$ and is uniformly bounded w.r.t. $\varepsilon$. Then for $\mu = 1, 2, \ldots, 4$ and $\forall \tau \in T$, there exists a constant $C > 0$ independent of $\varepsilon$ such that the unique solution of the two-scale system (2.4) with the initial condition (2.10) satisfies the following estimates

$$
\|U(t, \tau)\|_{L^\infty(H^s)} \leq C, \quad \|\partial^\alpha \partial^\beta U(t, \tau)\|_{L^\infty(H^{s-2\alpha})} \leq C\varepsilon^{\mu-\mu_m}.
$$

Proof. This proof will be presented in Section 4 as the first part of convergence analysis.

Step 3. Fully discrete scheme. We now present the fully discrete scheme for (2.4) which is constructed by making use of the spectral semi-discretisation (see [36]) in $\tau$ and exponential integrators (see [31]) in time.

For the spectral semi-discretisation used in $\tau$, let $\mathcal{M} := \{-N_\tau/2, -N_\tau/2 + 1, \ldots, N_\tau/2\}$ with a positive integer $N_\tau > 1$ and $Y_M = \text{span}\{e^{ik\tau}, \ k \in \mathcal{M}, \ \tau \in [-\pi, \pi]\}$. For any periodic function $v(\tau)$ on $[-\pi, \pi]$, define the standard projection operator $P_M : L^2([-\pi, \pi]) \to Y_M$ and the trigonometric interpolation operator $I_M : C([-\pi, \pi]) \to Y_M$ respectively as

$$(P_M v)(\tau) = \sum_{k \in \mathcal{M}} \hat{v}_k e^{ik\tau}, \quad (I_M v)(\tau) = \sum_{k \in \mathcal{M}} \hat{v}_k e^{ik\tau},$$

where $i = \sqrt{-1}$, $\hat{v}_k$ for $k \in \mathcal{M}$ are the Fourier transform coefficients of the periodic function $v(\tau)$ and $\hat{\hat{v}}_k$ are the discrete Fourier transform coefficients of the vector $\{v(\tau_k)\}_\kappa = \frac{\pi}{N_\tau} k$. For consistency reasons, we assume that the first term and the last one in the summation are taken with a factor $1/2$ here and after. Then the Fourier spectral method is given by finding the trigonometric polynomials

$$X^M_j(t, \tau) = \left(X_j^M(t, \tau)\right)_{j=1, 2, \ldots, d}, \quad V^M_j(t, \tau) = \left(V_j^M(t, \tau)\right)_{j=1, 2, \ldots, d}$$

such that

$$\begin{align*}
\partial_t X^M(t, \tau) + \frac{1}{\varepsilon} \partial_\tau X^M(t, \tau) &= -\varepsilon^{1-m} \Lambda^{-1} \sin(\tau \Lambda) F(\cos(\tau \Lambda) X^M(t, \tau) + \Lambda^{-1} \sin(\tau \Lambda) V^M(t, \tau)), \\
\partial_t V^M(t, \tau) + \frac{1}{\varepsilon} \partial_\tau V^M(t, \tau) &= \varepsilon^{1-m} \cos(\tau \Lambda) F(\cos(\tau \Lambda) X^M(t, \tau) + \Lambda^{-1} \sin(\tau \Lambda) V^M(t, \tau)).
\end{align*}$$

It follows from the orthogonality of the Fourier functions and collecting all the $\hat{X}_{k,j}$, $\hat{V}_{k,j}$ in $(N_\tau + 1)$-periodic coefficient vectors $\hat{X}(t) = (X_{k,j}(t))$, $\hat{V}(t) = (V_{k,j}(t))$ that

$$\begin{align*}
\frac{d}{dt} \hat{X}(t) &= i\Omega \hat{X}(t) - \varepsilon^{1-m} \mathcal{F}\left(\mathcal{C}\mathcal{F}^{-1} \hat{X}(t) + \mathcal{S}\mathcal{F}^{-1} \hat{V}(t)\right), \\
\frac{d}{dt} \hat{V}(t) &= i\Omega \hat{V}(t) + \varepsilon^{1-m} \mathcal{F}\left(\mathcal{C}\mathcal{F}^{-1} \hat{X}(t) + \mathcal{S}\mathcal{F}^{-1} \hat{V}(t)\right),
\end{align*}$$

(2.11)

where the vectors $\hat{X}$, $\hat{V}$ are in dimension $D := d \times (N_\tau + 1)$, $\mathcal{F}$ denotes the discrete Fourier transform, $\mathcal{S} = \text{diag}(\sin(\Omega_l \Omega^{-1}))_{l=0, 1, \ldots, N_\tau}$, $\mathcal{C} = \text{diag}(\cos(\Omega_l \Omega^{-1}))_{l=0, 1, \ldots, N_\tau}$, $\hat{\Omega} = \text{diag}(\Omega_1, \Omega_2, \ldots, \Omega_d)$ with $\Omega_1 = \Omega_2 = \ldots = \Omega_d := \frac{1}{\varepsilon} \text{diag}(\frac{\pi}{N_\tau}, \frac{\pi}{N_\tau} - 1, \ldots, \frac{-\pi}{N_\tau})$. Our analysis presented below will use the entries of $\hat{X}$ and $\hat{V}$, which are denoted by

$$\begin{align*}
\hat{X} &= (X_{X,1}, \ldots, X_{X,1}, X_{X,2}, \ldots, X_{X,2}, \ldots, X_{X,d}, \ldots, X_{X,d}), \\
\hat{V} &= (V_{V,1}, \ldots, V_{V,1}, V_{V,2}, \ldots, V_{V,2}, \ldots, V_{V,d}, \ldots, V_{V,d}).
\end{align*}$$

The same notation is used for all the vectors and diagonal matrices with the same dimension as $\hat{X}$. We also use the notations $\hat{X}_{:,l} = (X_{X,1}, \ldots, X_{X,1}, X_{X,2}, \ldots, X_{X,2}, \ldots, X_{X,d}, \ldots, X_{X,d})$ for $l = 0, 1, \ldots, N_\tau$ and the $\mathcal{F}$
denotes the discrete Fourier transform acting on each $\mathbf{X}_{n,t}$ of $\mathbf{X}$. Then the fully discrete scheme (FS-F) can read

$$
\begin{align*}
X_{M,j}^{n+1}(\tau) &= \sum_{k \in M} \tilde{X}_{k,j}^{n+1} e^{ik\tau}, \\
V_{M,j}^{n+1}(\tau) &= \sum_{k \in M} \tilde{V}_{k,j}^{n+1} e^{ik\tau},
\end{align*}
$$

where we consider the following s-stage exponential integrators (31) applied to (2.11):

$$
\begin{align*}
\tilde{X}_{i,j}^{n} &= e^{c_i h M} \tilde{X}_{n}^{i} - \varepsilon^{-1-m} h \sum_{j=1}^{s} a_{ij}(h M) F \left( S F \left( C F^{-1} \tilde{X}_{n,j}^{i} + S F^{-1} \tilde{V}_{n,j}^{i} \right) \right), \\
\tilde{V}_{i,j}^{n} &= e^{c_i h M} \tilde{V}_{n}^{i} + \varepsilon^{-1-m} h \sum_{j=1}^{s} a_{ij}(h M) F \left( C F \left( C F^{-1} \tilde{X}_{n,j}^{i} + S F^{-1} \tilde{V}_{n,j}^{i} \right) \right),
\end{align*}
$$

Here $M = i \Omega$, $c_{i}$ for $i = 1, \ldots, s$ are constants belonging to $[0,1]$, and $a_{ij}(h M), b_{j}(h M)$ are matrix-valued functions of $h M$.

The above procedure, however, is unsuitable in practice because of the computation of Fourier transform coefficients. In order to find an efficient implementation, we now consider the discrete Fourier transform coefficients instead of Fourier transform coefficients. This gives the following fully discrete scheme.

Let $\tau_{l} = \frac{2\pi}{M} l$ with $l \in M$ and

$$
\begin{align*}
X_{l,j}^{n} &\approx X_{j}(t_{n} + c_{i} h, \tau_{l}), \\
X_{l,j}^{n+1} &\approx X_{j}(t_{n+1}, \tau_{l}), \\
V_{l,j}^{n} &\approx V_{j}(t_{n} + c_{i} h, \tau_{l}), \\
V_{l,j}^{n+1} &\approx V_{j}(t_{n+1}, \tau_{l})
\end{align*}
$$

for $j = 1, 2, \ldots, d$. An exponential Fourier spectral discretization (FS-D) is defined as

$$
\begin{align*}
X_{l,j}^{n} &= \sum_{k \in M} \tilde{X}_{k,j}^{n} e^{i k \tau_{l}}, \\
V_{l,j}^{n} &= \sum_{k \in M} \tilde{V}_{k,j}^{n} e^{i k \tau_{l}}, \\
X_{l,j}^{n+1} &= \sum_{k \in M} \tilde{X}_{k,j}^{n+1} e^{i k \tau_{l}}, \\
V_{l,j}^{n+1} &= \sum_{k \in M} \tilde{V}_{k,j}^{n+1} e^{i k \tau_{l}},
\end{align*}
$$

where

$$
\begin{align*}
\tilde{X}_{i,j}^{n} &= e^{c_{i} h M} \tilde{X}_{n}^{i} - \varepsilon^{-1-m} h \sum_{j=1}^{s} a_{ij}(h M) F \left( S F \left( C F^{-1} \tilde{X}_{n,j}^{i} + S F^{-1} \tilde{V}_{n,j}^{i} \right) \right), \\
\tilde{V}_{i,j}^{n} &= e^{c_{i} h M} \tilde{V}_{n}^{i} + \varepsilon^{-1-m} h \sum_{j=1}^{s} a_{ij}(h M) F \left( C F \left( C F^{-1} \tilde{X}_{n,j}^{i} + S F^{-1} \tilde{V}_{n,j}^{i} \right) \right),
\end{align*}
$$

The initial values are obtained from (2.10): $[\tilde{X}_{0}^{i}; \tilde{V}_{0}^{i}] = F U_{0}(\tau)$. We now obtain the numerical approximation of (2.2), i.e.,

$$
\begin{align*}
\tilde{q}^{n} &= \cos(t_{n} \Lambda / \varepsilon) x^{n} + \Lambda^{-1} \sin(t_{n} \Lambda / \varepsilon) v^{n}, \\
\tilde{p}^{n} &= -\Lambda \sin(t_{n} \Lambda / \varepsilon) x^{n} + \cos(t_{n} \Lambda / \varepsilon) v^{n},
\end{align*}
$$

where

$$
\begin{align*}
x_{j}^{n} &= X_{n,j}^{n} = \sum_{\ell \in M} \tilde{X}_{\ell,j}^{n} e^{i \tau_{\ell} h / \varepsilon}, \\
v_{j}^{n} &= V_{n,j}^{n} = \sum_{\ell \in M} \tilde{V}_{\ell,j}^{n} e^{i \tau_{\ell} h / \varepsilon},
\end{align*}
$$

Finally, the numerical approximation of the original system (1.1) is given by

$$
\begin{align*}
q^{n} &= \tilde{P} \tilde{q}^{n}, \\
p^{n} &= \tilde{P} \tilde{p}^{n} / \varepsilon.
\end{align*}
$$
Some practical integrators. Proposition 2.4. The practical integrators presented below will be based on these symmetric conditions and stiff order conditions. Proposition 2.5. The above procedure fails to be practical unless the coefficients $c_i$, $\tilde{a}_{ij}(hM)$ and $\tilde{b}_i(hM)$ appearing in (2.13) are determined. To this end, the symmetry and stiff order conditions of (2.13) are needed.

### Table 1. Stiff order conditions.

| Stiff order conditions | Order |
|------------------------|-------|
| $\psi_1(hM) = 0$       | 1     |
| $\psi_2(hM) = 0$       | 2     |
| $\psi_3(hM) = 0$       | 2     |
| $\psi_3,1(hM) = 0$     | 3     |
| $\psi_4(hM) = 0$       | 3     |
| $\psi_3,1(hM) = 0$     | 4     |

Remark 2.3. In the process described above, the operator $M$ is required to be positive definite such that $\Lambda$ is invertible. Under this condition, the solution of (2.4) is periodic in $\tau$ on the torus $\mathbb{T} = (0, 2\pi)$. If this requirement does not hold, we can formulate the methods as follows. Without loss of generality, assume that the first diagonal element of $\Lambda$ is zero and the others are not. Then the system (2.1) can be partitioned into $\ddot{y}(t) + \frac{1}{2}A^2y(t) = f(y(t))$ with $y = [y_1; y_2; \ldots; y_d]$ and $\tilde{y} = [y_1; y]$. Then standard numerical discretizations can be used on $y_1$ and the integrators proposed in this section are applicable to $y$.

2.2. Some practical integrators. The above procedure fails to be practical unless the coefficients $c_i$, $\tilde{a}_{ij}(hM)$ and $\tilde{b}_i(hM)$ appearing in (2.13) are determined. To this end, the symmetry and stiff order conditions of (2.13) are needed.

**Proposition 2.4. (Symmetry)** The $s$-stage implicit exponential integrator (2.13) is symmetric if and only if its coefficients satisfy

$$
c_i = 1 - c_{s+1} - i, \quad \tilde{b}_i(hM) = e^{hM}\tilde{b}_{s+1-i}(-hM), \quad i = 1, 2, \ldots, s,
\begin{align*}
\tilde{a}_{ij}(hM) &= e^{c_i hM}\tilde{b}_{s+1-j}(-hM) - \tilde{a}_{s+1-i,s+1-j}(-hM), \\
&\quad i, j = 1, 2, \ldots, s. 
\end{align*}
$$

(2.15)

**Proof.** Under the conditions (2.15), it is trivial to verify that the method (2.13) remains the same after exchanging $n + 1 \leftrightarrow n$ and $h \leftrightarrow -h$. This completes the proof immediately. 

**Proposition 2.5. (Stiff order conditions)** Assume that the solution $q(t)$ of (1.1) stays in a bounded open set of $K$ for $t \in [0, T]$. Let $F(q)$ be smooth and uniformly bounded on the closure of $K$ for all $\varepsilon$. Define

$$
\psi_j(z) = \varphi_j(z) - \sum_{k=1}^s \tilde{b}_k(z) \frac{c_k^{j-1}}{(j-1)!}, \quad \psi_{j,i}(z) = \varphi_j(c_i z) c_i^j - \sum_{k=1}^s \tilde{a}_{ik}(z) \frac{c_k^{j-1}}{(j-1)!}, \quad i = 1, 2, \ldots, s,
$$

where the notations $\varphi_k$ are defined by $\varphi_k(z) = \int_0^1 \theta^{k-1} e^{(1-\theta) z} / (k-1)! d\theta$ for $k = 1, 2, \ldots$ (3.1). For a fixed number $1 \leq r \leq 4$, the order conditions of Table 1 are assumed to be true up to order $r$ and the condition $\psi_r(hM) = 0$ is weakened to the form $\psi_r(0) = 0$. Under these assumptions and the local assumptions of $X^n = X(t_n)$, $\tilde{V}^n = \tilde{V}(t_n)$, there exists a constant $h_0$ independent of $\varepsilon$ such that for $0 < h \leq h_0$, the local error bounds satisfy the following inequalities

$$
\|X^n - X(t_n + c_i h)\|_{L^2} \leq C \varepsilon^{r-r_m} h^r, \quad \|\tilde{V}^n - V(t_n + c_i h)\|_{L^2} \leq C \varepsilon^{r-r_m} h^r, \quad i = 1, 2, \ldots, s,
$$

$$
\|X^{n+1} - X(t_{n+1})\|_{L^2} \leq C (\varepsilon^{r-r_m} h^r \psi_r(hM) + \varepsilon^{(r+1)(1-m)} h^{r+1}),
\|\tilde{V}^{n+1} - V(t_{n+1})\|_{L^2} \leq C (\varepsilon^{r-r_m} h^r \psi_r(hM) + \varepsilon^{(r+1)(1-m)} h^{r+1}), \quad 0 \leq n \leq T/h,
$$

where $C > 0$ is a constant independent of $\varepsilon$ and $h$.

**Proof.** The proof will be given in Section 4 combined with the analysis of convergence. 

The practical integrators presented below will be based on these symmetric conditions and stiff order conditions.
Second-order integrator. We first consider two-stage integrators, i.e., $s = 2$. Solving the order conditions

$$\psi_1(hM) = \psi_2(hM) = 0$$

leads to

$$\tilde{b}_1(hM) = \frac{-c_2\varphi_1(hM) + \varphi_2(hM)}{c_1 - c_2}, \quad \tilde{b}_2(hM) = \frac{c_1\varphi_1(hM) - \varphi_2(hM)}{c_1 - c_2}.$$ 

Then using some other order conditions

$$\psi_{1,1}(hM) = \psi_{1,2}(hM) = \psi_{2,2}(hM) = 0$$

and a symmetric condition

$$\tilde{a}_{12}(hM) + \tilde{a}_{21}(-hM) = \varphi_0(c_1hM)\tilde{b}_1(-hM),$$

we get the results of $\tilde{a}_{ij}$ as

$$\tilde{a}_{21}(hM) = \frac{c_2^2(-\varphi_1(c_2hM) + \varphi_2(c_2hM))}{c_1 - c_2}, \quad \tilde{a}_{12}(hM) = -\tilde{a}_{21}(-hM) + \varphi_0(c_1hM)\tilde{b}_1(-hM),$$

$$\tilde{a}_{11}(hM) = -\tilde{a}_{12}(hM) + c_1\varphi_1(c_1hM), \quad \tilde{a}_{22}(hM) = -\tilde{a}_{21}(hM) + c_2\varphi_1(c_2hM).$$

On noticing $c_1 = 1 - c_2$, it can be verified that this class of integrators is symmetric and is of at least order two. As an example, we choose $c_1 = 0$ and denote the corresponding method as S2O2.

Fourth-order integrator. We now continue with three-stage ($s = 3$) integrators and obtain their coefficients by solving

$$\psi_1(hM) = 0 \text{ and } \psi_{j,i}(hM) = 0 \text{ for } i, j = 1, 2, 3.$$ 

The choice of $c_1 = 1$, $c_2 = 1/2$, $c_3 = 0$ and the corresponding results

$$\tilde{a}_{31}(hM) = \tilde{a}_{32}(hM) = \tilde{a}_{33}(hM) = 0, \quad \tilde{a}_{21}(hM) = -\frac{1}{4}\varphi_2(c_2hM) + \frac{1}{2}\varphi_3(c_2hM),$$

$$\tilde{a}_{22}(hM) = \varphi_2(c_2hM) - \varphi_3(c_2hM), \quad \tilde{a}_{23}(hM) = \frac{1}{2}\varphi_1(c_2hM) - \frac{3}{4}\varphi_2(c_2hM) + \frac{1}{2}\varphi_3(hM),$$

$$\tilde{a}_{11}(hM) = \tilde{b}_1(hM) = 4\varphi_3(hM) - \varphi_2(hM), \quad \tilde{a}_{12}(hM) = \tilde{b}_2(hM) = 4\varphi_2(hM) - 8\varphi_3(hM),$$

$$\tilde{a}_{13}(hM) = \tilde{b}_3(hM) = \varphi_1(hM) - 3\varphi_2(hM) + 4\varphi_3(hM),$$

determine this integrator. It is noted that this method satisfies all the stiff order conditions of order four and symmetric conditions. This integrator is referred as S3O4.

We end this section by noting that, with the same arguments stated above, higher-order stiff order conditions as well as the corresponding integrators can be derived. This process can be succinctly presented by B-series and rooted trees [8]. This is an issue which we will focus on in the future work.

3. Main results and numerical tests

In this section, we shall present the main results of this paper. The first one is about optimal uniformly high accuracy and the second is devoted to long time energy conservation. To support these two results, two numerical experiments with numerical results are carried out in the second part of this section.

3.1. Main results.

Theorem 3.1. (Optimal uniformly high accuracy) Under the conditions of Propositions 2.2 and 2.3, for the final numerical solutions $q^n$, $p^n$ (2.14) produced by S2O2 or S3O4, the global errors are

$$S2O2: \|q^n - q(t_n)\|_{L^2} \leq C(\varepsilon^{3-3m}h^2 + \delta_\varepsilon), \quad \|p^n - p(t_n)\|_{L^2} \leq C(\varepsilon^{2-3m}h^2 + \delta_\varepsilon), \quad 0 \leq n \leq T/h,$$

$$S3O4: \|q^n - q(t_n)\|_{L^2} \leq C(\varepsilon^{4-4m}h^4 + \delta_\varepsilon), \quad \|p^n - p(t_n)\|_{L^2} \leq C(\varepsilon^{3-4m}h^4 + \delta_\varepsilon), \quad 0 \leq n \leq T/h,$$

where $m$ is the parameter in the system (11), $C$ is independent of $n, h, \varepsilon$, and $\delta_\varepsilon$ denotes the projection error brought by the Fourier pseudo-spectral method.
Remark 3.2. It is noted that for \( m = 0 \), these two methods have a very nice improved accuracy which is \( \mathcal{O}(\varepsilon^3 h^2) \) for S2O2 and \( \mathcal{O}(\varepsilon^4 h^4) \) for S3O4 in \( q \), and \( \mathcal{O}(\varepsilon^2 h^2) \) for S2O2 and \( \mathcal{O}(\varepsilon^3 h^4) \) for S3O4 in \( p \). This is very significant for the numerical methods applied to highly oscillatory systems where \( \varepsilon \) is a very small value. When \( m = 1 \), our methods share the same uniform accuracy as the existing UA algorithms \([10,14]\). However, compared with these UA algorithms, our two methods also have a long time conservation in energy which will be stated below.

The next theorem requires a non-resonance condition and to describe it, we introduce the notations (111)

\[
\mathbf{k} = (k_{-\infty,1}, \ldots, k_{-\infty,1}, k_{-\infty,2}, \ldots, k_{-\infty,2}, \ldots, k_{-\infty,d}, \ldots, k_{-\infty,d}),
\]

\[
|\mathbf{k}| = \sum_{j=1}^{d} \sum_{\omega \in \mathbb{Z}} |k_{j,l}|, \quad \omega = \text{(diagonal elements of } \mathcal{Q} \text{),} \quad \mathbf{k} \cdot \mathbf{\omega} = \sum_{i=1}^{d} \sum_{j=1}^{d} |k_{i,l}| \omega_{j,l}.
\]

Denote the resonance module by \( \mathcal{M} = \{ \mathbf{k} \in \mathbb{Q} : \mathbf{k} \cdot \mathbf{\omega} = 0 \} \), where \( \mathbb{Q} = \{ \mathbf{k} \in \mathbb{Z}^D : \text{there exists an } l \in \{1, \ldots, 2d\} \text{ such that } |\mathbf{k} | = |\mathbf{k}_{l} | \} \). Let \( \langle j \rangle \) be the unit coordinate vector \((0, \ldots, 0, 1, 0, \ldots, 0)^T \in \mathbb{R}^D \) with the only entry 1 at the \((j, l)\)-th position. Further let \( \mathcal{K} \) be a set of representatives of the equivalence classes in \( \mathcal{Q} / \mathcal{M} \). The set \( \mathcal{K} \) is determined by two requirements. The first is that if \( \mathbf{k} \in \mathcal{K} \), we have \(-\mathbf{k} \in \mathcal{K}\). The other is to minimize the sum \( |\mathbf{k}| \) in the equivalence class \( |\mathbf{k}| = \mathbf{k} + \mathcal{M} \) for each \( \mathbf{k} \in \mathcal{K} \). Meanwhile, for those elements having the same minimal sum \( |\mathbf{k}| \), all of them are kept in \( \mathcal{K} \). Denote \( \mathcal{N}_N = \{ \mathbf{k} \in \mathcal{K} : |\mathbf{k}| \leq N \} \) and \( \mathcal{N}_N^\prime = \mathcal{N} \cup \{(0)_1 \}_{1,2, \ldots, d} \) for a positive integer \( N \).

**Theorem 3.3. (Long time energy conservation)** The bound of \( \psi_1, \psi_2 \) appeared in the initial value is denoted by \( 0 < \delta_0 := \|\psi_1; \psi_2\| < 1 \). The non-linearity \( F(q) \) is assumed to be smooth and satisfies \( F(0) = 0 \). For the time stepsize \( h \), we assume a lower bound \( h/\sqrt{\varepsilon} \geq c_0 > 0 \) and \( h \leq \delta_0 \). It is further required that the numerical non-resonance condition \( |\sin \left( \frac{1}{2} h \omega_{j,l} \right) | \geq c_1 \sqrt{\varepsilon} \) holds for a constant \( c_1 > 0 \) and \( j = \mathcal{N}_{2, \ldots, \mathcal{N}_2} \). Then the long time energy conservation of \( q^n, p^n \) produced by S2O2 or S3O4 is estimated by

\[
\varepsilon^2 \begin{align*}
\frac{\delta_0^2}{\delta_0} \left( H(q^n, p^n) - H(q^0, p^0) \right) &= \mathcal{O}(\varepsilon^{4-2m}\delta_0^2) + \mathcal{O}(\delta_F), \\
0 &\leq nh \leq \frac{\varepsilon^{2-m} \delta_0^{-N+3}}{h},
\end{align*}
\]

where \( \delta_F \) denotes the error brought by the Fourier pseudospectral method and the constants symbolized by \( \mathcal{O} \) depend on \( N, N_r, c_0, c_1 \), but are independent of \( n, h, \varepsilon \). Since \( N \) can be arbitrarily large, the conservation law holds for a long time. If the system (1.1) has small initial value \( \delta_0 = \mathcal{O}(\varepsilon) \), the above result is improved to be

\[
H(q^n, p^n) - H(q^0, p^0) = \mathcal{O}(\varepsilon^{6-2m}) + \mathcal{O}(\delta_F), \quad 0 \leq nh \leq \frac{\varepsilon^{-N+5-m}}{h}.
\]

**Remark 3.4.** Although the smallness of the parameter \( \delta_0 \) is technically required, we should note here that \( \delta_0 \) is totally independent of \( \varepsilon \). This means that the initial value of (1.1) is large, which has not been considered yet in the long term analysis of any methods. In all the previous work on this topic, small initial data is required (see, e.g., [15, 16, 17, 28, 29, 39, 41]). Moreover, we only need the lower bound on the time stepsize \( h \geq c_0 \sqrt{\varepsilon} \), which means that large stepsize can be used to keep the long time energy conservation. Compared with the analysis of (111), a looser numerical non-resonance requirement is posed in this theorem and this is because the methods derived in this paper avoid \( \sin \left( \frac{1}{2} h \omega_{j,l} - (\mathbf{k} \cdot \mathbf{\omega}) \right) \) with \( \mathbf{k} \in \mathcal{N}_N \neq \langle j \rangle \) in the denominator of the ansatz (5.5) of the modulated Fourier functions.

### 3.2. Numerical tests

Two numerical experiments are presented in this section to test the optimal uniformly high accuracy and the long time energy conservation of the obtained integrators.

**Problem 1. (Duffing equation)** As the first numerical example, we consider the Duffing equation defined by \( \ddot{q} + \frac{1}{2} \dot{q}^2 q + k^2 q = 2k^2 q^3 \). It is a Hamiltonian system with the Hamiltonian \( H(q, \dot{q}) = \frac{1}{2} \dot{q}^2 + \frac{1}{2} q^2 + \frac{k}{2} (q^2 - q^4) \). For comparison, we choose another two methods. The first one is the trigonometric integrator given in [25] and here we call it as improved Störmer-Verlet method (ISV). This method is directly used to solve (1.1) without taking the process given in Section 2. The second
LARGE-STEP SIZE HIGHLY ACCURATE INTEGRATORS

Figure 1. Duffing equation: the log-log plot of the temporal error $err = |q^n - q(t_n)| / |q(t_n)| + |\dot{q}^n - \dot{q}(t_n)| / |\dot{q}(t_n)|$ at $t_n = 1$ under different $\varepsilon$, where $h = 1/2^k$ with $k = 1, 2, \ldots, 6$.

Figure 2. Duffing equation: the log-log plot of the temporal errors $err_q = |q^n - q(t_n)| / |q(t_n)|$ and $err_{\dot{q}} = |\dot{q}^n - \dot{q}(t_n)| / |\dot{q}(t_n)|$ at $t_n = 1$ under different $h$, where $\varepsilon = 1/2^k$ with $k = 1, 2, \ldots, 6$. 
one is obtained by replacing S2O2 with the following one-stage exponential integrator
\[
\begin{align*}
\dot{X}^{n+1} &= e^{hM/2}X^n - \varepsilon h/2F \left( SF(CF^{-1}X^n + SF^{-1}V^n) \right), \\
\dot{V}^{n+1} &= e^{hM/2}V^n + \varepsilon h/2F \left( CF(CF^{-1}X^n + SF^{-1}V^n) \right), \\
\dot{X}^{n+1} &= e^{hM}X^n - \varepsilon h\phi_1(hM)F \left( SF(CF^{-1}X^n + SF^{-1}V^n) \right), \\
\dot{V}^{n+1} &= e^{hM}V^n + \varepsilon h\phi_1(hM)F \left( CF(CF^{-1}X^n + SF^{-1}V^n) \right).
\end{align*}
\]
This method is non-symmetric and we shall denote it by NSM. For implicit methods, we use standard fixed point iteration as nonlinear solver in the practical computations. We set \(10^{-16}\) as the error tolerance and 200 as the maximum number of each iteration.

Accuracy. In this test, \(N_T\) is chosen as 32 to discretize the \(\tau\) direction and \(k = 2.5\). The initial value is chosen as \(\psi_1 = 0.1\) and \(\psi_2/\varepsilon = 0.2/\varepsilon\), and this is the large initial value case as \(\varepsilon\) decreases. Firstly the accuracy of all the methods is shown by displaying the global errors \(\text{err}_\varepsilon\) with \(\text{err}_\varepsilon = |q^n - q(t_n)| / |q(t_n)|\) and \(\text{err}_\dot{q} = |\dot{q}^n - \dot{q}(t_n)| / |\dot{q}(t_n)|\) at \(T = t_n = 1\) in Figure 3. We use the result given by the ‘ode45’ of MATLAB as the reference solution. In the light of these results, we have the following observations.

a) The two integrators given in this paper have optimal uniformly high accuracy, and when \(\varepsilon\) and \(h\) decrease, the accuracy is improved. S2O2 shows second order and S3O4 performs fourth order. These observations support the convergence result of Theorem 3.1.

b) The improved Störmer-Verlet method ISV shows non-uniform accuracy. The integrator NSM only shows uniformly second order but does not have improved accuracy when \(\varepsilon\) becomes small.

To show the dependence of global errors in \(\varepsilon\), we present the errors \(\text{err}_\varepsilon\) and \(\text{err}_\dot{q}\) at \(t_n = 1\) for our two methods in Figure 2. It can be seen that for a fixed \(h\), S2O2 has \(O(\varepsilon^3)\) and \(O(\varepsilon^2)\) convergence in \(q\) and \(\dot{q}\), respectively, and the corresponding results for S3O4 are \(O(\varepsilon^4)\) and \(O(\varepsilon^3)\). These observations agree with the theoretical results given in Theorem 5.1.

Energy conservation. Then we display the long time energy conservation of each method by presenting the energy error \(\text{err}_H = \frac{|H(q^n, \dot{q}^n) - H(q^n, \dot{q}^n)|}{|H(q^n, \dot{q}^n)|}\). For large initial value, the energy errors are

\[
\begin{align*}
\log_{10}(\text{err}_H) &\approx 12, \quad \varepsilon = 0.1/2; \\
\log_{10}(\text{err}_H) &\approx 10, \quad \varepsilon = 0.1/4; \\
\log_{10}(\text{err}_H) &\approx 8, \quad \varepsilon = 0.1/8;
\end{align*}
\]
Figure 4. Duffing equation: the log-log plot of the temporal error $\text{err} = \frac{|q^n - q(t_n)|}{|q(t_n)|} + \frac{|\dot{q}^n - \dot{q}(t_n)|}{|\dot{q}(t_n)|}$ at $t_n = 10$ against CPU time, where $h = 1/2^k$ with $k = 1, 2, \ldots, 8$.

shown in Figure 3 for different $\varepsilon$ and large $h$. According to these numerical results, the following observations are made.

a) The energy $H$ is nearly preserved numerically by our integrators and ISV with large time steps $h$ over long times. S2O2 and S3O4 have a nice long time conservation, and with large time steps $h$, the numerical error in the energy can be improved when $\varepsilon$ decreases. These observations agree with the results given in Theorem 3.3. It also shows that S3O4 has a better conservation accuracy than S2O2 and it is believed that this phenomenon here could be analysed in future.

b) In contrast, NSM shows substantial drift in the energy quantity and thus it does not have long-term performance in the energy conservation. The reason is that it is not a symmetric method. This observation demonstrates that symmetry plays an important role in the numerical behaviour of energy conservation.

c) Both S2O2 and S3O4 are more accurate in the energy conservation than ISV. The reason is that ISV has $O(h)$ accuracy in the long time behaviour [25].

Efficiency. Compared with ISV applied to (1.1) directly, the scheme of our integrators given in this paper is more complicated. For example, the two-scale method enlarges the dimension of the original system and this usually adds some computation cost. Fortunately, Fast Fourier Transform (FFT) techniques can be used in the integrators and we hope that the efficiency of our integrators is still acceptable even compared with methods applied to (1.1) directly. To show this point, we solve this problem on the time interval $[0, 10]$. The efficiency of each integrator (measured by the log-log plot of the temporal error at $t = 10$ against CPU time) is displayed in Figure 4. Clearly, our integrators are not expensive in terms of efficiency.

Problem 2. (Nonlinear relativistic Klein–Gordon equation) The second illustrative numerical test is devoted to the nonlinear relativistic Klein–Gordon equation (1.2) with $\lambda = -1, d = 1, p = 2, L = \pi$ and the initial values $\phi(x) = \frac{2 \sin(x)}{\exp(x^2/2) + \exp(-x^2/2)}, \gamma(x) = \frac{2 \exp(-x^2)}{\sqrt{\pi}}$. By the Fourier spectral collocation method, we consider the second-order Fourier differentiation matrix $A = (a_{kj})_{M \times M}$ whose entries are given by $a_{kj} = \begin{cases} \frac{1}{2} \sin^{-2} \left( \frac{(k-j)\pi}{M} \right), & k \neq j, \\ \frac{M^2 + 1}{12}, & k = j, \end{cases}$ with $M = \frac{2L}{N_x}$. In terms of classical concepts, the method is of an infinite order and $A$ is also a positive semi-definite matrix. With the notation $U(t) = (u(x_1, t), u(x_2, t), \ldots, u(x_{N_x}, t))^T$, the NRKG equation (1.2) is transformed into

$$
\frac{d^2}{dt^2} U(t) + \frac{1 + \varepsilon A}{\varepsilon} U(t) = -\frac{1}{\varepsilon} |U(t)|^2 U(t), \quad t > 0, \quad U(0) = \Phi, \quad U_t(0) = \frac{1}{\varepsilon} \Upsilon,
$$

This test is conducted in a sequential program in MATLAB R2020b on a laptop ThinkPad X1 nano (CPU: i7-1160G7 @ 1.20GHz 2.11 GHz, Memory: 16 GB, Os: Microsoft Windows 10 with 64bit).
where $\Phi = (\phi(x_1), \phi(x_2), \ldots, \phi(x_{N_x}))^T$ and $\Upsilon = (\gamma(x_1), \gamma(x_2), \ldots, \gamma(x_{N_x}))^T$ with $x_j = -\pi + (j - 1)\frac{\pi}{N_x}$ for $j = 1, 2, \ldots, N_x$. We apply the methods to solve this system with $N_x = 32$ and $N_T = 64$. The results of global errors $err = |U^n - U(t_n)| / |U(t_n)| + |U^n - U_t(t_n)| / |U_t(t_n)|$ at $t_n = 1$ under different $h$, where $\varepsilon = 1/2^k$ with $k = 4, 5, \ldots, 8$.

where $\Phi = (\phi(x_1), \phi(x_2), \ldots, \phi(x_{N_x}))^T$ and $\Upsilon = (\gamma(x_1), \gamma(x_2), \ldots, \gamma(x_{N_x}))^T$ with $x_j = -\pi + (j - 1)\frac{\pi}{N_x}$ for $j = 1, 2, \ldots, N_x$. We apply the methods to solve this system with $N_x = 32$ and $N_T = 64$. The results of global errors $err = |U^n - U(t_n)| / |U(t_n)| + |U^n - U_t(t_n)| / |U_t(t_n)|$, energy errors $err_H = \frac{|H(U^n, U^n_t) - H(U_0, U_0_t)|}{|H(U_0, U_0_t)|}$ and efficiency are presented in Figures 5, 8, respectively. All the numerical phenomena demonstrate that our methods have uniform accuracy, long time energy conservation and competitive efficiency.

4. Proof of optimal uniformly high accuracy (Theorem 3.1)

The convergence of the three-stage integrator of order four (S3O4 with $s = 3, r = 4$) is studied in this section. The proof is easily presented for the second order S2O2 and we omit it for brevity.
To prove the optimal uniformly accuracy, we will show that the transformed system formulated in Section 2 has an important and surprising property. Based on which and the stiff order conditions of exponential integrators, local errors of integrators for solving transformed system can be improved. Then the convergence of integrators will be derived for the transformed system and further for the original problem by taking the transformations of Section 2. Since the parameter \( \varepsilon \) is very small in highly oscillatory problems, this optimal uniformly accuracy makes the integrators be very effective and competitive in solving highly oscillatory systems.

Proof. The proof is presented in three steps.

Proof of Proposition 2.2 (bounds of the solution of the two-scale system). Noticing that the operators \( \Pi \) and \( A \) are both bounded on \( C^0(T; H^s) \), the initial value can be estimated that \( U_0 \) is uniformly bounded w.r.t. \( \varepsilon \). Combining this with Proposition 2.1 of [10], it is known that
the two-scale system \((2.3)\) as well as the initial value \((2.10)\) determines a unique solution satisfying \(U(t, \tau) = O(1)\). In what follows, we study the boundedness of the derivatives of \(U(t, \tau)\) w.r.t. \(t\) and hope to get a more rigorous result. To this end, we first consider the differential equation of the first derivative \(\partial_t U(t, \tau) \triangleq V(t, \tau)\) which reads

\[
\partial_t V(t, \tau) + \frac{1}{\varepsilon} \partial_{\tau} V(t, \tau) = \partial_U f_\tau(U(t, \tau)) V(t, \tau).
\]

The initial date of this system is

\[
V_0 := V(0, \tau) = \partial_t U(0, \tau) = f_\tau(U_0) - \frac{1}{\varepsilon} L U_0
\]

\[
= f_\tau(U_0) - L \kappa_1(\tau, U_1^{[0]}) - \varepsilon L \kappa_2(\tau, U_1^{[0]}) - \varepsilon^2 L \kappa_3(\tau, U_1^{[0]})
\]

\[
= f_\tau(U_0) - f_\tau(U_0) + \Pi f_\tau(U_0) - \varepsilon L \kappa_2(\tau, U_1^{[0]}) - \varepsilon^2 L \kappa_3(\tau, U_1^{[0]})
\]

\[
= \Pi f_\tau(U_0) + \varepsilon \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]}) + \varepsilon^2 \partial_U f_\tau(U_1^{[0]}) \kappa_2(\tau, U_1^{[0]}) - \varepsilon L \kappa_2(\tau, U_1^{[0]})
\]

\[
- \varepsilon^2 L \kappa_3(\tau, U_1^{[0]}) + \varepsilon^3 \frac{1}{2} \partial_{\tau}^2 f_\tau(U_1^{[0]}) \left( \kappa_1(\tau, U_1^{[0]}), \kappa_1(\tau, U_1^{[0]}) \right) + O(\varepsilon^3).
\]

According to the expressions of \(\kappa_1, \kappa_2, \kappa_3 \triangleq (2.9)\), one deduces that

\[\kappa_1 = O(\varepsilon^{1-m}), \quad \kappa_2 = O(\varepsilon^{2-2m}), \quad \kappa_3 = O(\varepsilon^{3-3m})\]

and further \(V_0 = O(\varepsilon^{1-m})\) based on \(f_\tau = O(\varepsilon^{1-m})\). This result and the Proposition 2.1 of \((10)\) yield

\[
\partial_t U(t, \tau) = O(\varepsilon^{1-m}).
\]

For the second derivative \(\partial_U^2 U(t, \tau) \triangleq W(t, \tau)\), the equation stands

\[
\partial_t W(t, \tau) + \frac{1}{\varepsilon} \partial_{\tau} W(t, \tau) = \partial_U f_\tau(U(t, \tau))(V(t, \tau), V(t, \tau)) + \partial_U f_\tau(U(t, \tau)) W(t, \tau),
\]

and the corresponding initial date is obtained by

\[
W_0 := W(0, \tau) = \partial_t V(0, \tau) = \partial_U f_\tau(U_0) V_0 - \frac{1}{\varepsilon} L V_0
\]

\[
= \partial_U f_\tau(U_0) \Pi f_\tau(U_1^{[0]}) + \varepsilon \partial_U f_\tau(U_1^{[0]}) \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]})
\]

\[
- \varepsilon L \partial_U f_\tau(U_1^{[0]}) \kappa_2(\tau, U_1^{[0]}) + \varepsilon^2 L \kappa_3(\tau, U_1^{[0]}) + \frac{1}{2} \partial_{\tau}^2 f_\tau(U_1^{[0]}) \left( \kappa_1(\tau, U_1^{[0]}), \kappa_1(\tau, U_1^{[0]}) \right) + O(\varepsilon^{4-2m}).
\]

We further simplify the parts of \(O(\varepsilon^{0})\) as

\[
\partial_U f_\tau(U_0) \Pi f_\tau(U_1^{[0]}) - L \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]})
\]

\[
+ L^2 A \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]}) - L^2 A \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]})
\]

\[
= \partial_U f_\tau(U_0) \Pi f_\tau(U_1^{[0]}) - L \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]})
\]

\[
+ (I - \Pi) \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]}) - (I - \Pi)^2 \partial_U f_\tau(U_1^{[0]}) \Pi f_\tau(U_1^{[0]})
\]

\[
= \partial_U f_\tau(U_0) \Pi f_\tau(U_1^{[0]}) - (I - \Pi) \partial_U f_\tau(U_1^{[0]}) \Pi f_\tau(U_1^{[0]})
\]

\[
= \Pi \partial_U f_\tau(U_1^{[0]}) \Pi f_\tau(U_1^{[0]}) + \varepsilon \partial_U f_\tau(U_1^{[0]}) \left( A f_\tau(U_1^{[0]}), \Pi f_\tau(U_1^{[0]}) \right) + O(\varepsilon^{4-2m}).
\]

Then \(W_0\) has the form

\[
W_0 = \Pi \partial_U f_\tau(U_1^{[0]}) \Pi f_\tau(U_1^{[0]}) + \varepsilon \partial_U f_\tau(U_1^{[0]}) \left( A f_\tau(U_1^{[0]}), \Pi f_\tau(U_1^{[0]}) \right)
\]

\[
+ \varepsilon \partial_U f_\tau(U_1^{[0]}) \partial_U f_\tau(U_1^{[0]}) A f_\tau(U_1^{[0]}) - \varepsilon \partial_U f_\tau(U_1^{[0]}) \kappa_2(\tau, U_1^{[0]})
\]

\[
- \varepsilon \partial_U f_\tau(U_1^{[0]}) \kappa_2(\tau, U_1^{[0]}) + \varepsilon^2 \kappa_3(\tau, U_1^{[0]})
\]

\[
= - \frac{1}{2} L \partial_U^2 f_\tau(U_1^{[0]}) \left( \kappa_1(\tau, U_1^{[0]}), \kappa_1(\tau, U_1^{[0]}) \right) + O(\varepsilon^{4-2m}).
\]
Therefore, one gets that \( W_0 = \mathcal{O}(\varepsilon^{2-2m}) \) and
\[
\partial_t^2 U(t, \tau) = \mathcal{O}(\varepsilon^{2-2m}).
\]
Consider \( \partial_t^3 U(t, \tau) \equiv Y(t, \tau) \) and its equation reads
\[
\partial_t Y(t, \tau) + \frac{1}{\varepsilon} \partial_\tau Y(t, \tau) = \partial_t \partial_\tau f_r(U(t, \tau))(V(t, \tau), V(t, \tau), V(t, \tau)) + 3\partial_t^2 f_r(U(t, \tau))(V(t, \tau), W(t, \tau)) + \partial_t f_r(U(t, \tau))Y(t, \tau).
\]
The initial value \( Y_0 := Y(0, \tau) \) is extracted from (1.1)
\[
Y_0 = \partial_t^2 f_r(U_0)(0, V_0) + \partial_t f_r(U_0)W_0 - \frac{1}{\varepsilon} \partial_\tau Y_0
= \partial_t^2 f_r(U_0)(0, V_0) + \partial_t f_r(U_0)W_0 - LA \partial_\tau f_r(U_0) \left( \partial_\tau Y_0 + \partial_\tau f_r(U_0) \frac{\Pi}{3} \right)
- \frac{1}{2} L^2 \partial_\tau f_r(U_0) \kappa_2 \left( \tau, \Pi \right)
- \frac{1}{2} L^2 \partial_\tau f_r(U_0) \kappa_3 \left( \tau, \Pi \right) + \mathcal{O}(\varepsilon^{3-2m}).
\]
Therefore, we obtain that \( Y_0 = \mathcal{O}(\varepsilon^{3-3m}) \) and
\[
\partial_t^3 U(t, \tau) = \mathcal{O}(\varepsilon^{3-3m}).
\]
This procedure can be proceeded in an analogous way for \( \partial_t^4 U(t, \tau) \equiv Z(t, \tau) \) and we get
\[
\partial_t Z(t, \tau) + \frac{1}{\varepsilon} \partial_\tau Z(t, \tau) = \partial_t \partial_\tau f_r(U(t, \tau))(V(t, \tau), V(t, \tau), V(t, \tau), V(t, \tau)) + 4\partial_t^2 f_r(U(t, \tau))(V(t, \tau), Y(t, \tau), Y(t, \tau)) + 3\partial_t^3 f_r(U(t, \tau))(W(t, \tau), W(t, \tau)) + \partial_t f_r(U(t, \tau))Z(t, \tau)
\]
with the initial value
\[
Z_0 := Z(0, \tau) = \partial_t^2 f_r(U_0)(0, V_0, V_0) + 3\partial_t^2 f_r(U_0)(0, W_0) + \partial_t f_r(U_0)Y_0 - \frac{1}{\varepsilon} L Y_0.
\]
The only concern of this initial value comes from the factor \( \frac{1}{\varepsilon} L Y_0 \) and thus we collect the terms in the bound \( \mathcal{O}(1) \) of \( Y_0 \) as follows
\[
Y_0 = \partial_t^2 f_r(U_0) \left( \Pi f_r(U_0), \Pi f_r(U_0) \right) + \partial_t f_r(U_0) \Pi \partial_\tau f_r(U_0) \Pi f_r(U_0) - L \partial_t \partial_\tau f_r(U_0) \left( \partial_\tau Y_0 \right) + L \partial_\tau f_r(U_0) \left( \partial_\tau Y_0 \right) + L^2 \partial_\tau f_r(U_0) \kappa_2 \left( \tau, \Pi \right) + L^2 \partial_\tau f_r(U_0) \kappa_3 \left( \tau, \Pi \right) + \mathcal{O}(\varepsilon^{5-4m}).
\]
In the light of the properties \( L \Pi = 0, LA = I - \Pi \) and \( L A^2 = A \) given in (2.5), one can further derive that
\[
L^3 A = L^2 (I - \Pi) = L^2, \quad L^2 A^2 = LA = I - \Pi, \quad L^3 A^2 = L(I - \Pi) = L, \quad L^3 A^3 = LA = I - \Pi.
\]
With these results, \( Y_0 \) can be simplified as
\[
Y_0 = \Pi \partial_t^2 f_r(U_0) \left( \Pi f_r(U_0), \Pi f_r(U_0) \right) + \Pi \partial_\tau f_r(U_0) \Pi \partial_\tau f_r(U_0) \Pi f_r(U_0) + \mathcal{O}(\varepsilon^{5-4m}).
\]
Thus $\frac{1}{\varepsilon} L_0 = \mathcal{O}(\varepsilon^{4-4m})$ and the initial condition $Z_0 = \mathcal{O}(\varepsilon^{4-4m})$. In a similar way, it is deduced that
\[
\partial_t^4 U(t, \tau) = \mathcal{O}(\varepsilon^{4-4m}).
\]

**Proof of Proposition 2.5** (local errors of exponential integrators). Then we prove Proposition 2.5 where the local errors of our integrators for the transformed system are stated.

For all $h \geq 0$, it is true that $\|\varphi_0(hM)\|_{L^2} = 1$, and $\|\varphi_j(hM)\|_{L^2}$ for $j = 1, 2, \ldots$, are uniformly bounded. Therefore, the coefficients of exponential integrators are bounded as
\[
\|\tilde{a}_{ij}(hM)\|_{L^2} \leq C, \quad \|\tilde{b}_{ij}(hM)\|_{L^2} \leq C \quad \text{for} \quad i, j = 1, 2, \ldots, 3,
\]
where the constant $C$ is independent of $h, \varepsilon$.

Define the error functions by
\[
eX^n_\tau(t) := X(t, \tau) - I_M X^n, \quad \eX^n_\tau(t) := X(t, \tau) - I_M X^n,
\]
and the projected errors as
\[
e\eta^n_{M,X}(t) := P_M X(t, \tau) - X^n_M, \quad \e\eta^n_{M,X}(t) := P_M X(t, \tau) - X^n_M,
\]
\[
e\eta^n_{M,V}(t) := P_M V(t, \tau) - V^n_M, \quad \e\eta^n_{M,V}(t) := P_M V(t, \tau) - V^n_M.
\]

By the triangle inequality and estimates on projection error [36], one has
\[
\|e^n_X\|_{L^2} \leq \|e\eta^n_{M,X}\|_{L^2} + \|X^n_M - I_M X^n\|_{L^2} + \|X(t, \tau) - P_M X(t, \tau)\|_{L^2} \lesssim \|e\eta^n_{M,X}\|_{L^2} + \delta_f,
\]
\[
\|E^n_X\|_{L^2} \leq \|E^n_{M,X}\|_{L^2} + \|X^n_M - I_M X^n\|_{L^2} + \|X(t, \tau) - P_M X(t, \tau)\|_{L^2} \lesssim \|E^n_{M,X}\|_{L^2} + \delta_f,
\]
and similar results for $e^n_V$, $E^n_V$. Therefore, the estimations for $e^n_X$, $e^n_V$, and $E^n_X$, $E^n_V$ could be converted to the estimations for $e^n_{M,X}$, $e^n_{M,V}$ and $E^n_{M,X}$, $E^n_{M,V}$.

Since the scheme (2.12) is implicit, iterative solutions are needed, and we consider the following iterative pattern
\[
(\tilde{X}^{ni})^{[0]} = e^{c_i h M} \tilde{X}^n - \varepsilon^{1-m} h \sum_{j=1}^{3} \tilde{a}_{ij}(hM) F \left( SF \left( CF^{-1} \tilde{X}^n + SF^{-1} \tilde{V}^n \right) \right),
\]
\[
(\tilde{V}^{ni})^{[0]} = e^{c_i h M} \tilde{V}^n + \varepsilon^{1-m} h \sum_{j=1}^{3} \tilde{a}_{ij}(hM) F \left( CF \left( CF^{-1} \tilde{X}^n + SF^{-1} \tilde{V}^n \right) \right),
\]
\[
(\tilde{X}^{ni})^{[j+1]} = e^{c_i h M} \tilde{X}^n - \varepsilon^{1-m} h \sum_{j=1}^{3} \tilde{a}_{ij}(hM) F \left( SF \left( CF^{-1} (\tilde{X}^{ni})^{[j]} + SF^{-1} (\tilde{V}^{ni})^{[j]} \right) \right), \quad j = 0, 1, \ldots,
\]
\[
(\tilde{V}^{ni})^{[j+1]} = e^{c_i h M} \tilde{V}^n + \varepsilon^{1-m} h \sum_{j=1}^{3} \tilde{a}_{ij}(hM) F \left( CF \left( CF^{-1} (\tilde{X}^{ni})^{[j]} + SF^{-1} (\tilde{V}^{ni})^{[j]} \right) \right), \quad j = 0, 1, \ldots.
\]

Then according to the property of $e^{c_i h M}$ and the boundedness of the coefficients, the following result can be proved. That is, there exists a small constant $0 < \tau_0 < 1$ such that when $0 < h \leq \tau_0$ and $\tilde{X}^0 \in L^2$ with $\|\tilde{X}^0\|_{L^2} \leq K_1$, we can obtain $\tilde{X}^n \in L^2$, $(\tilde{X}^{ni})^{[\text{stopped num}]} \in L^2$ as well as their bounds $\|\tilde{X}^n\|_{L^2} \leq C_0$, $\|\tilde{X}^{ni}^{[\text{stopped num}]}\|_{L^2} \leq C_0$, where the constant $C_0$ depends on $K_1$. The same bounds can be derived for $\tilde{V}^n \in L^2$, $(\tilde{V}^{ni})^{[\text{stopped num}]} \in L^2$.

The error system of FS-F method is to find $e^n_{M,X}(\tau)$, $e^n_{M,V}(\tau)$ and $E^n_{M,X}(\tau)$, $E^n_{M,V}(\tau)$ in the space $X_M$, i.e., we have
\[
e^n_{M,X}(\tau) = \sum_{k \in \mathcal{M}} (\tilde{e}_{M,X}^{ni})^k e^{ik\tau}, \quad \e^n_{M,X}(\tau) = \sum_{k \in \mathcal{M}} (\tilde{e}_{M,X}^{ni})^k e^{ik\tau},
\]
\[
e^n_{M,V}(\tau) = \sum_{k \in \mathcal{M}} (\tilde{e}_{M,V}^{ni})^k e^{ik\tau}, \quad \e^n_{M,V}(\tau) = \sum_{k \in \mathcal{M}} (\tilde{e}_{M,V}^{ni})^k e^{ik\tau},
\]
where

\[
\begin{align*}
\tilde{e}^{n+1}_{\lambda,M} & = e^{hM}e^{\frac{\tilde{c}_{\lambda}}{M}} + h\varepsilon^{1-m}\sum_{j=1}^{s} b_j(hM)\Delta f^n_{X_j} + \delta^{n+1}_X, \\
\tilde{E}^{n}_{\lambda,M} & = e^{c_{\lambda} hM}e^{\frac{c}{hM}} + h\varepsilon^{1-m}\sum_{j=1}^{s} \tilde{a}_{ij}(hM)\Delta f^n_{X_j} + \Delta^n_X, \\
\tilde{e}^{n+1}_{\lambda,V} & = e^{hM}e^{\frac{\tilde{c}_{\lambda}}{M}} + h\varepsilon^{1-m}\sum_{j=1}^{s} b_j(hM)\Delta f^n_{V_j} + \delta^{n+1}_V, \\
\tilde{E}^{n}_{\lambda,V} & = e^{c_{\lambda} hM}e^{\frac{c}{hM}} + h\varepsilon^{1-m}\sum_{j=1}^{s} \tilde{a}_{ij}(hM)\Delta f^n_{V_j} + \Delta^n_V,
\end{align*}
\]

and

\[
\begin{align*}
\Delta f^n_{X_j} & = -\mathcal{FS}(G(P_{\lambda,M}(t_n + c_j h, \tau), P_{\lambda,V}(t_n + c_j h, \tau)) - G(X^n_{\lambda}, V^n_{\lambda})), \\
\Delta f^n_{V_j} & = \mathcal{FC}(G(P_{\lambda,M}(t_n + c_j h, \tau), P_{\lambda,V}(t_n + c_j h, \tau)) - G(X^n_{\lambda}, V^n_{\lambda})),
\end{align*}
\]

and \(G(\tilde{X}, \tilde{V}) = F(\mathcal{F}^{-1}\tilde{X} + \mathcal{S}^{-1}\tilde{V})\). Here the remainders \(\delta^{n+1}_X\) and \(\delta^{n+1}_V\) are bounded by inserting the exact solution of (2.11) into the numerical approximation, i.e.,

\[
\begin{align*}
X(t_n + c_j h) & = e^{c_{\lambda} hM}X(t_n) - \varepsilon^{1-m}\sum_{j=1}^{3} \tilde{a}_{ij}(hM)\mathcal{FSG}(X(t_n + c_j h), V(t_n + c_j h)) + \Delta^n_X, \\
V(t_n + c_j h) & = e^{c_{\lambda} hM}V(t_n) + \varepsilon^{1-m}\sum_{j=1}^{3} \tilde{a}_{ij}(hM)\mathcal{FCG}(X(t_n + c_j h), V(t_n + c_j h)) + \Delta^n_V,
\end{align*}
\]

By the Duhamel principle and Taylor expansions, the remainders \(\delta^{n+1}_X\) and \(\delta^{n+1}_V\) can be represented as

\[
\begin{align*}
[\delta^{n+1}_X; \delta^{n+1}_V] & = h\varepsilon^{1-m}\int_{0}^{1}\left(e^{(1-\xi)c_{\lambda} hM} \otimes \text{diag}(1, 1)\right)\sum_{j=1}^{4} \frac{(\xi c_{\lambda} h^j)^{-1}}{(j-1)!} \frac{d^{j-1}}{dt^{j-1}} G(t_n) d\xi \\
& \quad - h\varepsilon^{1-m}\sum_{k=1}^{s} b_{k}(hM) \otimes \text{diag}(1, 1)\sum_{j=1}^{4} \frac{c_{k}^{-1} h^{j-1}}{(j-1)!} \frac{d^{j-1}}{dt^{j-1}} G(t_n) + [\delta^{n+1}_X; \delta^{n+1}_V] \\
& = \varepsilon^{1-m}\sum_{j=1}^{4} h^j \left(\psi_{j}(hM) \otimes \text{diag}(1, 1)\right)\frac{d^{j-1}}{dt^{j-1}} G(t_n) + [\delta^{n+1}_X; \delta^{n+1}_V],
\end{align*}
\]

where we take the notation \(G(t) = [\mathcal{FSG}(\tilde{X}(t), \tilde{V}(t)); \mathcal{FCG}(\tilde{X}(t), \tilde{V}(t))]\) and the Kronecker product \(\otimes\). With the bounds of the solution of the two-scale system proposed in Proposition 2.2, it is obtained that \(\frac{d}{dt} G(t_n) = O(\varepsilon^{2-jm})\). Thus we get

\[
[\delta^{n+1}_X; \delta^{n+1}_V] = O\left(\varepsilon^{1-m} h^5 \frac{d^4}{dt^4} G(t_n + \zeta h) d\xi\right) = O(\varepsilon^5 - 5 m h^5),
\]

Similarly, one has

\[
[\Delta^{n}_{X}; \Delta^{n}_{V}] = \varepsilon^{1-m}\sum_{j=1}^{3} h^j \left(\psi_{j,i}(hM) \otimes \text{diag}(1, 1)\right)\frac{d^{j-1}}{dt^{j-1}} G(t_n) + [\Delta^{n}_{X}; \Delta^{n}_{V}]
\]

with \([\Delta^{n}_{X}; \Delta^{n}_{V}] = O(\varepsilon^{4-2m} h^4)\). Then using the stiff order conditions presented in Proposition 2.3, we know that

\[
[\Delta^{n}_{X}; \Delta^{n}_{V}] = [\Delta^{n}_{X}; \Delta^{n}_{V}]
\]
and 
\[ \tilde{\delta}_{\nu}^{n+1}; \tilde{\omega}_{\nu}^{n+1} = \epsilon^{1-m} h^4 \left( \psi_4(hM) \otimes \text{diag}(1, 1) \right) \frac{d^3}{dt^3} \tilde{G}(t_n) + \left[ \tilde{\delta}_{\nu}^{n+1}; \tilde{\omega}_{\nu}^{n+1} \right]. \]

The proof of Proposition 3.4 is immediately complete.

**Proof of the global errors.** We are now in a position to derive the error bounds in a standard way. To make the analysis be more compact, here we only present main points but without details.

Using the concise expressions
\[
\tilde{E}_{\nu}^{n+1} = \left[ \tilde{E}_{\nu}^{n+1}; \tilde{E}_{\nu}^{n+1} \right], \quad \tilde{e}_{\nu}^{n+1} = \left[ \tilde{e}_{\nu}^{n+1}; \tilde{e}_{\nu}^{n+1} \right], \quad \tilde{\Delta}^{n+1} = \left[ \tilde{\Delta}_{\nu}^{n+1}; \tilde{\Delta}_{\nu}^{n+1} \right],
\]
the error recursion (4.2) becomes
\[
\tilde{E}_{\nu}^{n+1} = \left( e^{hM} \otimes I_2 \right) \tilde{E}_{\nu}^{n} + \epsilon \left( \sum_{j=1}^{3} \left( \tilde{\delta}_{\nu}^{n+1}(hM) \otimes I_2 \right) \tilde{\Delta}_{\nu}^{n+1} + \tilde{\Delta}_{\nu}^{n+1} \right),
\]

By Taylor series, one gets \( \tilde{\Delta}_{\nu}^{n+1} = J_n \tilde{E}_{\nu}^{n} + \text{with a matrix } J_n \). Then there exist bounded operators \( N^{ni}(\tilde{E}_{\nu}^{n}) \) such that \( \tilde{E}_{\nu}^{n+1} = \tilde{E}_{\nu}^{n+1}(\tilde{E}_{\nu}^{n}) + \tilde{\Delta}_{\nu}^{n+1} + h^4 \epsilon^{1-4m} R^{ni} \) with uniformly bounded remainders \( R^{ni} \). Now it is arrived at
\[
\tilde{E}_{\nu}^{n+1} = \left( e^{hM} \otimes I_2 \right) \tilde{E}_{\nu}^{n} + \epsilon \left( \sum_{j=1}^{3} \left( \tilde{\delta}_{\nu}^{n+1}(hM) \otimes I_2 \right) \tilde{\Delta}_{\nu}^{n+1} + \tilde{\Delta}_{\nu}^{n+1} \right) + \frac{d^3}{dt^3} \tilde{G}(t_n) + O(\epsilon^{5-5m} h^5)
\]

where we use the notation \( \tilde{\Delta}_{\nu}^{n+1}(\tilde{E}_{\nu}^{n}) = \sum_{j=1}^{s} \left( \tilde{\delta}_{\nu}^{n+1}(hM) \otimes I_2 \right) J_n \tilde{\Delta}_{\nu}^{n+1}(\tilde{E}_{\nu}^{n}) \). Solving this recursion leads to
\[
\tilde{E}_{\nu}^{n+1} = \epsilon \left( \sum_{j=1}^{n-1} \left( \tilde{\delta}_{\nu}^{n+1}(hM) \otimes I_2 \right) \tilde{\Delta}_{\nu}^{n+1}(\tilde{E}_{\nu}^{n}) \right) + \frac{d^3}{dt^3} \tilde{G}(t_n) + O(\epsilon^{5-5m}).
\]

The order condition \( \psi_4(0) = 0 \) shows that there exist bounded operator \( \tilde{\psi}_4(hM) \) with \( \psi_4(hM) = hM \tilde{\psi}_4(hM) \) and Lemma 4.8 of [39] contributes
\[
\sum_{j=0}^{n-1} \left( e^{(n-j-1)hM}(hM) \otimes I_2 \right) \frac{d^3}{dt^3} \tilde{G}(t_n) = \frac{d^3}{dt^3} \tilde{G}(t_n) = O(\epsilon^{3-3m}).
\]

Combined with the above results and using Gronwall inequality leads to \( \tilde{E}_{\nu}^{n+1} = O(h^2 \epsilon^{1-4m}) \). This result and the formulation of the scheme give the final convergence for the numerical solutions of the original system (1.1). The proof of Theorem 3.1 is complete. \( \square \)

**Remark 4.1.** With the same arguments, the accuracy of the second-order method S2O2 can be studied. It is noted that S2O2 satisfies a stronger order condition, i.e., \( \psi_2(hM) = 0 \) instead of \( \psi_2(0) = 0 \), and thus the error brought by \( \sum_{j=0}^{n-1} \left( e^{(n-j-1)hM}(hM) \otimes I_2 \right) \frac{d^3}{dt^3} \tilde{G}(t_n) \) disappears in the analysis. Therefore, we obtain \( \tilde{e}_{\nu}^{n+1} = O(h^2 \epsilon^{1-3m}) \) for S2O2 and its accuracy is improved as stated in Theorem 3.1.
5. **Proof of long time energy conservation (Theorem 3.3)**

Long time energy conservation is proved mainly based on the technology of modulated Fourier expansions, which was firstly developed in [25] and was used for the long-term analysis of many methods [15 16 17 23 27 39 40 41]. The main differences and contributions of long term analysis given in this section involve in two aspects. We extend the technology of modulated Fourier expansions to multi-stage schemes and prove the long-time result for both two-stage and three-stage methods. This provides some developments for studying long-term behavior of various methods. Moreover, in contrast to the existing work, we neither assume bounded energy, nor assume small initial value for the considered system. In the proof, the result is derived for the methods applied to the energy unbounded system [1] with large initial value.

**Proof. Modulated Fourier expansions.** We first derive the modulated Fourier expansions of the numerical integrators, i.e., the numerical scheme S2O2 has the formal expansions:

\[
\hat{X}^n = \Phi(t) := \sum_{k \in \mathbb{N}_\infty^*} e^{i(k \cdot \omega)t} \alpha^k(t), \quad \hat{V}^n = \Psi(t) := \sum_{k \in \mathbb{N}_\infty^*} e^{i(k \cdot \omega)t} \beta^k(t),
\]

where \(\alpha^k\) and \(\beta^k\) are smooth coefficient functions for \(t = nh\) and \(\mathbb{N}_\infty^*\) denotes the set of \(\mathbb{N}_\infty^*\) with \(N = +\infty\). With the same arguments of local errors, it can be shown that the error between \(\hat{X}^n\) and \(\Phi(t + c_i h)\) has the form \(O(\varepsilon^{3-3m}h^2)\Phi(t + \theta h)\) for some \(\theta \in [t, t + c_i h]\). Similar result is true for \(\hat{V}^n\) and \(\Psi(t + c_i h)\). Hence, one can assume that for \(i = 1, 2\)

\[
\hat{X}^n = \Phi(t + c_i h) + C\varepsilon^{3-3m}h^2D^2\Phi(t + c_i h), \quad \hat{V}^n = \Psi(t + c_i h) + C\varepsilon^{3-3m}h^2D^2\Phi(t + c_i h),
\]

where \(C\) is the constant which is independent of \(h, \varepsilon\) and \(D\) is referred to the differential operator (see [26]).

Inserting (5.1) into (2.13) and defining the operators

\[
\mathcal{L}_1(hD) = (e^{hD} - e^{hM})\left(\hat{b}_1(hM)e^{c_1hD} + \hat{b}_2(hM)e^{c_2hD}\right)^{-1},
\]

\[
\mathcal{L}_2(hD) = \left(\hat{b}_1(hM)(e^{c_1hD} + C\varepsilon^{3-3m}h^2D^2) + \hat{b}_2(hM)(e^{c_2hD} + C\varepsilon^{3-3m}h^2D^2)\right)^{-1} - \mathcal{L}_1(hD),
\]

\[
\mathcal{L}(hD) = \mathcal{L}_1(hD) + \mathcal{L}_2(hD),
\]

one has

\[
\mathcal{L}(hD)\Phi(t) = -h\varepsilon^{1-m}\mathcal{FS}(\hat{Y}(t)), \quad \mathcal{L}(hD)\Psi(t) = h\varepsilon^{1-m}\mathcal{FCF}(\hat{Y}(t)).
\]

Here we use the notation \(\hat{Y}(t) := \mathcal{CF}^{-1}\Phi(t) + \mathcal{SF}^{-1}\Psi(t) = \sum_{k \in \mathbb{N}_\infty^*} e^{i(k \cdot \omega)t}x^k(t)\) with \(x^k(t) = \mathcal{CF}^{-1}\alpha^k(t) + \mathcal{SF}^{-1}\beta^k(t)\). Expanding the nonlinearity into its Taylor series yields

\[
\mathcal{L}(hD)\Phi(t) = -h\varepsilon^{1-m}\mathcal{FS} \sum_{k \in \mathbb{N}_\infty^*} e^{i(k \cdot \omega)t} \sum_{m \geq 2} \frac{F^{(m)}(0)}{m!} \sum_{k^1 + \ldots + k^m = k} \left[\gamma^{k^1} \ldots \gamma^{k^m}\right](t),
\]

\[
\mathcal{L}(hD)\Psi(t) = h\varepsilon^{1-m}\mathcal{FC} \sum_{k \in \mathbb{N}_\infty^*} e^{i(k \cdot \omega)t} \sum_{m \geq 2} \frac{F^{(m)}(0)}{m!} \sum_{k^1 + \ldots + k^m = k} \left[\gamma^{k^1} \ldots \gamma^{k^m}\right](t).
\]

We remark that the assumption \(F(0) = 0\) and \(F'(0) = 0\) are used here since the linearization of \(F(u)\) leads to a new nonlinearity \(\hat{F}(u) = F(u) - F'(0)u\) with the property \(\hat{F}'(0) = 0\). Inserting the ansatz (5.1) into these expressions and comparing the coefficients of \(e^{i(k \cdot \omega)t}\), we obtain

\[
\mathcal{L}(hD + i(k \cdot \omega)h)\alpha^k(t) = -h\varepsilon^{1-m}\mathcal{FS} \sum_{m \geq 2} \frac{F^{(m)}(0)}{m!} \sum_{k^1 + \ldots + k^m = k} \left[\gamma^{k^1} \ldots \gamma^{k^m}\right](t),
\]

\[
\mathcal{L}(hD + i(k \cdot \omega)h)\beta^k(t) = h\varepsilon^{1-m}\mathcal{FC} \sum_{m \geq 2} \frac{F^{(m)}(0)}{m!} \sum_{k^1 + \ldots + k^m = k} \left[\gamma^{k^1} \ldots \gamma^{k^m}\right](t).
\]

This is the modulation system for the coefficients \(\alpha^k(t)\) and \(\beta^k(t)\) of the modulated Fourier expansion.
Similarly, we get
\[ \mathcal{L}_1(hD) = -h\Omega I + hD - \frac{1}{2} h\Omega^{-1}\left(-2I + h\Omega\cot(h\Omega/2)\right)iD^2 + \ldots, \] 
with \( \zeta := \frac{1}{2}(h(\Omega - (k \cdot \omega))I) \). Some particular components we need are expressed as
\[ (\mathcal{L}_1(hD + ih\langle j \rangle \cdot \omega))_{j,l} = \frac{h^2\omega_{j,l}^2}{4 \sin^2(h\omega_{j,l}/2)} hD - i\frac{h^2\omega_{j,l}^2}{16 \sin^4(h\omega_{j,l}/2)} (h\omega_{j,l} - \sin(h\omega_{j,l}))(hD)^2 + \ldots. \] 

Similarly, we get
\[ \mathcal{L}_2(hD) = -CD^2(D - i\Omega)e^{3\cdot3m}h^3 + \ldots \]
and this demonstrates that the main part of \( \mathcal{L}(hD) \) comes from \( \mathcal{L}_1(hD) \). In what follows, we use the notations
\[ t_1 = \frac{h^2\omega_{j,l}^2}{4 \sin^2(h\omega_{j,l}/2)}, \ t_2 = -\frac{h^2\omega_{j,l}^2}{16 \sin^4(h\omega_{j,l}/2)}, \ t_3 = -ih^2\Omega^2 \left( h\Omega - \cot \zeta + \cos \zeta \csc \zeta \right)^{-1}. \] 
With these Taylor expansions and in the spirit of Euler’s derivation of the Euler-Maclaurin summation formula (see Chapter II. 10 of [28] and [41]), the following ansatz of the modulated Fourier functions \( \alpha^k(t) \) is derived:
\[ \hat{\alpha}_{j,l}^{(j)}(t) = \frac{h^{1-m}}{t_1} F_{j,l}^1(\cdot) + \ldots, \ j = -N_{\ell}^-, \ldots, N_{\ell}^+, \ \alpha^k(t) = \frac{h^{1-m}}{t_3} \left( F_{j,l}^k(\cdot) + \ldots \right), \ k \neq \langle j \rangle_l, \] 
where the dots mean the power series in \( h \) and \( F^k \) and so on stand for formal series. The coefficients \( \beta^k(t) \) have the same ansatz as \( \alpha^k(t) \). We truncate the series after the \( O(h^{N_{\ell} + N_0}) \) terms for arbitrary positive integer \( N_0 \) since they often diverge. The initial values for the differential equations appeared in the ansatz are determined by considering \( \Psi(0) = \hat{X}^0 \). We thus get
\[ \hat{X}^0_{j,l} = \alpha_{j,l}^{(j)}(0) + O(h^{2-m}\delta_0^2), \]
which yields \( \alpha_{j,l}^{(j)}(0) = O(\delta_0) \).

Under the above analysis and the conditions given in Theorem 3.3, the numerical result \( \hat{X}^n \) and \( \hat{V}^n \) obtained from S2O2 can be expressed by the following modulated Fourier expansions at \( t = nh \)
\[ \hat{X}^n = \sum_{k \in N_{\ell}^s} e^{i(k \cdot \omega)t} \alpha^k(t) + R_{\hat{X},N}(t), \ \hat{V}^n = \sum_{k \in N_{\ell}^s} e^{i(k \cdot \omega)t} \beta^k(t) + R_{\hat{V},N}(t). \] 
From the construction of the coefficient functions, it follows that it is reasonable to assume \( \alpha_{0,l}^k = \beta_{0,l}^k = 0 \) if \( k \neq \langle 0 \rangle_l \) and \( \alpha_{k,m} = \beta_{k,m} = 0 \) if \( |k|_l > 0 \) and \( l \neq m \). Considering the fact \( \hat{X}^n, \hat{V}^n \in \mathbb{R}^D \) yields that \( \alpha_{-l,j}^{-k} = \alpha_{l,j}^k \) and \( \beta_{-l,j}^{-k} = \beta_{l,j}^k \). In what follows, we derive the bounds of the coefficient functions \( \alpha^k(t) \) and \( \beta^k(t) \).

By the first formula of (5.5), we obtain a coarse estimate as
\[ \hat{\alpha}_{j,l}^{(j)}(t) = O\left(\frac{h^{1-m}}{t_1} F^1\right) = O\left(\frac{h^{1-m}}{t_1}\right) \]
and by further considering the bound of \( \alpha_{j,l}^{(j)}(0) \), \( \alpha_{j,l}^{(j)}(t) = O(\delta_0) \). Based on this estimate, it is deduced that \( F^k = O(\delta_0^k|k|) \). Therefore, \( \alpha^k(t) \) is bounded as \( \alpha^k(t) = O\left(\frac{h^{1-m} \delta_0}{t_3}\right) \) by the second formula of (5.5). According to these estimates, a finer bound of \( F^1 \) is determined by
\[ \sum_{k+l+\ldots+k^m=\langle j \rangle_l} \left| \eta_{j,l}^k \right| \ldots \left| \eta_{j,l}^m \right|, \] 
which yields \( F^1 = O(\frac{h^{1-m}}{t_3}) \). Hence, \( \hat{\alpha}_{j,l}^{(j)}(t) = O\left(\frac{h^{1-m} \delta_0^3}{t_3} \right) \). In a same way, the bounds of \( \beta^k(t) \) can be deduced. We summary these results as follows. The
coefficient functions $\alpha^k(t)$ and $\beta^k(t)$ and their derivatives have the bounds
\[
\begin{align*}
\alpha_{j,l}^{(k)}(t) &= O(\delta_0), \quad \alpha_{j,l}^{(k)}(t) = O\left(\frac{h^{2-2n}}{t_3^2} \delta_0^{(n)}\right), \quad \alpha_k^{(k)}(t) = O\left(\frac{h^{1-m}}{t_3} \delta_0^{(0)}\right), \quad k \neq (j), \\
\beta_{j,l}^{(k)}(t) &= O(\delta_0), \quad \beta_{j,l}^{(k)}(t) = O\left(\frac{h^{2-2n}}{t_3^2} \delta_0^{(n)}\right), \quad \beta_k^{(k)}(t) = O\left(\frac{h^{1-m}}{t_3} \delta_0^{(0)}\right), \quad k \neq (j),
\end{align*}
\]  
(5.7) 
where $l = 1, \ldots, d$. The constants symbolised by the notation $O$ are independent of $h, \varepsilon$, but depend on $c_0, c_1$.

The remainede appearances in (5.6) are bounded by
\[
R_{\tilde{X}, \tilde{N}}(t) = O(\varepsilon h^{2-2n} \delta_0^{N+1}), \quad R_{\tilde{Y}, \tilde{N}}(t) = O(\varepsilon h^{2-2n} \delta_0^{N+1}),
\]  
(5.8) 
which are shown as follows. First insert $\Phi(t), \Psi(t)$ into the numerical scheme \(2.13\) and then the corresponding discrepancies are
\[
\begin{align*}
d_1(t) &= \Phi(t + c_1 h) - e^{c_1 h M} \Phi(t) - h\varepsilon^{1-m} \left(\overline{a}_{11} \mathcal{F} \mathcal{S} \mathcal{F}(\overline{Y}(t + c_1 h)) + \overline{a}_{12} \mathcal{F} \mathcal{S} \mathcal{F}(\overline{Y}(t + c_2 h))\right), \\
d_2(t) &= \Phi(t + c_2 h) - e^{c_2 h M} \Phi(t) - h\varepsilon^{1-m} \left(\overline{a}_{11} \mathcal{F} \mathcal{S} \mathcal{F}(\overline{Y}(t + c_1 h)) + \overline{a}_{22} \mathcal{F} \mathcal{S} \mathcal{F}(\overline{Y}(t + c_2 h))\right), \\
d_3(t) &= \Psi(t + c_1 h) - e^{c_1 h M} \Psi(t) + h\varepsilon^{1-m} \left(\overline{a}_{11} \mathcal{F} \mathcal{C} \mathcal{F}(\overline{Y}(t + c_1 h)) + \overline{a}_{12} \mathcal{F} \mathcal{C} \mathcal{F}(\overline{Y}(t + c_2 h))\right), \\
d_4(t) &= \Psi(t + c_2 h) - e^{c_2 h M} \Psi(t) + h\varepsilon^{1-m} \left(\overline{a}_{11} \mathcal{F} \mathcal{C} \mathcal{F}(\overline{Y}(t + c_1 h)) + \overline{a}_{22} \mathcal{F} \mathcal{C} \mathcal{F}(\overline{Y}(t + c_2 h))\right), \\
d_5(t) &= \Phi(t + h) - e^{h M} \Phi(t) - h\varepsilon^{1-m} \left(\overline{b}_1 \mathcal{F} \mathcal{S} \mathcal{F}(\overline{Y}(t + c_1 h)) + \overline{b}_2 \mathcal{F} \mathcal{S} \mathcal{F}(\overline{Y}(t + c_2 h))\right), \\
d_6(t) &= \Psi(t + h) - e^{h M} \Psi(t) + h\varepsilon^{1-m} \left(\overline{b}_1 \mathcal{F} \mathcal{C} \mathcal{F}(\overline{Y}(t + c_1 h)) + \overline{b}_2 \mathcal{F} \mathcal{C} \mathcal{F}(\overline{Y}(t + c_2 h))\right).
\end{align*}
\]
There are two aspects in the bounds of these discrepancies: $O\left(h^{1-m} \delta_0^{N+1}\right) = O(h^{2-2n} \delta_0^{N+1})$ in the truncation of modulated Fourier expansions and $O(h^{N+N_0})$ in the truncation of the ansatz \(\overline{X}, \overline{Y}\). Therefore, discrepancies are bounded by
\[
\begin{align*}
d_j(t) &= O(h^{N+N_0}) + O(h^{2-2n} \delta_0^{N+1}) = O(h^{2-2n} \delta_0^{N+1}) \quad \text{for } j = 1, 2, \ldots, 6
\end{align*}
\]
on the basis of the arbitrarily large number $N_0$. Then define the errors
\[
\begin{align*}
c_{\tilde{X}} = \tilde{X} - \Phi(t_n), \quad E_{\overline{X}n_i} = \tilde{X}_{n_i} - \Phi(t_n + c_i h), \quad c_{\overline{Y}} = \tilde{Y} - \Psi(t_n), \quad E_{\overline{Y}n_i} = \tilde{Y}_{n_i} - \Psi(t_n + c_i h).
\end{align*}
\]
They satisfy the error recursion
\[
\begin{align*}
E_{\overline{X}n_i} &= e^{c_i h M} E_{\overline{X}n_i} - h\varepsilon^{1-m} \sum_{j=1}^{s} \overline{a}_{ij}(h M) \mathcal{F} \mathcal{S} \mathcal{F}(G(\overline{X}_{n_j}, \overline{V}_{n_j})) - F(\overline{Y}(t_n + c_i h)) \right) + d_i(t), \quad i = 1, 2, \\
E_{\overline{Y}n_i} &= e^{c_i h M} E_{\overline{Y}n_i} + h\varepsilon^{1-m} \sum_{j=1}^{s} \overline{b}_{ij}(h M) \mathcal{F} \mathcal{C} \mathcal{F}(G(\overline{X}_{n_j}, \overline{V}_{n_j})) - F(\overline{Y}(t_n + c_i h)) \right) + d_i(t), \quad i = 1, 2, \\
c_{\overline{X}n+1} &= e^{h M} E_{\overline{X}n} - h\varepsilon^{1-m} \sum_{j=1}^{s} \overline{b}_j(h M) \mathcal{F} \mathcal{S} \mathcal{F}(G(\overline{X}_{n+1}, \overline{V}_{n+1})) - F(\overline{Y}(t_n + c_i h)) \right) + d_i(t), \\
c_{\overline{Y}n+1} &= e^{h M} E_{\overline{Y}n} + h\varepsilon^{1-m} \sum_{j=1}^{s} \overline{b}_j(h M) \mathcal{F} \mathcal{C} \mathcal{F}(G(\overline{X}_{n+1}, \overline{V}_{n+1})) - F(\overline{Y}(t_n + c_i h)) \right) + d_i(t).
\end{align*}
\]
Taking the Lipschitz condition of $F$ into account, we obtain
\[
\begin{align*}
\left\|F(C \mathcal{F}^{-1} \overline{X}_{n} + S \mathcal{F}^{-1} \overline{V}_{n}) - F(\overline{Y}(t_n + c_i h))\right\| &\leq L \left\|C \mathcal{F}^{-1} \overline{X}_{n} + S \mathcal{F}^{-1} \overline{V}_{n} - \overline{Y}(t_n + c_i h)\right\| \\
\leq L \left\|C \mathcal{F}^{-1} \overline{X}_{n} + S \mathcal{F}^{-1} \overline{V}_{n} - C \mathcal{F}^{-1} \Phi(t_n + c_i h) - S \mathcal{F}^{-1} \Psi(t_n + c_i h)\right\| &\leq L \left\|E_{\overline{X}n} + L \left\|E_{\overline{Y}n}\right\|.
\end{align*}
\]
The application of the Gronwall inequality now shows the bounds of the defects \(\overline{X}, \overline{Y}\).
where the following notations are used here and after

\[ X_h(t) = \sum_{k \in \mathbb{N}_N^d} X_h^k(t), \quad V_h(t) = \sum_{k \in \mathbb{N}_N^d} V_h^k(t), \quad \Upsilon(t) = \sum_{k \in \mathbb{N}_N^d} \Upsilon_h^k(t), \]

with

\[ X_h^k(t) = e^{i(k \cdot \omega)t} \alpha^k(t), \quad V_h^k(t) = e^{i(k \cdot \omega)t} \beta^k(t), \quad \Upsilon_h^k(t) = e^{i(k \cdot \omega)t} \gamma^k(t). \]

Switching the formulation to \( X_h^k \) and \( V_h^k \), we obtain

\[
L(hD)X_h^k(t) = -h \varepsilon^{1-m} \nabla_{-k} \mathcal{V}(Y(t)) + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1}),
\]

\[
L(hD)V_h^k(t) = h \varepsilon^{1-m} \nabla_{X-k} \mathcal{V}(Y(t)) + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1}),
\]

where the vector \( Y(t) \) is defined as \( Y(t) = (Y_h^k(t))_{k \in \mathbb{N}_N^d} \) with \( Y_h(t) = [X_h(t); V_h(t)] \), and the function \( \mathcal{V}(Y(t)) \) is given by

\[
\mathcal{V}(Y(t)) = \sum_{m=1}^{N} \frac{V^{(m+1)}(0)}{(m+1)!} \sum_{k_1 + \ldots + k_m + 1 = 0} (\Upsilon_h^{k_1} \ldots \Upsilon_h^{k_m+1})(t) \tag{5.9}
\]

with the potential

\[
\mathcal{V}(\tilde{Y}(t)) = \frac{1}{d(N+1)} \sum_{l=1}^{d} \sum_{k \in \mathbb{N}_N^d} U(PCF^{-1}X(t) + PSSF^{-1}V(t))_{k,l} \text{ with } \tilde{Y}(t) = [X(t); V(t)].
\]

By this reformulation, we further switch to the quantities \( \alpha^k(t) \) and \( \beta^k(t) \), and then get

\[
L(hD + ih(k \cdot \omega)) \alpha^k(t) = -h \varepsilon^{1-m} \nabla_{-k} \mathcal{V}(\tilde{\vartheta}(t)) + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1}),
\]

\[
L(hD + ih(k \cdot \omega)) \beta^k(t) = h \varepsilon^{1-m} \nabla_{X-k} \mathcal{V}(\tilde{\vartheta}(t)) + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1}). \tag{5.10}
\]

Here \( \alpha^k \) and \( \beta^k \) determine a new vector \( \vartheta^k = [\alpha^k; \beta^k] \) and then compose \( \tilde{\vartheta} = (\vartheta^k)_{k \in \mathbb{N}_N^d} \).

To derive an almost-invariant of the coefficient functions, we consider the vector functions \( \tilde{\vartheta}(\lambda, t) = (e^{i(k \cdot \mu) \lambda} \vartheta^k(t))_{k \in \mathbb{N}_N^d} \) for any real sequence \( \mu \). Then it follows from the definition \( \text{(5.9)} \) that \( k^1 + \ldots + k^{m+1} = 0 \). This shows that the function \( \mathcal{V}(\tilde{\vartheta}(\lambda, t)) \) is independent of \( \lambda \). Therefore, it is clear that

\[
0 = \frac{d}{d\lambda} |_{\lambda = 0} \mathcal{V}(\tilde{\vartheta}(\lambda, t)) = \sum_{k \in \mathbb{N}_N^d} i(k \cdot \mu) (\alpha^{-k}(t))^\top \nabla_{-k} \mathcal{V}(\tilde{\vartheta}(t))
\]

\[
= \sum_{k \in \mathbb{N}_N^d} i(k \cdot \mu) [\alpha^k; \beta^k]^\top [\nabla_{-k} \mathcal{V}(\tilde{\vartheta}(t)); \nabla_{-k} \mathcal{V}(\tilde{\vartheta}(t))].
\]

Combining with \( \text{(5.10)} \), it is arrived that

\[
0 = \frac{1}{h} \sum_{k \in \mathbb{N}_N^d} i(k \cdot \mu) [\alpha^k; \beta^k]^\top \mathcal{J}[L(hD + ih(k \cdot \omega)) \alpha^k; L(hD + ih(k \cdot \omega)) \beta^k + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1})]
\]

\[
= \mathcal{J}\mathcal{S}\mathcal{J}[L(hD + ih(k \cdot \omega)) \vartheta^k(t) + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1})], \tag{5.11}
\]

with \( \mathcal{J} = \begin{pmatrix} 0 & \Lambda & 0 \\ -\Lambda & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \). By using the properties \( \alpha_{-l,j} = \overline{\alpha_{l,j}} \) and \( \beta_{-l,j} = \overline{\beta_{l,j}} \), \( \text{(5.11)} \) can be reformulated as

\[
0 = \frac{1}{h} \sum_{k \in \mathbb{N}_N^d} i(k \cdot \mu) (\overline{\vartheta^k(t)})^\top \mathcal{S}\mathcal{J}[L(hD + ih(k \cdot \omega)) \vartheta^k(t) + \mathcal{O}(h^2 \varepsilon^{2-m} \delta_0^{N+1})],
\]

where \( \mathcal{S} = \text{diag}(S_1, S_2, \ldots, S_{2d}) \) with

\[
S_1 = S_2 = \ldots = S_{2d} := \begin{pmatrix} 0 & \cdots & 0 & 1 \\ 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \cdots & 0 & 0 \end{pmatrix}_{(N_r+1) \times (N_r+1)}.
\]
It follows from the skew-symmetry of $\mathbf{S} \mathbf{J}$ that the matrix decomposition $\mathbf{S} \mathbf{J} = i \mathbf{P} \mathbf{H} \bar{\mathbf{A}} \mathbf{P}$ is clear, where $\mathbf{P}$ is a unitary matrix and $\bar{\mathbf{A}}$ is a diagonal matrix of the form $\bar{\mathbf{A}} = \text{diag}(-I,I)$. These formulations lead to

$$\frac{1}{\epsilon} \sum_{k \in \mathcal{N}_N} (k \cdot \mathbf{\mu})(\mathbf{\zeta}^k)^\top \bar{\mathbf{A}} L(h\mathbf{D} + i h(k \cdot \mathbf{\omega})) \zeta^k = \mathcal{O}(h \varepsilon^{2m} \delta_0^{N+1}),$$

where $\zeta^k = (\mathbf{P} \mathbf{\phi}^k)$ and $\bar{L}_{j,l} = L_{-j,l}$ for $j = -N_ε/2, \ldots, N_ε/2$ and $l = 1, \ldots, d$. It is worth pointing out that $\bar{L}$ has another possible scheme $\bar{L}_{j,l} = L_{j,l}$ and this does not affect the proof described below.

The following analysis is mainly based on the arguments of [25, 26, 41] and thus we only present the main points here. With the Taylor expansions of $L(h\mathbf{D})$, it is easy to get a function $\mathcal{I}$ which satisfies $\frac{d}{dt} \mathcal{I}[\mathbf{\mu}](t) = \mathcal{O}(h \varepsilon^{2m} \delta_0^{N+1})$ and then

$$\mathcal{I}[\mathbf{\mu}](t) = \mathcal{I}[\mathbf{\mu}](0) + \mathcal{O}(\varepsilon^{2m} \delta_0^{N+1})$$

by an integration. In the light of (5.12) and (5.13), the construction of $\mathcal{I}$ is obtained as follows

$$\mathcal{I}(t) = \sum_{l=1}^{d} \sum_{j=-N_ε/2}^{N_ε/2} \left( \Omega^2(l,l) \left| \alpha^{(j)}_{j,l} \right|^2 (t) + \left| \beta^{(j)}_{j,l} \right|^2 (t) \right) + \sum_{l=1}^{d} \sum_{j=-N_ε/2}^{N_ε/2} \frac{t_2}{t_1} \text{Re} \left( \alpha^{(j)}_{j,l} \bar{\alpha}^{(j)}_{j,l} \right)(t) + \mathcal{O}(\varepsilon^{6-2m} \delta_0^4)

+ \sum_{l=1}^{d} \sum_{j=-N_ε/2}^{N_ε/2} \frac{t_2}{t_1} \text{Re} \left( \beta^{(j)}_{j,l} \bar{\beta}^{(j)}_{j,l} \right)(t) + \mathcal{O}(\varepsilon^{6-2m} \delta_0^4)

= \sum_{l=1}^{d} \sum_{j=-N_ε/2}^{N_ε/2} \left( \Omega^2(l,l) \left| \alpha^{(j)}_{j,l} \right|^2 (t) + \left| \beta^{(j)}_{j,l} \right|^2 (t) \right) + \mathcal{O}(\varepsilon^{6-2m} \delta_0^4)

= \sum_{l=1}^{d} \sum_{j=-N_ε/2}^{N_ε/2} \left( \Omega^2(l,l) \left| \alpha^{(j)}_{j,l} \right|^2 (t) + \left| \beta^{(j)}_{j,l} \right|^2 (t) \right) + \mathcal{O}(\varepsilon^{4-2m} \delta_0^4),$$

where the arbitrary $\mu$ is chosen as $\mu_{j,l} = (-1)^{\left\lfloor \frac{l+1}{2} \right\rfloor} \frac{\sin^2(\frac{1}{2} h \omega_{j,l})}{(\frac{1}{2} h \omega_{j,l})^2}$ for $\alpha^k$ and $\mu_{j,l} = (-1)^{\left\lfloor \frac{l+1}{2} \right\rfloor} \frac{\sin^2(\frac{1}{2} h \omega_{j,l})}{(\frac{1}{2} h \omega_{j,l})^2}$ for $\beta^k$ in the analysis. By multiplying (5.10) with $(\mathbf{\phi}^{-k})^\top$ and summing up the terms, one gets

$$\mathcal{O}(h \varepsilon \delta_0^{N+1}) = \frac{1}{h \varepsilon^{1-m}} \sum_{k \in \mathcal{N}_N} (\mathbf{\phi}^{-k})^\top \mathbf{J} L(h\mathbf{D} + i h(k \cdot \mathbf{\omega})) \mathbf{\phi}^k + \frac{d}{dt} V(\mathbf{\tilde{\phi}}(t))

= \frac{1}{h \varepsilon^{1-m}} \sum_{k \in \mathcal{N}_N} (\mathbf{\zeta}^k)^\top \bar{\mathbf{A}} L(h\mathbf{D} + i h(k \cdot \mathbf{\omega})) \zeta^k + \frac{d}{dt} V(\mathbf{\tilde{\phi}}(t)).$$

Then it can be shown that there exists a function $\mathcal{H}_1$ of the form

$$\mathcal{H}_1(t) = V(\mathbf{\tilde{\phi}}(t)) + \frac{t_2}{t_1} \sum_{j=-N_ε/2}^{N_ε/2} \frac{(\frac{1}{2} h \omega_{j,l})^2}{\sin^2(\frac{1}{2} h \omega_{j,l})} \left( \mathbf{\tilde{\phi}}^{(j)}_{j,l} + \ldots = V(\mathbf{\tilde{\phi}}(t)) + \mathcal{O}(\varepsilon^{3-2m} \delta_0^4)$$

such that $\frac{d}{dt} \mathcal{H}_1[\mathbf{\tilde{\phi}}](t) = \mathcal{O}(h \varepsilon \delta_0^{N+1})$. We are now in a position to give the almost-invariant by defining

$$\mathcal{H} = \frac{1}{\varepsilon^2} \mathcal{I} + \mathcal{H}_1.$$

It has an important property that

$$\varepsilon^2 \mathcal{H}(t) = \varepsilon^2 \mathcal{H}(0) + \mathcal{O}(h \varepsilon^{2-m} \delta_0^{N+1}).$$

Moreover, the relationship between this almost-invariant and the result $H_2$ of the numerical method is derived as

$$\varepsilon^2 \mathcal{H}(t_n) = \mathcal{I}(t_n) + \varepsilon^2 V(\mathbf{\tilde{U}}^n) + \mathcal{O}(\varepsilon^{5-2m} \delta_0^4) + \mathcal{O}(\delta_F) = \varepsilon^2 H_2(\mathbf{\tilde{\phi}}^n, \mathbf{\tilde{p}}^n) + \mathcal{O}(\varepsilon^{4-2m} \delta_F^4) + \mathcal{O}(\delta_F).$$
With the above results, it is easy to get
\[ \varepsilon^2 H_2(\hat{q}^n, \hat{p}^n) = \varepsilon^2 H(t_n) + O(\varepsilon^{4-2m} \delta_0^4) + O(\delta x) \]
\[ = \varepsilon^2 H(t_{n-1}) + hO(\varepsilon^{2-m} \delta_0^{N+1}) + O(\varepsilon^{4-2m} \delta_0^4) + O(\delta x) \]
\[ = \ldots = \varepsilon^2 H(0) + nhO(h) + O(\varepsilon^{4-2m} \delta_0^4) + O(\delta x) \]
as long as \( nh \varepsilon^{2-m} \delta_0^{N+1} \leq \varepsilon^{4-2m} \delta_0^4 \). Then using the connection of \( H_2 \) with \( H \) completes the proof of Theorem 3.3 for S2O2.

**Proof for S3O4.** For the integrator S3O4, it follows from its coefficients that
\[ \hat{X}^{n1} = \Phi(t + c_1 h) + C \varepsilon^{5-5m} h^4 D^4 \Phi(t + c_1 h), \quad \hat{V}^{n1} = \Psi(t + c_1 h) + C \varepsilon^{5-5m} h^4 D^4 \Psi(t + c_1 h), \]
\[ \hat{X}^{n2} = \Phi(t + c_2 h) + C \varepsilon^{5-5m} h^4 D^4 \Phi(t + c_2 h), \quad \hat{V}^{n2} = \Psi(t + c_2 h) + C \varepsilon^{5-5m} h^4 D^4 \Psi(t + c_2 h), \]
\[ \hat{X}^{n3} = \Phi(t + c_3 h) + C \varepsilon^{5-5m} h^4 D^4 \Phi(t + c_3 h), \quad \hat{V}^{n3} = \Psi(t + c_3 h) + C \varepsilon^{5-5m} h^4 D^4 \Psi(t + c_3 h), \]
with the error constant \( C \). We define the operator
\[ \mathcal{L}_{S3}(hD) = (e^{hD} - e^{hM}) (b_1(hM)(c_1 hD + C \varepsilon^{5-5m} h^4 D^4) + b_2(hM)(c_1 hD + C \varepsilon^{5-5m} h^4 D^4))^{-1} \]
for S3O4. Then the rest proceeds are similar to that stated above for S2O2. It should be noted that the bounds of the coefficients in modulated expansions have the same expression as S2O2. For S3O4, the notations \( t_1, t_2, t_3 \) appeared in the above proof (5.3) become
\[ t_1 = \frac{h^4 \omega_4^3}{\sin^4(h \omega_{j,4}/4)(64 \cos(h \omega_{j,4}/4) + 16 \sin(h \omega_{j,4}/4))^4} \]
\[ t_2 = \frac{h^4 \omega_4^3 (-4 + 6 \omega^2_{j,4} + 4 \cos(h \omega_{j,4}))}{256 \sin^4(h \omega_{j,4}/4)(4 \cos(h \omega_{j,4}/4) + \sin(h \omega_{j,4}/4))^2}, \quad t_3 = O(h \Omega), \]
based on the Taylor expansion of \( \mathcal{L}_{S3} \). Therefore, the energy at S3O4 has the following relation with the almost-invariant \( \mathcal{H} \):
\[ \varepsilon^2 \mathcal{H}(t_n) = \mathcal{I}(t_n) + \varepsilon^2 V(\hat{U}^n) + O(\frac{t_2}{t_1 t_3} h^2 \varepsilon^{2-2m} \delta_0^4) + O(\varepsilon^{5-2m} \delta_0^4) + O(\delta x) \]
\[ = \mathcal{I}(t_n) + \varepsilon^2 V(\hat{U}^n) + O(\varepsilon^{4-2m} \delta_0^4) + O(\varepsilon^{5-2m} \delta_0^4) + O(\delta x) \]
\[ = \varepsilon^2 H_2(\hat{q}^n, \hat{p}^n) + O(\varepsilon^{4-2m} \delta_0^4) + O(\delta x). \]
This result yields the estimate of S3O4 given in Theorem 3.3.

6. Conclusion

In this paper, we have designed and analyzed numerical integrators for a class of highly oscillatory second-order differential equations with large initial values. Using three transformations of the original system, two-scale formulation approach, spectral semi-discretisation and general s-stage exponential integrators, a class of large-stepsize highly accurate integrators was formulated as the numerical approximation of (1.1) with large initial data. Stiff order conditions and symmetric property were used in the construction of practical methods. The proposed integrators were shown to have not only optimal uniformly high accuracy but also good long-term energy conservation even for large time stepsizes. The numerical results of two numerical experiments supported the properties of the obtained integrators.

Last but not least, we point out that the main contribution of this paper is that we have established a new framework to design optimal uniform higher-order trigonometric integrators with long time behavior for solving highly oscillatory differential equations with large initial values. We believe that the methodology presented in this paper can be extended to a range of nonlinear Hamiltonian PDEs such as the Dirac equation. The rigorous analysis on this topic will be considered in our next work. Another issue for future exploration is the study of uniform higher-order integrators with exact structure conservation such as symplecticity and energy.
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