Optimal convergence and long-time conservation of exponential integration for Schrödinger equations in a normal or highly oscillatory regime

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Abstract

In this paper, we formulate and analyse exponential integrations when applied to nonlinear Schrödinger equations in a normal or highly oscillatory regime. A kind of exponential integrators with energy preservation, optimal convergence and long time near conservations of actions, momentum and density will be formulated and analysed. To this end, we derive continuousstage exponential integrators and show that the integrators can exactly preserve the energy of Hamiltonian systems. Three practical energy-preserving integrators are presented. It is shown that these integrators exhibit optimal convergence and have near conservations of actions, momentum and density over long times. A numerical experiment is carried out to support all the theoretical results presented in this paper. Some applications of the integrators to other kinds of ordinary/partial differential equations are also presented.

Keywords: Schrödinger equations; exponential integration; energy-preserving methods; optimal convergence; modulated Fourier expansion

MSC: 65P10, 65M70.

1 Introduction

The main aim of this paper is to present the formulation and analysis of exponential integration when applied to the nonlinear Schrödinger equation (NSE) with periodic boundary conditions (see [16, 17])

$$\begin{cases} iu_t(t,x) = -\frac{1}{\varepsilon} \Delta u(t,x) + \lambda |u(t,x)|^2 u(t,x), & (t,x) \in [0,T] \times [-\pi,\pi]^d, \\ u(0,x) = u^0(x), & x \in [-\pi,\pi]^d, \end{cases}$$
(1)

where λ is a parameter and ε determines the regime of the solution. In this paper, we consider two different regimes: the normal regime $\varepsilon = 1$ and the highly oscillatory regime $0 < \varepsilon \ll 1$ which

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means that the solution is highly oscillatory. It is known that the solution of this equation exactly conserves the following energy

$$H[u,\bar{u}] = \frac{1}{2(2\pi)^d} \int_{[-\pi,\pi]^d} \left(\frac{1}{\varepsilon} |\nabla u|^2 + \frac{1}{2}\lambda |u|^4\right) dx,$$
(2)

where $|\cdot|$ denotes the Euclidean norm. Apart from this, the solution also has the conservations of the momentum

$$K[u,\bar{u}] = \mathrm{i}\frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} (u\nabla\bar{u} - \bar{u}\nabla u) dx,\tag{3}$$

and of the density or mass

$$m[u,\bar{u}] = i \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} |u|^2 dx.$$
 (4)

For the linear Schrödinger equation, its solution exactly conserves the actions

$$I_j(u, \bar{u}) = \frac{1}{2} |u_j|^2, \qquad j \in \mathbb{Z}^d,$$
(5)

where u_j is defined by $u(t,x) = \sum_{j \in \mathbb{Z}^d} u_j(t)e^{i(j \cdot x)}$ with $j \cdot x = j_1 x_1 + \dots + j_d x_d$. For nonlinear

equation (1), it has been shown that these actions are approximately conserved over long times under conditions of small initial data and non-resonance (see [29, 30]). In this paper, only cubic Schrödinger equation with $x \in [-\pi, \pi]^d$ is considered for brevity, although all our ideas, algorithms and analysis can be easily extended to the solutions of other NSEs.

As is known, NSEs often arise in a wide range of applications such as in fiber optics, physics, quantum transport and other applied sciences, and we refer the reader to [23, 40, 43]. In order to effectively solve NSEs, various numerical methods have been developed and researched in recent decades. With regard to some related methods of this topic, we refer the reader to exponential-type integrators (see, e.g. [5, 8, 12, 14, 19, 21, 52]), splitting methods (see, e.g. [1, 9, 17, 22, 30, 45, 50]), multi-symplectic methods (see, e.g. [5]), Fourier integrators (see, e.g. [24, 42, 47]), waveform relaxation algorithms (see, e.g. [27]) and other effective methods (see, e.g. [2, 3, 6, 31, 38, 41]).

In the last two decades, structure-preserving algorithms of Hamiltonian partial differential equations (PDEs) have also been received much attention and we refer to [10, 35, 38, 57]. Amongst the typical subjects of structure-preserving algorithms are energy-preserving (EP) schemes (see, e.g. [20, 26, 32, 39, 49, 46, 53, 54]). One important property of EP methods is that they can exactly preserve the energy of the considered system. On the other hand, long-time conservation properties of different methods when applied to Hamiltonian systems have been researched in many research publications (see, e.g. [19, 29, 30, 34, 35]). All the long-time analyses can be achieved by using the technique of modulated Fourier expansions, which was developed by Hairer and Lubich in [33].

With regard to the existing researches on these two topics for Schrödinger equations, we have comments as follows:

a) Concerning EP methods for NSEs, although the average vector field method (see [15]) and Hamiltonian Boundary Value Methods (see [11]) were considered, exponential EP methods have not been studied well for Schrödinger equations in the literature. Recently, the authors in [55] derived a kind of exponential collocation methods, but the energy conservation only holds under some special conditions. Exponential structure-preserving Runge-Kutta methods have been studied in [10] for first-order ODEs and the methods are shown to exactly preserve conformal symplecticity and decay (or growth) rates in linear and quadratic invariants. However, energy-preserving exponential Runge-Kutta methods have not been considered there. Exponential EP integrators as well as their convergence have not been established rigorously for NSEs.

b) For the long time analysis of numerical methods applied to NSEs, there have also been many publications, and we refer the reader to [19, 28, 29, 30]. Unfortunately, however, all the methods described in these publications are not EP methods. Too little attention has been paid to the long term analysis of EP methods in other qualitative aspects for solving NSEs in the literature.

The above facts motivate this paper and the main contributions will be made as follows:

A) By using the idea of continuous-stage methods, we formulate a kind of exponential integration. This formulation will provide novel energy-preserving methods and this will be discussed in detail in Sect. 2.

B) For the obtained EP methods, we analyze their optimal convergence for the first time. We prove by using the averaging technique [17], that some schemes exhibit improved error bounds for highly oscillatory NSEs (Sect. 3).

C) It is also shown that these EP integrators have near conservations of actions, momentum and density over long times by using modulated Fourier expansions (Sect. 4).

After these steps, a novel kind of exponential integration with energy preservation, optimal convergence and long time near conservations of actions, momentum and density is obtained. All the theoretical results presented in this paper will be supported numerically by a numerical experiment carried out in Sect. 5. The last section concerns some applications of the integrators and some issues which will be studied further.

2 Energy-preserving exponential integrators

In order to derive energy-preserving exponential integrators, we consider the simple but classical way: Duhamel formulation of the equation and the discretization of the integral, which has been used in many publications (see, e.g. [3, 8, 10, 12, 14, 19, 21, 36, 44, 47]). Although this formulation is not new, the obtained methods will have some advantages and we will make some important notes in Remark 1 below.

Rewrite the NSE (1) as

$$\frac{\partial u}{\partial t}(t,x) = i\mathcal{A}u(t,x) + f(u(t,x)), \quad u(0,x) = u^0(x), \tag{6}$$

where \mathcal{A} is the differential operator defined by $(\mathcal{A}u)(t,x) = \frac{1}{\varepsilon} \Delta u(t,x)$ and $f(u) = -i\lambda |u|^2 u$. The Duhamel principle of this system gives

$$u(t_n + h, x) = e^{ih\mathcal{A}}u(t_n, x) + h \int_0^1 e^{(1-\xi)ih\mathcal{A}} f(u(t_n + \xi h, x))d\xi$$
(7)

with the time stepsize h and $t_n = nh$. Then we define the operator-argument functions φ_j by

$$\varphi_0(\mathbf{i}t\mathcal{A}) := e^{\mathbf{i}t\mathcal{A}}, \quad \varphi_j(\mathbf{i}t\mathcal{A}) := \int_0^1 e^{\mathbf{i}(1-\xi)t\mathcal{A}} \frac{\xi^{j-1}}{(j-1)!} \mathrm{d}\xi, \quad j = 1, 2, \dots$$
(8)

We deal with the integral appearing in (7) by the idea of continuous-stage methods and define the novel integrators as follows. **Definition 1** (*Exponential time integrators.*) For solving the NSE (1), a continuous-stage exponential time integrator is defined as follows:

$$u^{n+\tau}(x) = \Phi^{\tau h}(u^n(x)) := C_{\tau}(\mathcal{V})u^n(x) + h \int_0^1 A_{\tau,\sigma}(\mathcal{V})f(u^{n+\sigma}(x))d\sigma, \quad 0 \le \tau \le 1, \ n = 0, 1, \dots,$$

where $\mathcal{V} = ih\mathcal{A}$, $C_{\tau}(\mathcal{V})$ and $A_{\tau,\sigma}(\mathcal{V})$ are bounded operator-argument functions and $C_{\tau}(\mathcal{V})$ is required to satisfy $C_{c_j}(\mathcal{V}) = e^{c_j \mathcal{V}}$ for $j = 0, \ldots, s$ with the fitting nodes c_j and $s \ge 1$. It is required that $c_0 = 0$ and $c_s = 1$. The numerical solution after one time stepsize h is obtained by letting $\tau = 1$ in (9).

Remark 1 Although this exponential time integrator is formulated by the Duhamel formulation and the discretization of the integral, which is a very simple and classical way, it is important to note that this scheme has the following advantages.

- At the first sight, for a p-th order exponential integrator, it will produce errors of order $\mathcal{O}(\frac{h^p}{\varepsilon^p})$ when it is used to solving (1) with a time step size h. However, for the scheme (9) presented above, we will show that some obtained methods exhibit improved error bounds such as $\mathcal{O}(\frac{h^2}{\varepsilon})$ or $\mathcal{O}(\frac{h^3}{\varepsilon^2})$.
- We have noticed that some novel methods with improved or uniform accuracy have been presented (see, e.g. [3, 16, 17, 42, 47]). These methods have good even better convergence result than the methods given in this paper but they do not have energy, actions, momentum and density conservations. Based on the scheme (9), we will obtain some energy-preserving exponential integrators with improved error bounds. We will also show that this scheme (9) can provide methods with near conservations of actions, momentum and density over long times. In other words, the scheme (9) can produce some practical methods with three properties simultaneously: energy preservation, improved error bounds and near conservations of actions, momentum and density.

For the integrator (9), its energy conservation property is shown as follows.

Theorem 1 (Energy-preserving conditions.) Let $\mathcal{K} = hJ\mathcal{M}$ with $\mathcal{M} = \begin{pmatrix} \mathcal{A} & 0 \\ 0 & \mathcal{A} \end{pmatrix}$ and $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. If the coefficients of the scheme (9) satisfy $\begin{cases} A_{0,\sigma}(\mathcal{K}) = \mathbf{0}, \\ (e^{\mathcal{K}})^{\mathsf{T}} \mathcal{M} A_{1,\tau}(\mathcal{K}) \mathcal{K} + (C'_{\tau}(\mathcal{K}))^{\mathsf{T}} \mathcal{M} = \mathbf{0}, \\ \mathcal{K}^{\mathsf{T}}(A_{1,\tau}(\mathcal{K}))^{\mathsf{T}} \mathcal{M} A_{1,\sigma}(\mathcal{K}) \mathcal{K} + \mathcal{M} A'_{\tau,\sigma}(\mathcal{K}) \mathcal{K} + (\mathcal{M} A'_{\sigma,\tau}(\mathcal{K}) \mathcal{K})^{\mathsf{T}} = \mathbf{0}, \end{cases}$ (10)

with $C_{\tau}'(\mathcal{K}) = \frac{d}{d\tau}C_{\tau}(\mathcal{K})$ and $A_{\tau,\sigma}'(\mathcal{K}) = \frac{\partial}{\partial\tau}A_{\tau,\sigma}(\mathcal{K})$, then the integrator (9) exactly preserves the energy (2), i.e., $H[u^{n+1}, \bar{u}^{n+1}] = H[u^n, \bar{u}^n]$ for $n = 0, 1, \ldots$

<u>Proof</u> By letting u = p + iq, we rewrite the equation (1) as a infinite-dimensional real Hamiltonian system

$$\frac{\partial y}{\partial t} = J\mathcal{M}y + J\nabla_y U(y) \quad y_0(x) = \begin{pmatrix} \operatorname{Re}(u_0(x)) \\ \operatorname{Im}(u_0(x)) \end{pmatrix}, \tag{11}$$

where $y = \begin{pmatrix} p \\ q \end{pmatrix}$ and $U(y) = -\frac{\lambda}{4}(p^2 + q^2)^2$. The energy of this system accordingly becomes

$$\mathcal{H}(p,q) = \frac{-1}{2(2\pi)^d} \int_{\mathbf{T}^d} \left(p\mathcal{A}p + q\mathcal{A}q - \frac{\lambda}{2}(p^2 + q^2)^2 \right) dx.$$
(12)

Our continuous-stage exponential integrator (9) applying to (11) gives

$$\begin{cases} Y^{n+\tau}(x) = C_{\tau}(\mathcal{K})y^{n}(x) + h \int_{0}^{1} A_{\tau,\sigma}(\mathcal{K})g(Y^{n+\sigma}(x))d\sigma, & 0 \le \tau \le 1, \\ y^{n+1}(x) = e^{\mathcal{K}}y^{n}(x) + h \int_{0}^{1} A_{1,\tau}(\mathcal{K})g(Y^{n+\tau}(x))d\tau, \end{cases}$$
(13)

where $g(y) = J\nabla_y U(y)$.

Inserting the numerical scheme (13) into (12) yields

$$\mathcal{H}[y^{n+1}] = \frac{-1}{2(2\pi)^d} \int_{\mathbf{T}^d} \left\{ \frac{1}{2} (y^n)^{\mathsf{T}} \mathcal{M} y^n + (y^n)^{\mathsf{T}} (e^{\mathcal{K}})^{\mathsf{T}} \mathcal{M} \int_0^1 A_{1,\tau}(\mathcal{K}) \mathcal{K} \tilde{g}(Y^{n+\tau}) d\tau + \frac{1}{2} \int_0^1 \left(A_{1,\tau}(\mathcal{K}) \mathcal{K} \tilde{g}(Y^{n+\tau}) \right)^{\mathsf{T}} d\tau \mathcal{M} \int_0^1 A_{1,\tau}(\mathcal{K}) \mathcal{K} \tilde{g}(Y^{n+\tau}) d\tau + U(y^{n+1}) \right\} dx,$$

$$(14)$$

where $\tilde{g} = \mathcal{M}^{-1} \nabla_y U(y)$ and we have used the result $(e^{\mathcal{K}})^{\intercal} \mathcal{M} e^{\mathcal{K}} = \mathcal{M}$ (see [44]). It follows from the first condition of (10) that $Y^n = y^n$ and $Y^{n+1} = y^{n+1}$. Then one arrives at

$$\begin{split} U(y^{n+1}) - U(y^n) &= \int_0^1 \left(\nabla_y U(Y^{n+\tau}) \right)^\mathsf{T} dY^{n+\tau} \\ &= \int_0^1 \left(\nabla_y U(Y^{n+\tau}) \right)^\mathsf{T} d \left(C_\tau(\mathcal{K}) y^n + h \int_0^1 A_{\tau,\sigma}(\mathcal{K}) g(Y^{n+\sigma}) d\sigma \right) \\ &= (y^n)^\mathsf{T} \int_0^1 (C'_\tau(\mathcal{K}))^\mathsf{T} \mathcal{M} \tilde{g}(Y^{n+\tau}) d\tau + \int_0^1 \int_0^1 \left(\tilde{g}(Y^{n+\tau}) \right)^\mathsf{T} \mathcal{M} A'_{\tau,\sigma}(\mathcal{K}) \mathcal{K} \tilde{g}(Y^{n+\sigma}) d\tau d\sigma. \end{split}$$

Therefore, using the above results and the second condition of (10), we obtain

$$\begin{aligned} \mathcal{H}[y^{n+1}] &- \mathcal{H}[y^n] \\ = \frac{-1}{2(2\pi)^d} \int_{\mathbf{T}^d} \frac{1}{2} \int_0^1 \int_0^1 \left(\tilde{g}(Y^{n+\tau}) \right)^{\mathsf{T}} \Big\{ (\mathcal{K})^{\mathsf{T}} (A_{1,\tau}(\mathcal{K}))^{\mathsf{T}} \mathcal{M} A_{1,\sigma}(\mathcal{K}) \mathcal{K} + 2\mathcal{M} A_{\tau,\sigma}'(\mathcal{K}) \mathcal{K} \Big\} \tilde{g}(Y^{n+\sigma}) d\tau d\sigma dx \\ = \frac{-1}{2(2\pi)^d} \int_{\mathbf{T}^d} \frac{1}{2} \int_0^1 \int_0^1 \left(\tilde{g}(Y^{n+\sigma}) \right)^{\mathsf{T}} \Big\{ (\mathcal{K})^{\mathsf{T}} (A_{1,\sigma}(\mathcal{K}))^{\mathsf{T}} \mathcal{M} A_{1,\tau}(\mathcal{K}) \mathcal{K} + 2\mathcal{M} A_{\sigma,\tau}'(\mathcal{K}) \mathcal{K} \Big\} \tilde{g}(Y^{n+\tau}) d\sigma d\tau dx \\ = \frac{-1}{2(2\pi)^d} \int_{\mathbf{T}^d} \frac{1}{2} \int_0^1 \int_0^1 \left(\tilde{g}(Y^{n+\tau}) \right)^{\mathsf{T}} \Big\{ (\mathcal{K})^{\mathsf{T}} (A_{1,\tau}(\mathcal{K}))^{\mathsf{T}} \mathcal{M} A_{1,\sigma}(\mathcal{K}) \mathcal{K} + (2\mathcal{M} A_{\sigma,\tau}'(\mathcal{K}) \mathcal{K})^{\mathsf{T}} \Big\} \tilde{g}(Y^{n+\sigma}) d\tau d\sigma dx. \end{aligned}$$

It is clear from the third equality of (10) that

$$2(\mathcal{H}[y^{n+1}] - \mathcal{H}[y^n]) = \frac{-1}{2(2\pi)^d} \int_{\mathbf{T}^d} \int_0^1 \int_0^1 \left(\tilde{g}(Y^{n+\tau}) \right)^{\mathsf{T}} \Big\{ (\mathcal{K})^{\mathsf{T}} (A_{1,\tau}(\mathcal{K}))^{\mathsf{T}} \mathcal{M} A_{1,\sigma}(\mathcal{K}) \mathcal{K} + \mathcal{M} A'_{\sigma,\tau}(\mathcal{K}) \mathcal{K} + (\mathcal{M} A'_{\sigma,\tau}(\mathcal{K}) \mathcal{K})^{\mathsf{T}} \Big\} \tilde{g}(Y^{n+\sigma}) d\tau d\sigma dx$$
$$=0.$$

The proof is completed.

In what follows, we present three practical energy-preserving algorithms based on the scheme (9) and on the conditions (10) of energy preservation. The coefficients are obtained by solving the conditions (10) and we omit the details of calculations for brevity.

Algorithm 1 (Energy-preserving algorithm 1.) For the integrator given in Definition 1, consider s = 1 and define a practical method (9) with the coefficients

$$C_{\tau}(\mathcal{V}) = (1-\tau)I + \tau e^{\mathcal{V}}, \ A_{\tau,\sigma}(\mathcal{V}) = \tau \varphi_1(\mathcal{V}).$$

We shall refer to this integrator by EP1.

Algorithm 2 (Energy-preserving algorithm 2.) We choose s = 2 and the coefficients of (9) are given by

$$C_{\tau}(\mathcal{V}) = \frac{(\tau-1)(\tau-m)}{m}I + \frac{\tau(\tau-1)}{m(m-1)}e^{m\mathcal{V}} + \frac{\tau(m-\tau)}{m-1}e^{\mathcal{V}}, \ A_{\tau,\sigma}(\mathcal{V}) = \sum_{l=1}^{2}\sum_{n=1}^{2}a_{ln}(\mathcal{V})\tau^{l}\sigma^{n-1},$$

where m is a parameter required that $m \neq 0, 1$, and

$$\begin{aligned} a_{11}(\mathcal{V}) &= \frac{1+m}{m(1-m)}\varphi_1(m\mathcal{V}) + \frac{m+1}{m-1}\varphi_1(\mathcal{V}) + \frac{1}{1-m}\varphi_1((1-m)\mathcal{V}), \\ a_{22}(\mathcal{V}) &= \frac{2}{m(1-m)} \left(\varphi_1(m\mathcal{V}) - \varphi_1(\mathcal{V}) + \varphi_1((1-m)\mathcal{V})\right), \\ a_{21}(\mathcal{V}) &= (1+1/m)\varphi_1(\mathcal{V}) - 1/m\varphi_1((1-m)\mathcal{V}) - a_{11}(\mathcal{V}), \\ a_{12}(\mathcal{V}) &= -2/m(\varphi_1(\mathcal{V}) - \varphi_1((1-m)\mathcal{V})) - a_{22}(\mathcal{V}). \end{aligned}$$

As an example of this method, we choose m = 1/2 and denoted it by EP2.

Algorithm 3 (Energy-preserving algorithm 3.) As another example, we choose s = 3 and

$$C_{\tau}(\mathcal{V}) = \sum_{k=0}^{3} l_{k}(\tau) e^{c_{k}\mathcal{V}}, \ A_{\tau,\sigma}(\mathcal{V}) = \sum_{l=1}^{3} \sum_{n=1}^{3} a_{ln}(\mathcal{V}) \tau^{l} \sigma^{n-1},$$

where $l_j(\tau) = \prod_{k \neq j} \frac{\tau - c_k}{c_j - c_k}$ for $j = 0, \dots, 3$ and

$$\begin{aligned} a_{jj}(\mathcal{V}) &= -\left(c_1C_{j0}C_{j1}\varphi_{1,c_1} + c_2C_{j0}C_{j2}\varphi_{1,c_2} + (c_2 - c_1)C_{j1}C_{j2}\varphi_{1,c_2 - c_1} \right. \\ &+ C_{j0}C_{j3}\varphi_{1,1} + (1 - c_1)C_{j1}C_{j3}\varphi_{1,1 - c_1} + (1 - c_2)C_{j2}C_{j3}\varphi_{1,1 - c_2}\right)/j, \ j = 1, 2, 3, \\ a_{j+1,1}(\mathcal{V}) &= -\left(c_1C_{j1}C_{00}\varphi_{1,c_1} + c_2C_{j2}C_{00}\varphi_{1,c_2} + (c_2 - c_1)C_{j2}C_{01}\varphi_{1,c_2 - c_1} \right. \\ &+ C_{j3}C_{00}\varphi_{1,1} + (1 - c_1)C_{j3}C_{01}\varphi_{1,1 - c_1} + (1 - c_2)C_{j3}C_{02}\varphi_{1,1 - c_2}\right)/j, \ j = 1, 2, \\ a_{1,j+1}(\mathcal{V}) &= -\left(c_1C_{j0}C_{01}\varphi_{1,c_1} + c_2C_{j0}C_{02}\varphi_{1,c_2} + (c_2 - c_1)C_{j1}C_{02}\varphi_{1,c_2 - c_1} \right. \\ &+ C_{j0}C_{03}\varphi_{1,1} + (1 - c_1)C_{j1}C_{03}\varphi_{1,1 - c_1} + (1 - c_2)C_{j2}C_{03}\varphi_{1,1 - c_2}\right)/j, \ j = 1, 2, \\ a_{32}(\mathcal{V}) &= -\left(c_1C_{21}C_{10}\varphi_{1,c_1} + c_2C_{22}C_{10}\varphi_{1,c_2} + (c_2 - c_1)C_{22}C_{11}\varphi_{1,c_2 - c_1} \right. \\ &+ C_{23}C_{10}\varphi_{1,1} + (1 - c_1)C_{23}C_{11}\varphi_{1,1 - c_1} + (1 - c_2)C_{23}C_{12}\varphi_{1,1 - c_2}\right), \\ a_{23}(\mathcal{V}) &= -\left(c_1C_{20}C_{11}\varphi_{1,c_1} + c_2C_{20}C_{12}\varphi_{1,c_2} + (c_2 - c_1)C_{21}C_{12}\varphi_{1,c_2 - c_1} \right. \\ &+ C_{20}C_{13}\varphi_{1,1} + (1 - c_1)C_{21}C_{13}\varphi_{1,1 - c_1} + (1 - c_2)C_{22}C_{13}\varphi_{1,1 - c_2}\right). \end{aligned}$$

Here we choose $c_1 = 1/3$, $c_2 = \frac{1}{18}(14 + (71 - 9\sqrt{58})^{\frac{1}{3}} + (71 + 9\sqrt{58})^{\frac{1}{3}})$ and use the notations

$$\begin{split} \varphi_{1,1} &= \varphi_1(\mathcal{V}), & \varphi_{1,c_1} = \varphi_1(c_1\mathcal{V}), & \varphi_{1,c_2} = \varphi_1(c_2\mathcal{V}), \\ \varphi_{1,1-c_1} &= \varphi_1((1-c_1)\mathcal{V}), & \varphi_{1,1-c_2} = \varphi_1((1-c_2)\mathcal{V}), & \varphi_{1,c_2-c_1} = \varphi_1((c_2-c_1)\mathcal{V}), \\ C_{00} &= \frac{c_1+c_2+c_1c_2}{-c_1c_2}, & C_{01} = \frac{c_2}{(-1+c_1)c_1(c_1-c_2)}, & C_{02} = \frac{-c_1}{(c_1-c_2)(-1+c_2)c_2}, \\ C_{10} &= \frac{2(1+c_1+c_2)}{c_1c_2}, & C_{11} = \frac{2(1+c_2)}{(-c_1+c_2)(-c_1+c_2)}, & C_{12} = \frac{2(1+c_1)}{(c_1-c_2)(-1+c_2)c_2}, \\ C_{20} &= -\frac{3}{c_1c_2}, & C_{21} = \frac{3}{(-1+c_1)c_1(c_1-c_2)}, & C_{22} = \frac{-3}{(c_1-c_2)(-1+c_2)c_2}. \end{split}$$

We shall refer to this semi-discrete integrator by EP3.

The presented three algorithms EP1-EP3 are obtained by considering the conditions (10) of energy preservation and this shows that all of them are energy-preserving schemes. It is noted that some more energy-preserving schemes can be derived from other value of s and (10) and we omit them for brevity. The main observation of the paper is that some of these energy-preserving algorithms show optimal error bound and good near conservations of actions, momentum and density over long times. All of these observations will be illustrated by numerical experiments in Sect. 5. The next two sections are devoted to the optimal convergence and long time conservations in actions, momentum and density.

3 Optimal convergence

In this section, we analyze the convergence of the presented three schemes EP1-EP3.

3.1 Notations and auxiliary results

In this part, we present some auxiliary results which will be used in the analysis. For the exact solution to (1), we require the following assumption.

Assumption 1 It is assumed that the initial value $u^0(x)$ is chosen in H^{α} with the sufficiently large exponent $\alpha > 0$. Then the exact solution to (1) is sufficiently regular.

In the analysis of convergence, we will reparametrize the time variable t as

$$\kappa := t/\varepsilon. \tag{15}$$

By letting

$$w(\kappa, x) := u(t, x), \tag{16}$$

it is obtained that

$$w_{\kappa}(\kappa, x) = \frac{\partial}{\partial \kappa} u(t, x) = \varepsilon u_t(t, x)$$

Thus in this section, we consider the following equivalent long-term NSE ([17])

$$\begin{cases} \mathrm{i}w_{\kappa}(\kappa,x) = -\Delta w(\kappa,x) + \varepsilon \lambda |w(\kappa,x)|^2 w(\kappa,x), & (\kappa,x) \in [0,T/\varepsilon] \times [-\pi,\pi]^d, \\ w(0,x) = w^0(x) := u^0(x), & x \in [-\pi,\pi]^d, \end{cases}$$
(17)

which helps to zoom-in to see the different scales between ε and time step, and to see the averaging effect which will be used in the proof of the convergence. The solution of (17) satisfies the following properties.

Theorem 2 (See [13].) For any $\varepsilon > 0$ and $w^0 \in H^{\alpha}$, there exists a constant T > 0 such that, the long-term NSE (17) has a unique solution which satisfies

$$w \in C^0([0, T/\varepsilon]; H^{\alpha}) \bigcap C^1([0, T/\varepsilon]; H^{\alpha-2})$$

and

$$\|w(\kappa,\cdot)\|_{H^{\alpha}} \leq K \|w^0\|_{H^{\alpha}}$$
 for any $\kappa \in [0, T/\varepsilon]$,

where $\alpha > d/2 + 2$ and K > 1.

Proposition 1 (See [17].) Let $f(w) = -i\lambda |w|^2 w$ and the following two estimates hold for this function.

• For the function $f(w) \in C^{\infty} : H^{\alpha} \to H^{\alpha}$, there exists a constant M > 0 such that for all $(w, v) \in H^{\alpha} \times H^{\alpha}$, it has the estimates

$$||f(w)||_{H^{\alpha}} \le M, ||f'(w)(v)||_{H^{\alpha}} \le M ||v||_{H^{\alpha}}.$$

Moreover, similar estimates for higher derivatives also hold. If α is changed into $\alpha - 2 > 0$, all the results are still true.

• The function has the Lipschitz estimate

$$||f(w) - f(v)||_{H^{\beta}} \le L ||u - v||_{H^{\beta}}, \quad (w, v) \in H^{\alpha - 2} \times H^{\alpha - 2},$$

where $\beta \in [0, \alpha - 2]$ and L > 0 is a constant.

Proposition 2 (See [21].) Denote by φ a bounded function (bounded by $C \ge 0$) from $i\mathbb{R}$ to \mathbb{C} and then the operator-argument function $\varphi(ih\Delta)$ is bounded by

$$\|\varphi(ih\Delta)\|_{H^{\alpha} \hookrightarrow H^{\alpha}} \le C$$

for all h > 0 and $\alpha \ge 0$. For example, the estimate $\|e^{ih\Delta}\|_{H^{\alpha} \hookrightarrow H^{\alpha}} = 1$ holds.

3.2 Main result

We first note that for the long term NSE (17), the evolution operator $e^{it\Delta}$ is periodic with period T_0 ([17]). For simplicity, it is assumed that $T_0 = 1$ in this section since this can be achieved by a simple rescaling of time. For simplicity of notations, we shall denote

 $A \lesssim B$

for $A \leq CB$ with a generic constant C > 0 independent of n or the time step size or ε but depends on T and the constants appeared in Theorem 2 and Propositions 1-2. We use the abbreviation $w(\kappa)$ instead of $w(\kappa, x)$ for brevity. For solving the long term NSE (17), the exponential time integrator becomes

$$w^{n+\tau}(x) = \Phi^{\tau\delta\kappa}(w^n(x)) := C_{\tau}(\mathcal{W})w^n(x) + \varepsilon\delta\kappa \int_0^1 A_{\tau,\sigma}(\mathcal{W})f(w^{n+\sigma}(x))d\sigma, \quad 0 \le \tau \le 1,$$
(18)

where $\delta \kappa := \kappa_{n+1} - \kappa_n$ is the time step size and $\mathcal{W} = i\delta\kappa\Delta$. Then EP1-EP3 for solving (17) can also be obtained by considering Algorithms 1-3, respectively. The optimal convergence of these algorithms is given by the following theorem.

Theorem 3 (Optimal convergence of algorithms for the long term system.) There exists a constant $N_0 > 0$ independent of ε , such that for any time step $\delta \kappa = \frac{T_0}{N}$ with any integer $N \ge N_0$, the EP1-EP3 for solving the long term system (17) have the following error bounds for both regimes ε :

$$EP1: \quad \left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-4}} \lesssim \delta\kappa^2, \qquad \alpha > \max(d/2+2,4)$$

$$EP2: \quad \left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-6}} \lesssim \varepsilon \delta\kappa^2 + \delta\kappa^3, \quad \alpha > \max(d/2+2,6), \qquad (19)$$

$$EP3: \quad \left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-8}} \lesssim \varepsilon \delta\kappa^3 + \delta\kappa^4, \quad \alpha > \max(d/2+2,8),$$

where $n\delta\kappa \leq \frac{T}{\varepsilon}$. When $\varepsilon = 1$, the above results of EP2 and EP3 can be given in the $H^{\alpha-4}$ -norm and $H^{\alpha-6}$ -norm, respectively.

Remark 2 Similarly to [17, 56], the time step $\delta \kappa = T_0/N$ with some integer N is only a technique condition for rigorous proof and we only need $\delta \kappa \leq 1$ in practice, which will be shown numerically in Sect. 5. In the whole paper, it is noted that estimates are considered in non-negative Sobolev spaces.

Before we present the proof of Theorem 3, some remarks are given here. By the relation (16) and by directly comparing (9) and (18), it is clear that for $h = \varepsilon \delta \kappa$ and for all $n \ge 0$,

$$u(t_n, x) = w(\kappa_n \varepsilon, x), \quad u^n(x) = w^n(x).$$

Therefore, the convergence of EP1-EP3 in the original scaling (1) is equivalently presented as follows.

Corollary 1 (Optimal convergence of algorithms for the original system.) For the methods EP1-EP3 with a time step size $h \leq \varepsilon$ applied to the original system (1), their error bounds are given by

$$EP1: \| (\Phi^{h})^{n}(u^{0}) - u(t_{n}) \|_{H^{\alpha-4}} \lesssim \frac{h^{2}}{\varepsilon^{2}}, \qquad \alpha > \max(d/2 + 2, 4),$$

$$EP2: \| (\Phi^{h})^{n}(u^{0}) - u(t_{n}) \|_{H^{\alpha-6}} \lesssim \frac{h^{2}}{\varepsilon} + \frac{h^{3}}{\varepsilon^{3}}, \quad \alpha > \max(d/2 + 2, 6),$$

$$EP3: \| (\Phi^{h})^{n}(u^{0}) - u(t_{n}) \|_{H^{\alpha-8}} \lesssim \frac{h^{3}}{\varepsilon^{2}} + \frac{h^{4}}{\varepsilon^{4}}, \quad \alpha > \max(d/2 + 2, 8),$$
(20)

where $nh \leq T$. The results of EP2 and EP3 can be respectively given in the $H^{\alpha-4}$ -norm and $H^{\alpha-6}$ -norm when $\varepsilon = 1$.

3.3 Proof of Theorem 3

In the light of Proposition 2, it is obtained that the coefficients of integrators EP1-EP3 are bounded as $\|C_{\kappa}(\mathcal{W})\|_{H^{\alpha} \hookrightarrow H^{\alpha}} \leq 1$ and $\|A_{\tau,\sigma}(\mathcal{W})\|_{H^{\alpha} \hookrightarrow H^{\alpha}} \leq C_A$, where the constant C_A is independent of $\|\mathcal{W}\|_{H^{\alpha} \hookrightarrow H^{\alpha}}$. For simplicity, the proof will be given only for EP2 because with little modifications it can be adapted to EP1 and EP3. We begin with the local errors and stability of EP2.

Lemma 1 (Local errors.) For the local errors

$$\delta^{n+\tau} := \Phi^{\tau\delta\kappa}(w(\kappa_n)) - w(\kappa_n + \tau\delta\kappa), \quad \text{for } 0 < \tau < 1,$$

$$\delta^{n+1} := \Phi^{\delta\kappa}(w(\kappa_n)) - w(\kappa_{n+1}),$$

there exits $\widehat{\delta\kappa_0} > 0$ independent of ε such that for any $0 < \delta\kappa < \widehat{\delta\kappa_0}$, the following bounds hold for EP2

$$\begin{split} \|\delta^{n+\tau}\|_{H^{\alpha-2}} &\lesssim \delta\kappa, \qquad \|\delta^{n+\tau}\|_{H^{\alpha-4}} \lesssim \delta\kappa^2, \quad for \ 0 < \tau < 1, \\ \|\delta^{n+1}\|_{H^{\alpha-2}} &\lesssim \varepsilon\delta\kappa^2, \qquad \|\delta^{n+1}\|_{H^{\alpha-4}} \lesssim \varepsilon\delta\kappa^3. \end{split}$$

<u>Proof</u> Firstly, according to the scheme (9), the Duhamel principle (7) and the fact that

$$\left\| C_{\tau}(\mathcal{W})w(\kappa_n) - e^{\mathrm{i}\tau\delta\kappa\Delta}w(\kappa_n) \right\|_{H^{\alpha-2}} \lesssim \delta\kappa_n$$

it is clearly that $\|\delta^{n+\tau}\|_{H^{\alpha-2}} \lesssim \delta\kappa$. Then it follows from the Duhamel principle (7) that

$$w(\kappa_n + \tau\delta\kappa) = e^{i\tau\delta\kappa\Delta}w(\kappa_n) + \varepsilon\tau\delta\kappa\varphi_1(\tau\mathcal{W})f(w(\kappa_n)) + \varepsilon\tau^2\delta\kappa^2 \int_0^1 \int_0^1 \xi e^{(1-\xi)i\tau\delta\kappa\Delta}f'(w(\kappa_n + \zeta\xi\tau\delta\kappa))w'(\kappa_n + \zeta\xi\tau\delta\kappa)d\zeta d\xi.$$

For the integrator (9), we have

$$\begin{split} \Phi^{\tau\delta\kappa}(w(\kappa_n)) = & C_{\tau}(\mathcal{W})w(\kappa_n) + \varepsilon\delta\kappa \int_0^1 A_{\tau,\sigma}(\mathcal{W})d\sigma f(w(\kappa_n)) + \delta\kappa^2 C_1 \\ & + \varepsilon\delta\kappa^2 \int_0^1 \int_0^1 \sigma A_{\tau,\sigma}(\mathcal{W})f'(w(\kappa_n + \zeta\sigma\delta\kappa))w'(\kappa_n + \zeta\sigma\delta\kappa)d\zeta d\sigma \end{split}$$

with $||C_1||_{H^{\alpha-4}} \lesssim 1$, where we replace $\Phi^{\sigma\delta\kappa}(w(\kappa_n))$ by $w(\kappa_n + \sigma\delta\kappa)$ in the numerical scheme and the error brought by this is denoted by $\delta\kappa^2 C_1$. The combination of the above two equalities yields $||\delta^{n+\tau}||_{H^{\alpha-4}} \lesssim \delta\kappa^2$ for $0 < \tau < 1$, where the inequality

$$\left\|\int_0^1 A_{\tau,\sigma}(\mathcal{W})d\sigma - \tau\varphi_1(\tau\mathcal{W})\right\|_{H^{\alpha-4}} \lesssim \delta\kappa$$

and the result of Lagrange interpolation have been used.

Then by the same arguments given above and by noticing $C_1(\mathcal{W}) = e^{i\delta\kappa\Delta}$, the bound of $\|\delta^{n+1}\|_{H^{\alpha-2}}$ can be derived.

Finally, in the light of

$$w(\kappa_{n+1}) = e^{i\delta\kappa\Delta}w(\kappa_n) + \varepsilon\delta\kappa\varphi_1(\mathcal{W})f(w(\kappa_n)) + \varepsilon\delta\kappa^2\varphi_2(\mathcal{W})f'(w(\kappa_n))w'(\kappa_n) + \varepsilon\delta\kappa^3\int_0^1\int_0^1(1-\zeta)\xi^2e^{(1-\xi)i\delta\kappa\Delta}(f''(w(\kappa_n+\zeta\xi\delta\kappa))(w'(\kappa_n+\zeta\xi\delta\kappa))^2 + f'(w(\kappa_n+\zeta\xi\delta\kappa))w''(\kappa_n+\zeta\xi\delta\kappa))d\zeta d\xi,$$

and

$$\begin{split} \Phi^{\delta\kappa}(w(\kappa_n)) = & e^{\mathrm{i}\delta\kappa\bigtriangleup}w(\kappa_n) + \varepsilon\delta\kappa\int_0^1 A_{1,\sigma}(\mathcal{W})d\sigma f(w(\kappa_n)) + \varepsilon\delta\kappa^2\int_0^1\sigma A_{1,\sigma}(\mathcal{W})d\sigma f'(w(\kappa_n))w'(\kappa_n) \\ & + \varepsilon\delta\kappa^3C_2 + \varepsilon\delta\kappa^3\int_0^1\int_0^1(1-\zeta)\sigma^2A_{1,\sigma}(\mathcal{W})\big(f''(w(\kappa_n+\zeta\sigma\delta\kappa))(w'(\kappa_n+\zeta\sigma\delta\kappa)))w'(\kappa_n+\zeta\sigma\delta\kappa)\big)d\zeta d\sigma, \end{split}$$

with $\|C_2\|_{H^{\alpha-4}} \lesssim 1$, we obtain the bound of $\|\delta^{n+1}\|_{H^{\alpha-4}}$ as follows

$$\|\delta^{n+1}\|_{H^{\alpha-4}} \lesssim \sum_{j=0}^{1} \varepsilon \delta \kappa^{j+1} \left\| \varphi_{j+1}(\mathcal{W}) - \int_{0}^{1} A_{1,\sigma}(\mathcal{W}) \frac{\sigma^{j}}{j!} \mathrm{d}\sigma \right\|_{H^{\alpha-4}} + \varepsilon \delta \kappa^{3}.$$

Using the results of $A_{1,\sigma}$:

$$\left\|\int_0^1 A_{1,\sigma}(\mathcal{W})d\sigma - \varphi_1(\mathcal{W})\right\|_{H^{\alpha-4}} \lesssim 0, \quad \left\|\int_0^1 A_{1,\sigma}(\mathcal{W})\sigma d\sigma - \varphi_2(\mathcal{W})\right\|_{H^{\alpha-4}} \lesssim \delta\kappa,$$

the last local error can be bounded.

Lemma 2 (Stability.) Consider the abbreviations $R = 2K \|w^0\|_{H^{\alpha}}$, $\mathcal{H}_R^s = \{w \in H^s, \|w\|_{H^s} \leq R\}$. For the numerical solution $\Phi^{\tau\delta\kappa}$ of EP2 applied to $v, w \in \mathcal{H}_{3R/4}^{\alpha-2}$, there exist $\varepsilon_0 > 0$ and $\delta\kappa_0 > 0$ independent of ε such that for any $0 < \varepsilon < \varepsilon_0$ and $0 < \delta\kappa < \delta\kappa_0$, it holds that $\Phi^{\tau\delta\kappa}(v), \Phi^{\tau\delta\kappa}(w) \in \mathcal{H}_R^{\alpha-2}$ and

$$\|\Phi^{\tau\delta\kappa}(v) - \Phi^{\tau\delta\kappa}(w)\|_{H^{\beta}} \le e^{\varepsilon\tau\delta\kappa LC_{A}} \|v - w\|_{H^{\beta}}, \quad 0 \le \tau \le 1,$$

$$\|(\Phi^{\delta\kappa}(v) - e^{i\delta\kappa\Delta}v) - (\Phi^{\delta\kappa}(w) - e^{i\delta\kappa\Delta}w)\|_{H^{\beta}} \le \varepsilon\delta\kappa LC_{A}e^{\varepsilon\tau\delta\kappa LC_{A}} \|v - w\|_{H^{\beta}},$$

(21)

where $\beta \in [0, \alpha - 2]$.

<u>Proof</u> Employing the definition of the method, the isometry $C_{\tau}(\mathcal{W})$ and the Lipschitz estimate of f, one gets

$$\|\Phi^{\tau\delta\kappa}(v) - \Phi^{\tau\delta\kappa}(w)\|_{H^{\beta}} \le \|v - w\|_{H^{\beta}} + \varepsilon LC_A \int_0^{\delta\kappa} \|\Phi^{\sigma}(v) - \Phi^{\sigma}(w)\|_{H^{\beta}} d\sigma,$$

as long as $\Phi^{\sigma}(v)$, $\Phi^{\sigma}(w) \in \mathcal{H}_{R}^{\alpha-2}$ for $\sigma \in [0, \delta \kappa]$. Considering $\tau = 1$ and using the Gronwall's lemma yields

$$\|\Phi^{\delta\kappa}(v) - \Phi^{\delta\kappa}(w)\|_{H^{\beta}} \le e^{\varepsilon\delta\kappa LC_A} \|v - w\|_{H^{\beta}},$$

which gives the first statement of (21) by modifying $\delta \kappa$ to $\tau \delta \kappa$. Setting in particular w = 0 implies $\Phi^{\tau \delta \kappa}(v) \in \mathcal{H}_R^{\alpha-2}$ under the condition that $0 < \delta \kappa < \delta \kappa_0$. It is also direct to have

$$\|(\Phi^{\delta\kappa}(v) - e^{\mathrm{i}\delta\kappa\triangle}v) - (\Phi^{\delta\kappa}(w) - e^{\mathrm{i}\delta\kappa\triangle}w)\|_{H^{\beta}} \le \varepsilon\delta\kappa LC_A \|\Phi^{\tau\delta\kappa}(v) - \Phi^{\tau\delta\kappa}(w)\|_{H^{\beta}}.$$

The second result of (21) follows immediately from this inequality and the first statement.

We are now in a position to prove Theorem 3.

Proof of Theorem 3. <u>Proof</u> **Boundedness of the method.** The stated local errors and stability imply

$$\left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-2}} = \left\| \sum_{l=1}^n \left((\Phi^{\delta\kappa})^{n-l} \Phi^{\delta\kappa} (w(\kappa_{l-1})) - (\Phi^{\delta\kappa})^{n-l} (w(\kappa_l)) \right) \right\|_{H^{\alpha-2}}$$
$$\leq \sum_{l=1}^n e^{\varepsilon(n-l)\delta\kappa LC_A} \left\| \delta^l \right\|_{H^{\alpha-2}} \leq C\varepsilon\delta\kappa^2 \sum_{l=1}^n e^{\varepsilon(n-l)\delta\kappa LC_A} \leq \tilde{C} \frac{e^{LTC_A} - 1}{L} \delta\kappa.$$

Therefore, there exist $\widetilde{\delta\kappa_0} > 0$ independent of ε such that $0 < \delta\kappa < \widetilde{\delta\kappa_0}$, the time-discrete solutions satisfy $(\Phi^{\delta\kappa})^n(w^0) \in \mathcal{H}^{\alpha-2}_{3R/4}$, where $w(\kappa_n) \in \mathcal{H}^{\alpha-2}_{R/2}$ has been used here. Using a stability estimate with respect to the $H^{\alpha-4}$ -norm and considering the local error result in this norm yields

$$\left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-4}} \le \tilde{C} \frac{e^{LTC_A} - 1}{L} \delta\kappa^2.$$

Refined local error. For the method (9), we expand the nonlinear function f at $C_{\xi}w(\kappa_n)$ and then get

$$\begin{split} \Phi^{\delta\kappa}(w(\kappa_n)) = & e^{i\delta\kappa \bigtriangleup} w(\kappa_n) + \varepsilon \delta\kappa \int_0^1 A_{1,\xi} f(C_{\xi}w(\kappa_n)) d\xi \\ & + \varepsilon^2 \delta\kappa^2 \int_0^1 \int_0^1 A_{1,\xi} A_{\xi,\sigma} f'(C_{\xi}w(\kappa_n)) f(\Phi^{\sigma\delta\kappa}(w(\kappa_n))) d\xi d\sigma \\ & + \varepsilon^3 \delta\kappa^3 \int_0^1 \int_0^1 (1-\zeta) A_{1,\xi} f'' \Big(C_{\xi}w(\kappa_n) + \zeta\varepsilon\delta\kappa \int_0^1 A_{\xi,\sigma} f(\Phi^{\sigma\delta\kappa}(w(\kappa_n))) d\sigma \Big) \\ & \Big(\int_0^1 A_{\xi,\sigma} f(\Phi^{\sigma\delta\kappa}(w(\kappa_n))) d\sigma \Big)^2 d\xi d\zeta \\ = & e^{i\delta\kappa\bigtriangleup} w(\kappa_n) + \varepsilon\delta\kappa \int_0^1 A_{1,\xi} f(C_{\xi}w(\kappa_n)) d\xi \\ & + \varepsilon^2 \delta\kappa^2 \int_0^1 \int_0^1 A_{1,\xi} A_{\xi,\sigma} f'(C_{\xi}w(\kappa_n)) f(C_{\sigma}w(\kappa_n)) d\xi d\sigma + \varepsilon^3 \delta\kappa^3 \Xi_{\Phi}, \end{split}$$

with

$$\begin{split} \Xi_{\Phi} &= \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} A_{1,\xi} A_{\xi,\sigma} f' \left(C_{\xi} w(\kappa_{n}) \right) f' (C_{\sigma} w(\kappa_{n}) + \zeta (\Phi^{\sigma\delta\kappa}(w(\kappa_{n})) - C_{\sigma} w(\kappa_{n}))) \right) \\ &\qquad \left(\int_{0}^{1} A_{\sigma,\varsigma} f(\Phi^{\varsigma\delta\kappa}(w(\kappa_{n}))) d\varsigma \right) d\zeta d\xi d\sigma \\ &\qquad + \int_{0}^{1} \int_{0}^{1} (1-\zeta) A_{1,\xi} f'' \left(C_{\xi} w(\kappa_{n}) + \zeta \varepsilon \delta\kappa \int_{0}^{1} A_{\xi,\sigma} f(\Phi^{\sigma\delta\kappa}(w(\kappa_{n}))) d\sigma \right) \\ &\qquad \left(\int_{0}^{1} A_{\xi,\sigma} f(\Phi^{\sigma\delta\kappa}(w(\kappa_{n}))) d\sigma \right)^{2} d\xi d\zeta. \end{split}$$

For the exact solution (7), similarly we obtain its expansion as

$$w(\kappa_{n+1}) = e^{i\delta\kappa\Delta}w(\kappa_n) + \varepsilon\delta\kappa \int_0^1 e^{(1-\xi)i\delta\kappa\Delta}f(e^{i\xi\delta\kappa\Delta}w(\kappa_n))d\xi + \varepsilon^2\delta\kappa^2 \int_0^1 \int_0^1 \xi e^{(1-\xi)i\delta\kappa\Delta}f'(e^{i\xi\delta\kappa\Delta}w(\kappa_n))e^{(1-\sigma)i\xi\delta\kappa\Delta}f(e^{i\sigma\delta\kappa\Delta}w(\kappa_n))d\xi d\sigma + \varepsilon^3\delta\kappa^3\Xi_w,$$

with

$$\Xi_{w} = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} e^{(1-\xi)i\delta\kappa\triangle} e^{(1-\sigma)\xi i\delta\kappa\triangle} f'(e^{\xi i\delta\kappa\triangle}w(\kappa_{n}))f'(e^{i\sigma\delta\kappa\triangle}w(\kappa_{n})) + \zeta(w(\kappa_{n}+\sigma\delta\kappa-e^{i\sigma\delta\kappa\triangle}w(\kappa_{n}))) \Big(\int_{0}^{1} e^{(1-\varsigma)i\sigma\delta\kappa\triangle}f(w(\kappa_{n}+\varsigma\delta\kappa))d\varsigma\Big)d\zeta d\xi d\sigma + \int_{0}^{1} \int_{0}^{1} (1-\zeta)e^{(1-\xi)i\delta\kappa\triangle}f''(e^{\xi i\delta\kappa\triangle}w(\kappa_{n})+\zeta\varepsilon\delta\kappa\int_{0}^{1} e^{(1-\sigma)i\xi\delta\kappa\triangle}f(w(\kappa_{n}+\sigma\delta\kappa))d\sigma\Big) - \Big(\int_{0}^{1} e^{(1-\sigma)i\xi\delta\kappa\triangle}f(w(\kappa_{n}+\sigma\delta\kappa))d\sigma\Big)^{2}d\xi d\zeta.$$

Then the local error δ^{n+1} can be refined as

$$\delta^{n+1} = \varepsilon \delta \kappa \Psi(\kappa_n) + \varepsilon^2 \delta \kappa^2 \Delta(\kappa_n), \tag{22}$$

where

$$\begin{split} \Psi(\kappa_n) &= \int_0^1 A_{1,\xi} f(C_{\xi} w(\kappa_n)) d\xi - \int_0^1 e^{(1-\xi)\mathbf{i}\delta\kappa\bigtriangleup} f(e^{\xi\mathbf{i}\delta\kappa\bigtriangleup} w(\kappa_n)) d\xi, \\ \Delta(\kappa_n) &= \int_0^1 \int_0^1 A_{1,\xi} A_{\xi,\sigma} f'(C_{\xi} w(\kappa_n)) f(C_{\sigma} w(\kappa_n)) d\xi d\sigma \\ &- \int_0^1 \int_0^1 \xi e^{(1-\xi)\mathbf{i}\delta\kappa\bigtriangleup} f'(e^{\xi\mathbf{i}\delta\kappa\bigtriangleup} w(\kappa_n)) e^{(1-\sigma)\xi\mathbf{i}\delta\kappa\bigtriangleup} f(e^{\mathbf{i}\sigma\delta\kappa\bigtriangleup} w(\kappa_n)) d\xi d\sigma + \varepsilon\delta\kappa\Xi_{\Phi} - \varepsilon\delta\kappa\Xi_{W}. \end{split}$$

Concerning the previous local errors given in Lemma 1, one has

$$\|\Psi(\kappa_n)\|_{H^{\alpha-4}} \lesssim \delta \kappa^2, \quad \|\Delta(\kappa_n)\|_{H^{\alpha-4}} \lesssim \delta \kappa.$$

Refined convergence over one period. In this part, we consider convergence over one period, that is $n\delta\kappa = T_0 = 1$. For the global error

$$(\Phi^{\delta\kappa})^n(w^0) - w(\kappa_n) = \sum_{l=1}^n \left((\Phi^{\delta\kappa})^{n-l} \Phi^{\delta\kappa}(w(\kappa_{l-1})) - (\Phi^{\delta\kappa})^{n-l}(w(\kappa_l)) \right),$$

we introduce $\Theta_{n-l}^{\delta\kappa} := (\Phi^{\delta\kappa})^{n-l} - e^{i(n-l)\delta\kappa\Delta}$ and then rewrite it as

$$(\Phi^{\delta\kappa})^n(w^0) - w(\kappa_n) = \underbrace{\sum_{l=1}^n e^{i(n-l)\delta\kappa\triangle\delta^l}}_{\mathbb{E}_1} + \underbrace{\sum_{l=1}^n \left(\Theta^{\delta\kappa}_{n-l}(\Phi^{\delta\kappa}(w(\kappa_{l-1}))) - \Theta^{\delta\kappa}_{n-l}(w(\kappa_l))\right)}_{\mathbb{E}_2}.$$
(23)

For the part \mathbb{E}_2 , we first estimate

$$\begin{split} & \left\|\Theta_{l}^{\delta\kappa}v - \Theta_{l}^{\delta\kappa}w\right\|_{H^{\beta}} = \left\|(\Phi^{\delta\kappa})^{l}v - e^{il\delta\kappa\Delta}v - (\Phi^{\delta\kappa})^{l}w + e^{il\delta\kappa\Delta}w\right\|_{H^{\beta}} \\ & \leq \sum_{k=1}^{l} \left\|\Theta_{1}^{\delta\kappa}(\Phi^{\delta\kappa})^{k-1}v - \Theta_{1}^{\delta\kappa}(\Phi^{\delta\kappa})^{k-1}w\right\|_{H^{\beta}} \leq \varepsilon\delta\kappa LC_{A}e^{\varepsilon\tau\delta\kappa LC_{A}}\sum_{k=1}^{l} \left\|(\Phi^{\delta\kappa})^{k-1}v - (\Phi^{\delta\kappa})^{k-1}w\right\|_{H^{\beta}} \\ & \leq \varepsilon\delta\kappa LC_{A}e^{\varepsilon\tau\delta\kappa LC_{A}}\sum_{k=1}^{l} e^{\varepsilon(k-1)\delta\kappa LC_{A}} \left\|v - w\right\|_{H^{\beta}} \leq \varepsilon LC_{A}T_{0}e^{\varepsilon LC_{A}T_{0}} \left\|v - w\right\|_{H^{\beta}}. \end{split}$$

Then the following bound holds

$$\|\mathbb{E}_2\|_{H^{\alpha-4}} \le \varepsilon L C_A T_0 e^{\varepsilon L C_A T_0} \sum_{l=1}^n \|\delta^l\|_{H^{\alpha-4}} \lesssim \varepsilon^2 \delta \kappa^2.$$
(24)

For the part \mathbb{E}_1 , we use the refined local error (22) and then have

$$\mathbb{E}_{1} = \sum_{l=1}^{n} e^{i(n-l)\delta\kappa\triangle} \varepsilon \delta\kappa \Psi(\kappa_{l-1}) + \sum_{l=1}^{n} e^{i(n-l)\delta\kappa\triangle} \varepsilon^{2} \delta\kappa^{2} \Delta(\kappa_{l-1}).$$
(25)

According to (23)-(25) and the following bound

$$\left\|\sum_{l=1}^{n} e^{\mathrm{i}(n-l)\delta\kappa\triangle}\varepsilon^{2}\delta\kappa^{2}\Delta(\kappa_{l-1})\right\|_{H^{\alpha-4}} \leq \varepsilon^{2}\delta\kappa^{3}\sum_{l=1}^{n}\left\|e^{\mathrm{i}(n-l)\delta\kappa\triangle}\right\|_{H^{\alpha-4}} \lesssim \varepsilon^{2}\delta\kappa^{2},$$

the global error is bounded by

$$\left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-4}} \lesssim \varepsilon \delta \kappa \left\| \sum_{l=1}^n e^{i(n-l)\delta\kappa \bigtriangleup} \Psi(\kappa_{l-1}) \right\|_{H^{\alpha-4}} + \varepsilon^2 \delta \kappa^2.$$
(26)

In what follows, we derive the optimal bound for $\varepsilon \delta \kappa \left\| \sum_{l=1}^{n} e^{i(n-l)\delta \kappa \bigtriangleup} \Psi(\kappa_{l-1}) \right\|_{H^{\alpha-4}}$, which satisfies

$$\begin{split} \varepsilon \delta \kappa \left\| \sum_{l=1}^{n} e^{\mathrm{i}(n-l)\delta\kappa \bigtriangleup} \Psi(\kappa_{l-1}) \right\|_{H^{\alpha-4}} \\ \lesssim \varepsilon \delta \kappa \left\| \sum_{l=1}^{n} e^{\mathrm{i}(n-l)\delta\kappa \bigtriangleup} \int_{0}^{1} A_{1,\xi} f(C_{\xi} e^{\mathrm{i}(l-1)\delta\kappa \bigtriangleup} w_{0}) d\xi - \varepsilon \sum_{l=1}^{n} e^{\mathrm{i}(n-l+1)\delta\kappa \bigtriangleup} \int_{0}^{\delta\kappa} e^{-\mathrm{i}\xi \bigtriangleup} f(e^{\mathrm{i}\xi \bigtriangleup} e^{\mathrm{i}(l-1)\delta\kappa \bigtriangleup} w_{0}) d\xi \right\|_{H^{\alpha-4}} \\ + \varepsilon^{2} \delta \kappa^{2} \\ \lesssim \left\| \varepsilon \delta \kappa \sum_{l=1}^{n} e^{-\mathrm{i}l\delta\kappa \bigtriangleup} \int_{0}^{1} A_{1,\xi} f(C_{\xi} e^{\mathrm{i}(l-1)\delta\kappa \bigtriangleup} w_{0}) d\xi - \varepsilon \int_{0}^{1} e^{-\mathrm{i}\xi \bigtriangleup} f(e^{\mathrm{i}\xi \bigtriangleup} w_{0}) d\xi \right\|_{H^{\alpha-4}} + \varepsilon^{2} \delta \kappa^{2}. \end{split}$$

Here we used the result $\|w(\kappa_{l-1}) - e^{i(l-1)\delta\kappa\Delta}w_0\|_{H^{\alpha-4}} \lesssim \varepsilon$. We first consider Fourier expansion $F_{\xi}(w) = \sum_{k\in\mathbb{Z}} e^{i2k\pi\xi} \hat{F}_k(w)$ of $F_{\kappa}(w) := e^{-i\xi\Delta}f(e^{i\xi\Delta}w)$, which yields that $\int_0^1 e^{-i\xi\Delta}f(e^{i\xi\Delta}w_0)d\xi = \hat{F}_0(w_0)$. Then let $G_{l\delta\kappa}(w) = e^{-il\delta\kappa\Delta} \int_0^1 A_{1,\xi}f(C_{\xi}e^{il\delta\kappa\Delta}w)d\xi$ and the Fourier expansion of $G_{l\delta\kappa}(w)$ is given by $G_{l\delta\kappa}(w) = \sum_{k\in\mathbb{Z}} e^{i2k\pi l\delta\kappa} \hat{G}_k(w)$. Therefore, it is obtained that

$$\varepsilon\delta\kappa\sum_{l=1}^{n}e^{-\mathrm{i}l\delta\kappa\Delta}\int_{0}^{1}A_{1,\xi}f(C_{\xi}e^{\mathrm{i}(l-1)\delta\kappa\Delta}w_{0})d\xi = \varepsilon\delta\kappa e^{-\mathrm{i}\delta\kappa\Delta}\sum_{l=0}^{n-1}\sum_{k\in\mathbb{Z}}e^{\mathrm{i}2k\pi l\delta\kappa}\hat{G}_{k}(w)$$
$$=\varepsilon e^{-\mathrm{i}\delta\kappa\Delta}\sum_{k\in\mathbb{Z}}\left(\frac{1}{n}\sum_{l=0}^{n-1}e^{\mathrm{i}2k\pi l\delta\kappa}\hat{G}_{k}(w)\right) = \varepsilon e^{-\mathrm{i}\delta\kappa\Delta}\sum_{k\in\mathbb{Z}}\hat{G}_{nk}(w).$$

Based on the above results, it follows that

...

$$\varepsilon\delta\kappa \left\| \sum_{l=1}^{n} e^{i(n-l)\delta\kappa\Delta} \Psi(\kappa_{l-1}) \right\|_{H^{\alpha-6}} \\ \lesssim \varepsilon \left\| \hat{F}_{0}(w_{0}) - e^{-i\delta\kappa\Delta} \hat{G}_{0}(w) \right\|_{H^{\alpha-6}} + \varepsilon \left\| \sum_{k\in\mathbb{Z}^{*}} \hat{G}_{nk}(w) \right\|_{H^{\alpha-6}} + \varepsilon^{2}\delta\kappa^{2} \\ \lesssim \varepsilon \left\| \int_{0}^{1} e^{-i\xi\Delta} f(e^{i\xi\Delta}w_{0})d\xi - \int_{0}^{1} e^{-i\xi\Delta} \left[e^{-i\delta\kappa\Delta} \int_{0}^{1} A_{1,\xi} f(C_{\xi}e^{i\xi\Delta}w_{0})d\xi \right] d\xi \right\|_{H^{\alpha-6}} \\ + \varepsilon\delta\kappa^{3} + \varepsilon^{2}\delta\kappa^{2} \\ \lesssim \varepsilon\delta\kappa^{3} + \varepsilon\delta\kappa^{3} + \varepsilon^{2}\delta\kappa^{2}.$$

$$(27)$$

Here Lemma A.1 of [17] and the results $A_{1,\xi}$ and C_{ξ} of EP2 are used to obtain the last two inequalities, respectively. Finally, combining (26) with (27), we obtain the global error over one period

$$\left\| (\Phi^{\delta\kappa})^n (w^0) - w(\kappa_n) \right\|_{H^{\alpha-6}} \lesssim \varepsilon \delta \kappa^3 + \varepsilon^2 \delta \kappa^2, \quad n\delta\kappa = T_0.$$
⁽²⁸⁾

Refined global error.

For $n\delta\kappa \leq T/\varepsilon$, the global error of EP2 given in (19) can be derived by considering (28) and by using the same way presented in Sect. 5 of [17].

The whole proof is complete.

Remark 3 It is noted that for EP1, the estimate of (27) is only $\varepsilon \delta \kappa^2$. Therefore, EP1 does not have optimal convergence.

4 Long time conservations in actions, momentum and density

In this section, we turn back to the methods applied to the original system (1) and in order to make the analysis be succinct, we choose $\lambda = 1$. For our integrator (9), spectral semi-discretisation (see [18, 19, 29, 30]) with the points $x_k = \frac{\pi}{M}k$, $k \in \mathcal{M}$ is used in space, where $\mathcal{M} = \{-M, \ldots, M-1\}^d$ and 2M presents the number of internal discretisation points in space. Then the fully discrete scheme of (9) is

$$u^{n+\tau} = C_{\tau}(V)u^{n} + h \int_{0}^{1} A_{\tau,\sigma}(V)f(u^{n+\sigma})d\sigma, \quad 0 \le \tau \le 1,$$
(29)

where $V = ih\Omega$, $\Omega = -\text{diag}((\omega_j)_{j \in \mathcal{M}})$ and $f(u) = -i\mathcal{Q}(|u|^2 u)^1$. Here, $\omega_j = \frac{1}{\varepsilon} |j|^2 = \frac{1}{\varepsilon} (j_1^2 + \dots + j_d^2)$ for $j = (j_1, \dots, j_d) \in \mathcal{M}$ are the eigenvalues of the linear part of (1) after spectral semi-discretisation in space, and the notation $\mathcal{Q}(v)$ denotes the trigonometric interpolation of a periodic function $v = \sum_{j \in \mathbb{Z}^d} v_j e^{i(j \cdot x)}$ in the collocation points, i.e., $\mathcal{Q}(v) = \sum_{j \in \mathcal{M}} (\sum_{l \in \mathbb{Z}^d} v_{j+2Ml}) e^{i(j \cdot x)}$.

¹We still use the notation f in this section without any confusion.

The following notations are needed in this section which have been used in [19, 29, 30]. For a sequence $k = (k_j)_{j \in \mathcal{M}}$ of integers k_j and the sequence $\omega = (\omega_j)_{j \in \mathcal{M}}$, denote

$$||k|| = \sum_{j \in \mathcal{M}} |k_j|, \ k \cdot \omega = \sum_{j \in \mathcal{M}} k_j \omega_j, \ \omega^{\sigma|k|} = \prod_{j \in \mathcal{M}} \omega_j^{\sigma|k_j|}$$

for a real σ . Denote by $\langle j \rangle$ the unit coordinate vector $(0, \ldots, 0, 1, 0, \ldots, 0)^{\intercal}$ with the only entry 1 at the |j|-th position.

4.1 Result of near-conservation properties

Theorem 4 (Long time near-conservations.) Consider the small initial data

$$\left\| u^0 \right\|_{H^s} \le \tilde{\epsilon} \ll 1,\tag{30}$$

and define the set

$$\mathcal{R}_{\tilde{\epsilon},M,h} = \left\{ (j,k) : j = j(k), \ k \neq \langle j \rangle, \ \left| \sin\left(\frac{1}{2}h(\omega_j - k \cdot \omega)\right) \right| \le \frac{1}{2}\tilde{\epsilon}^{1/2}h, \ \|k\| \le 2N + 2 \right\},$$
(31)

where $j(k) := \sum_{l \in \mathcal{M}} k_l l \mod 2M \in \mathcal{M}$. For the near-resonant indices (j,k) in $\mathcal{R}_{\tilde{\epsilon},M,h}$, they are required such that

$$\sup_{(j,k)\in\mathcal{R}_{\tilde{\epsilon},M,h}} \frac{|\omega_j|^{s-\frac{d+1}{2}}}{\omega^{(s-\frac{d+1}{2})|k|}} \tilde{\epsilon}^{||k||+1} \le \tilde{C}\tilde{\epsilon}^{2N+4}$$
(32)

with a constant \tilde{C} independent of $\tilde{\epsilon}$. For given $N \geq 1$ and $s \geq d+1$, the numerical solution u^n of EP1 has the following conservations of actions, momentum and density, respectively

$$\sum_{j \in \mathcal{M}} |\omega_j|^s \frac{|I_j(u^n, \bar{u}^n) - I_j(u^0, \bar{u}^0)|}{\tilde{\epsilon}^2} \le C\tilde{\epsilon}^{\frac{3}{2}},$$
$$\sum_{r=1}^d \frac{|K_r[u^n, \bar{u}^n] - K_r[u^0, \bar{u}^0]|}{\tilde{\epsilon}^2} \le C\tilde{\epsilon}^{\frac{3}{2}},$$
$$\frac{|m[u^n, \bar{u}^n] - m[u^0, \bar{u}^0]|}{\tilde{\epsilon}^2} \le C\tilde{\epsilon}^{\frac{3}{2}},$$

where $0 \leq t_n = nh \leq \tilde{\epsilon}^{-N}$ and the constant *C* depends on \tilde{C} , $\max_{j \in \mathcal{M}} \left\{ \frac{1}{|\cos(\frac{1}{2}h\omega_j)|} \right\}$, the dimension d, N, s and the norm of the potential but is independent of *n*, the size of the initial value $\tilde{\epsilon}$, the regime of the solution ε , and the discretisation parameters *M* and *h*. Here K_r is referred to the *r*th component of *K*. For the schemes EP1-EP2, if the midpoint rule is used to the integral appearing in these methods, the above near conservations still hold.

Remark 4 We remark that the method EP3 does not have such near conservations and the reason will be explained at the end of this section.

Remark 5 It is noted that the authors in [19, 28, 30] analysed the long-time behaviour of exponential integrators, splitting integrators and split-step Fourier method for Schrödinger equations. However, those methods cannot preserve the energy (12) exactly. We remark that Theorem 4 shows that our energy-preserving integrators also have a near conservation of actions, momentum and density over long times.

4.2 The proof of Theorem 4

The proof makes use of a modulated Fourier expansion [19, 29, 30, 54] in time of the numerical solution. We will use the following expansion

$$\tilde{u}(t,x) = \sum_{\|k\| \le K} z^k(\tilde{\epsilon}t,x) \mathrm{e}^{-\mathrm{i}(k\cdot\omega)t} = \sum_{\|k\| \le K} \sum_{j \in \mathcal{M}} z_j^k(\tilde{\epsilon}t) \mathrm{e}^{\mathrm{i}(j\cdot x)} \mathrm{e}^{-\mathrm{i}(k\cdot\omega)t}$$
(33)

to describe the numerical solution u^n at time $t_n = nh$ after n time steps, where the functions z^k are termed the modulation functions which evolve on a slow time-scale $\tilde{\tau} = \tilde{\epsilon}t$. Following [19], these functions can be assumed to be single spatial waves: $z^k(\tilde{\epsilon}t, x) = z^k_{j(k)}(\tilde{\epsilon}t)e^{i(j(k)\cdot x)}$, i.e., their Fourier coefficients z^k_j vanish for $j \neq j(k)$ with $j(k) = \sum_{l \in \mathcal{M}} k_l l \mod 2M \in \mathcal{M}$.

It is noted that as a standard approach to the study of the long-time behavior of numerical methods, modulated Fourier expansion is also used in the analysis of [19, 29, 30, 54]. However, in this paper, there are novel modifications adapted to our integrators, which come from the implicitness of the integrator and the integral appearing in the integrator. We present the main differences in the proof. For the similar derivations as those of [19, 29, 30], we skip them in the analysis for brevity.

4.2.1 Modulation equations

Proposition 3 (Modulation equations.) Define

$$\begin{split} L^k &:= (L_2^k)^{-1} L_1^k, \\ L_1^k &:= \mathrm{e}^{-\mathrm{i}(k\cdot\omega)h} \mathrm{e}^{\tilde{\epsilon}hD} - 2\cos(h\Omega) + \mathrm{e}^{\mathrm{i}(k\cdot\omega)h} \mathrm{e}^{-\tilde{\epsilon}hD}, \\ L_2^k &:= \varphi_1(ih\Omega) \mathrm{e}^{-\frac{1}{2}\mathrm{i}(k\cdot\omega)h} \mathrm{e}^{\frac{1}{2}\tilde{\epsilon}hD} - \varphi_1(-ih\Omega) \mathrm{e}^{\frac{1}{2}\mathrm{i}(k\cdot\omega)h} \mathrm{e}^{-\frac{1}{2}\tilde{\epsilon}hD} \end{split}$$

where D is the differential operator (see [35]). The modulation equations for the coefficients z_j^k appearing in (33) are given by

$$L^{k}z_{j}^{k}(\tilde{\epsilon}t) = -i\hbar \sum_{k^{1}+k^{2}-k^{3}=k} \int_{0}^{1} w_{j(k^{1})}^{k^{1}}(\tilde{\epsilon}t,\sigma) w_{j(k^{2})}^{k^{2}}(\tilde{\epsilon}t,\sigma) \overline{w_{j(k^{3})}^{k^{3}}}(\tilde{\epsilon}t,\sigma) d\sigma,$$
(34)

where

$$w_{j(k)}^{k}(\tilde{\epsilon}t,\sigma) = L_{3}^{k}(\sigma)z_{j(k)}^{k}(\tilde{\epsilon}t)$$
(35)

with

$$L_3^k(\sigma) := (1 - \sigma) \mathrm{e}^{\frac{1}{2}\mathrm{i}(k \cdot \omega)h} \mathrm{e}^{-\frac{h}{2}\tilde{\epsilon}D} + \sigma \mathrm{e}^{-\frac{1}{2}\mathrm{i}(k \cdot \omega)h} \mathrm{e}^{\frac{h}{2}\tilde{\epsilon}D}.$$

The initial condition for modulation equations is given by

$$u_j^0 = \sum_k z_{j(k)}^k(0).$$
(36)

<u>Proof</u> In order to derive the modulation equations for EP1, a new approach different from [19, 29, 30] is considered here. To this end, we define the operator L^k and it can be expressed in Taylor

expansions as follows:

$$L_{j}^{\langle j \rangle} = \frac{1}{2} \tilde{\epsilon} h^{2} \omega_{j} \csc\left(\frac{1}{2} h \omega_{j}\right) D + \frac{1}{48} \tilde{\epsilon}^{3} h^{4} \omega_{j} \csc\left(\frac{1}{2} h \omega_{j}\right) D^{3} + \cdots,$$

$$L^{k} = ih\Omega \csc\left(\frac{1}{2} h\Omega\right) \sin\left(\frac{1}{2} h(-\Omega - (k \cdot \omega)I)\right)$$

$$+ \frac{1}{2} \tilde{\epsilon} h^{2}\Omega \csc\left(\frac{1}{2} h\Omega\right) \cos\left(\frac{1}{2} h((k \cdot \omega)I + \Omega)\right) D + \cdots.$$
(37)

Moreover, for the operator $L_3^k(\sigma)$, we have

$$L_3^k(\frac{1}{2}) = \cos\left(\frac{h(k\cdot\omega)}{2}\right) + \frac{1}{2}\sin\left(\frac{h(k\cdot\omega)}{2}\right)(\mathrm{i}h\tilde{\epsilon}D) + \cdots$$

By using the symmetry of the EP1 integrator and

$$\int_{0}^{1} f((1-\sigma)u^{n} + \sigma u^{n-1})d\sigma = \int_{0}^{1} f((1-\sigma)u^{n-1} + \sigma u^{n})d\sigma$$

we can rewrite the scheme of EP1 as 2

$$u^{n+1} - 2\cos(h\Omega)u^n + u^{n-1} = h \Big[\varphi_1(V) \int_0^1 f((1-\sigma)u^n + \sigma u^{n+1}) d\sigma - \varphi_1(-V) \int_0^1 f((1-\sigma)u^{n-1} + \sigma u^n) d\sigma \Big].$$
(38)

For the term $(1 - \sigma)u^n + \sigma u^{n+1}$, we look for a modulated Fourier expansion of the form

$$\tilde{u}_h(t+\frac{h}{2},x,\sigma) = \sum_{\|k\| \le K} w_{j(k)}^k \left(\tilde{\epsilon}(t+\frac{h}{2}),\sigma\right) \mathrm{e}^{\mathrm{i}(j(k)\cdot x)} \mathrm{e}^{-\mathrm{i}(k\cdot\omega)(t+\frac{h}{2})},$$

which leads to

$$w_{j(k)}^{k}\left(\tilde{\epsilon}(t+\frac{h}{2}),\sigma\right) = L_{3}^{k}(\sigma)z_{j(k)}^{k}\left(\tilde{\epsilon}(t+\frac{h}{2})\right).$$
(39)

Likwise, for $(1 - \sigma)u^{n-1} + \sigma u^n$, we have the following modulated Fourier expansion

$$\tilde{u}_h(t-\frac{h}{2},x,\sigma) = \sum_{\|k\| \le K} w_{j(k)}^k \left(\tilde{\epsilon}(t-\frac{h}{2}),\sigma\right) \mathrm{e}^{\mathrm{i}(j(k)\cdot x)} \mathrm{e}^{-\mathrm{i}(k\cdot\omega)(t-\frac{h}{2})}.$$

Inserting (33) and (39) into (38) yields

$$\tilde{u}(t+h,x) - 2\cos(h\Omega)\tilde{u}(t,x) + \tilde{u}(t-h,x)$$

= $h\left[\varphi_1(V)\int_0^1 f\left(\tilde{u}_h(t+\frac{h}{2},x,\sigma)\right)d\sigma - \varphi_1(-V)\int_0^1 f\left(\tilde{u}_h(t-\frac{h}{2},x,\sigma)\right)d\sigma\right]$

which can be expressed by operators as

$$(\varphi_1(ih\Omega)e^{\frac{1}{2}hD} - \varphi_1(-ih\Omega)e^{-\frac{1}{2}hD})^{-1}(e^{hD} - 2\cos(h\Omega) + e^{-hD})\tilde{u}(t,x) = h \int_0^1 f(\tilde{u}_h(t,x,\sigma))d\sigma.$$
(40)

²This form has been given in [44] for first-order ODEs.

On the other hand, we rewrite the nonlinearity f as:

$$f(u) = -\mathbf{i} \sum_{\|k\| \le K} \sum_{j(k) \in \mathcal{M}} \sum_{k^1 + k^2 - k^3 = k} w_{l_1}^{k^1} w_{l_2}^{k^2} \overline{w_{l_3}^{k^3}} e^{\mathbf{i}(j(k) \cdot x)} e^{-\mathbf{i}(k \cdot \omega)t},$$

where $j(k) = (j(k^1) + j(k^2) - j(k^3)) \mod 2M$ if $k = k^1 + k^2 - k^3$. On the basis of this fact and (40), considering the *j*th Fourier coefficient and comparing the coefficients of $e^{-i(k \cdot \omega)t}$, the result of this proposition is obtained.

4.2.2 Iterative solution of modulation system

In order to achieve an approximate solution of the modulation system (34)-(36), we introduce an iterative procedure in this subsection which was used in [19, 30].

For j = j(k) with $k \neq \langle j \rangle$, the modulation system takes the form

$$i\hbar\omega_j\csc\left(\frac{1}{2}\hbar\omega_j\right)\sin\left(\frac{1}{2}\hbar(\omega_j-k\cdot\omega)\right)z_{j(k)}^k(\tilde{\epsilon}t) = \mathbf{N}(w(\tilde{\epsilon}t))_{j(k)}^k + \mathbf{B}(z(\tilde{\epsilon}t))_{j(k)}^k,\tag{41}$$

and for $j = j(\langle j \rangle)$, the modulation system becomes

$$\frac{1}{2}\tilde{\epsilon}h^2\omega_j\csc\left(\frac{1}{2}h\omega_j\right)\dot{z}_j^{\langle j\rangle}(\tilde{\epsilon}t) = \mathbf{N}(w(\tilde{\epsilon}t))_j^{\langle j\rangle} + \mathbf{A}(z(\tilde{\epsilon}t))_j^{\langle j\rangle},\tag{42}$$

where $\dot{z}_{j}^{(j)}$ stands for the derivative with respect to $\tilde{\tau} = \tilde{\epsilon}t$ and we have used the differential operators

$$\mathbf{B}(z(\tilde{\epsilon}t))_{j(k)}^{k} = -\frac{1}{2}\tilde{\epsilon}h^{2}\omega_{j}\csc\left(\frac{1}{2}h\omega_{j}\right)\cos\left(\frac{1}{2}h(k\cdot\omega-\omega_{j})\right)\dot{z}(\tilde{\epsilon}t)_{j(k)}^{k} - \dots$$
$$\mathbf{A}(z(\tilde{\epsilon}t))_{j}^{\langle j \rangle} = -\frac{1}{48}\tilde{\epsilon}^{3}h^{4}\omega_{j}\csc\left(\frac{1}{2}h\omega_{j}\right)z^{\langle 3 \rangle}(\tilde{\epsilon}t)_{j}^{\langle j \rangle} - \dots,$$

and

$$\mathbf{N}(w(\tilde{\epsilon}t))_{j(k)}^{k} = -\mathrm{i}h \sum_{k^{1}+k^{2}-k^{3}=k} \int_{0}^{1} w_{j(k^{1})}^{k^{1}}(\tilde{\epsilon}t,\sigma) w_{j(k^{2})}^{k^{2}}(\tilde{\epsilon}t,\sigma) \overline{w_{j(k^{3})}^{k^{3}}}(\tilde{\epsilon}t,\sigma) d\sigma.$$

Denote by $[\cdot]^l$ the *l*th iterate and we choose the starting iterates (l = 0) as $[z_j^k(\tilde{\tau})]^0 = 0$ for $k \neq \langle j \rangle$, and $[z_j^{\langle j \rangle}(\tilde{\tau})]^0 = u_j^0$. Then the modulation functions are distinguished as follows.

Definition 2 (Iterative solution of modulation system.)

- For near-resonant indices $(j,k) \in \mathcal{R}_{\tilde{\epsilon},M,h}$ or ||k|| > K = 2N + 2, it is set for $0 \leq \tilde{\epsilon}t = \tilde{\tau} \leq 1$ that $[z_{i}^{k}(\tilde{\tau})]^{l+1} = 0$.
- For near-resonant indices $(j,k) = (j,\langle j \rangle)$, in the light of (42), $[z_j^{\langle j \rangle}]^{l+1}$ is defined as the solution of the differential equation

$$\left[\dot{z}_{j}^{\langle j \rangle}(\tilde{\epsilon}t)\right]^{l+1} = \left[\frac{\operatorname{sinc}\left(\frac{1}{2}h\omega_{j}\right)}{h\tilde{\epsilon}}\mathbf{N}(w(\tilde{\epsilon}t))_{j}^{\langle j \rangle} + \frac{\operatorname{sinc}\left(\frac{1}{2}h\omega_{j}\right)}{h\tilde{\epsilon}}\mathbf{A}(z(\tilde{\epsilon}t))_{j}^{\langle j \rangle}\right]^{l}$$

with the initial value $\left[z_j^{\langle j \rangle}(0)\right]^{l+1} = u_j^0 - \left[\sum_{k \neq \langle j \rangle} z_j^k(0)\right]^l$ and $\operatorname{sinc}(x) = \sin(x)/x$.

• For the remaining indices (j, k) in the set

$$\mathcal{L}_{\tilde{\epsilon},M,h} = \{ (j,k) : j = j(k), \ k \neq \langle j \rangle, \ (j,k) \notin \mathcal{R}_{\tilde{\epsilon},M,h}, \ \|k\| \le K \},$$
(43)

it follows from (41) that

$$\left[z_{j(k)}^{k}(\tilde{\epsilon}t)\right]^{l+1} = \left[\frac{\operatorname{sinc}\left(\frac{1}{2}h\omega_{j}\right)}{2i\sin\left(\frac{1}{2}h(\omega_{j}-k\cdot\omega)\right)} \left(\mathbf{N}(w(\tilde{\epsilon}t))_{j(k)}^{k} + \mathbf{B}(z(\tilde{\epsilon}t))_{j(k)}^{k}\right)\right]^{l}.$$
(44)

It is noted that by this iterative construction, the iterated modulation functions $[z_{i(k)}^k(\tilde{\epsilon}t)]^l$ are polynomials in $\tilde{\epsilon}t$ of degree bounded in terms of the number of iterations l.

4.2.3Rescaling

Following [19, 30], this subsection rescales and splits the modulation functions in order to make good use of the powers of $\tilde{\epsilon}$. By letting

$$[[k]] = \begin{cases} \max(2, (||k|| + 1)/2), & k \neq \langle j \rangle, \\ (||k|| + 1)/2 = 1, & k = \langle j \rangle, \end{cases}$$

we split the functions z_j^k into two parts $z_j^k = \tilde{\epsilon}^{[[k]]} a_j^k + \tilde{\epsilon}^{[[k]]} b_j^k$, where a_j^k denotes the "diagonal" entries (i.e., $a_j^k \neq 0$ only for $k = \langle j \rangle$) and b_j^k presents the "off-diagonal" entries (i.e., $b_j^k \neq 0$ only for $k = \langle j \rangle$) $k \neq \langle j \rangle$). We use the following notations

$$\mathbf{a} = (a^k)_k = (a^k_{j(k)}e^{i(j(k)\cdot x)})_k, \quad \mathbf{b} = (b^k)_k = (b^k_{j(k)}e^{i(j(k)\cdot x)})_k$$
(45)

and define the operator

$$(\mathbf{\Omega c})_{j}^{k} = \begin{cases} \frac{2\mathrm{i}\sin\left(\frac{1}{2}h(\omega_{j}-k\cdot\omega)\right)}{\mathrm{sinc}\left(\frac{1}{2}h\omega_{j}\right)}c_{j}^{k}, & (j,k) \in \mathcal{L}_{\tilde{\epsilon},M,h},\\ \\ \tilde{\epsilon}^{\frac{1}{2}}hc_{j}^{k}, & \text{else.} \end{cases}$$
(46)

Furthermore, we rescale the non-linearity $\mathbf{N}(\mathbf{w})$ by

$$\mathbf{F}(\mathbf{v})_{i}^{k} = \tilde{\epsilon}^{-\max([[k]],2)} \mathbf{N}(\mathbf{w}), \tag{47}$$

where $\mathbf{v} = (v^k)_k$ is defined by $v^k = \tilde{\epsilon}^{-[[k]]} w^k = \tilde{\epsilon}^{-[[k]]} w^k_{j(k)} e^{i(j(k) \cdot x)}$. We are now in a position to rewrite the iteration from the previous subsection in these rescaled variables.

Proposition 4 (*Rescaling.*) Using the above rescaled variables, the iteration given by Definition 2 can be formulated as

$$\begin{bmatrix} b_j^k \end{bmatrix}^{l+1} = \begin{bmatrix} (\mathbf{\Omega}^{-1} \mathbf{B}(\mathbf{b}))_j^k \end{bmatrix}^l + \begin{bmatrix} (\mathbf{\Omega}^{-1} \mathbf{F}(\mathbf{v}))_j^k \end{bmatrix}^l, \quad (j,k) \in \mathcal{L}_{\tilde{\epsilon},M,h}, \\ \begin{bmatrix} \dot{a}_j^{\langle j \rangle} \end{bmatrix}^{l+1} = \frac{\operatorname{sinc}(\frac{1}{2}h\omega_j)}{h\tilde{\epsilon}} \begin{bmatrix} (\mathbf{A}(\mathbf{a}))_j^{\langle j \rangle} \end{bmatrix}^l + \frac{\operatorname{sinc}(\frac{1}{2}h\omega_j)}{h} \begin{bmatrix} (\mathbf{F}(\mathbf{v}))_j^{\langle j \rangle} \end{bmatrix}^l, \\ \begin{bmatrix} a_j^{\langle j \rangle}(0) \end{bmatrix}^{l+1} = \tilde{\epsilon}^{-1} u_j^0 - \begin{bmatrix} \sum_{k \neq \langle j \rangle} \tilde{\epsilon}^{[[k]]-1} b_j^k(0) \end{bmatrix}^l, \end{aligned}$$
(48)

where $[v_j^k]^l = \tilde{\epsilon}^{-[[k]]} [w_j^k]^l$ defined by (35).

Another rescaling of the variables will be used in this section

$$\hat{a}_{j}^{k} = \left| \omega^{\frac{2s-d-1}{4}|k|} \right| a_{j}^{k}, \quad \hat{b}_{j}^{k} = \left| \omega^{\frac{2s-d-1}{4}|k|} \right| b_{j}^{k}, \quad \hat{v}_{j}^{k} = \left| \omega^{\frac{2s-d-1}{4}|k|} \right| v_{j}^{k}.$$

For these rescaled variables, the iteration for $\hat{\mathbf{b}}$ becomes

$$\left[\hat{b}_{j}^{k}\right]^{l+1} = \left[\left(\mathbf{\Omega}^{-1}\mathbf{B}(\hat{\mathbf{b}})\right)_{j}^{k}\right]^{l} + \left[\left(\mathbf{\Omega}^{-1}\hat{\mathbf{F}}(\hat{\mathbf{v}})\right)_{j}^{k}\right]^{l}, \quad (j,k) \in \mathcal{L}_{\tilde{\epsilon},M,h},$$

where $\hat{\mathbf{F}}(\hat{\mathbf{v}})_j^k = \left| \omega^{\frac{2s-d-1}{4}|k|} \right| \mathbf{F}(\mathbf{v})_j^k.$

4.2.4 Size of the iterated modulation functions

In this subsection, we will control the size of the iterated modulation functions. The norm $|||\mathbf{z}|||_s^2 = \sum_j |\omega_j|^s \left(\sum_k |z_j^k|\right)^2$ (see, e.g. [19]) will be used in the rest of this paper.

Before presenting the size of the iterated modulation functions, we first need to estimate the bounds of the operator Ω (46) and the non-linearity **F** (47).

Proposition 5 (Bounds of the operator Ω and the non-linearity **F**.) The following bounds hold

$$\begin{aligned} |||\mathbf{\Omega}^{-1}\mathbf{v}|||_{s} &\leq \tilde{\epsilon}^{-\frac{1}{2}}h^{-1}|||\mathbf{v}|||_{s}, \quad |||\mathbf{F}(\mathbf{v})|||_{s} &\leq C\tilde{\epsilon}h|||\check{\mathbf{v}}|||_{s}^{3}, \\ |||\mathbf{F}(\mathbf{v_{1}}) - \mathbf{F}(\mathbf{v_{2}})|||_{s} &\leq C\tilde{\epsilon}h|||\check{\mathbf{v}}_{1} - \check{\mathbf{v}}_{2}|||_{s}\max(|||\check{\mathbf{v}}_{1}|||_{s}, |||\check{\mathbf{v}}_{2}|||_{s})^{2}, \end{aligned}$$

$$\tag{49}$$

where $\check{\mathbf{v}} = \sup_{0 \le \sigma \le 1} \{\mathbf{v}(\tilde{\tau}, \sigma)\}$ and the constant *C* is independent of $\tilde{\epsilon}$ but depends on *d*, *s*, and *V*. The same estimates are ture for $\hat{\mathbf{v}}, \hat{\mathbf{F}}$ and $||| \cdot |||_{\frac{d+1}{2}}$ instead of \mathbf{v}, \mathbf{F} and $||| \cdot |||_s$, respectively.

<u>Proof</u> The proof is given in Appendix I.

We next consider the iterated modulation functions given in (45). Their sizes are controlled by the following result.

Proposition 6 (Size of the iterated modulation functions.) For $0 \le \tilde{\tau} = \tilde{\epsilon}t \le 1$ and for all $l \ge 0$, it is true that

$$|||[\mathbf{a}(\tilde{\tau})]^{l}|||_{s} \leq C, \quad |||[\mathbf{a}^{(n)}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}, \quad for \quad n \geq 1,$$

$$|||[\mathbf{b}^{(n)}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}^{\frac{1}{2}}, \quad for \quad n \geq 0,$$

(50)

where the constant C depends only on C_0, d, n, s and the norm of V. For $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ instead of \mathbf{a} and \mathbf{b} , the same estimates are true if $||| \cdot |||_s$ is replaced by $||| \cdot |||_{\frac{d+1}{2}}$. It follows from these bounds that the modulated Fourier expansion of the numerical scheme \tilde{u} is bounded by

$$\|\tilde{u}(t,\cdot)\|_{s} \le C\tilde{\epsilon} \tag{51}$$

and its coefficients z are controlled by

$$\sum_{j \in \mathcal{M}} |\omega_j|^s \left| z_j^{\langle j \rangle} \right|^2 \le C \tilde{\epsilon}^2, \quad \sum_{j \in \mathcal{M}} |\omega_j|^s \left(\sum_{k \neq \langle j \rangle} \left| z_j^k \right| \right)^2 \le C \tilde{\epsilon}^5.$$
(52)

<u>Proof</u> The proof is given in Appendix II.

4.2.5 Defect of the iterated modulation functions

After l iterations, the defect in the modulation system (44) with the initial value (36) has the form

$$\begin{bmatrix} d_j^k \end{bmatrix}^l = \begin{bmatrix} \mathrm{i}\hbar\omega_j \csc\left(\frac{1}{2}\hbar\omega_j\right) \sin\left(\frac{1}{2}\hbar(\omega_j - k \cdot \omega)\right) z_j^k - \mathbf{B}(\mathbf{z})_j^k - \mathbf{N}(\mathbf{w})_j^k \end{bmatrix}^l, \\ \begin{bmatrix} \tilde{d}_j^{\langle j \rangle}(0) \end{bmatrix}^l = u_j^0 - \begin{bmatrix} \sum_k z_{j(k)}^k(0) \end{bmatrix}^l.$$
(53)

Clearly, it can be decomposed into four parts: $[d_j^k]^l = [e_j^k + f_j^k + g_j^k + \dot{h}_j^k]^l$, where $[e_j^k]^l = 0$ for $(j,k) \in \mathcal{L}_{\tilde{\epsilon},M,h}, [f_j^k]^l = 0$ for non-near resonant indices $(j,k) \in \mathcal{R}_{\tilde{\epsilon},M,h}, [\dot{h}_j^k]^l = 0$ for $k \neq \langle j \rangle$, and $[g_j^k]^l = 0$ for $\|k\| \leq K$. The size of each part can be estimated as follows.

Proposition 7 (Defect of the iterated modulation functions.) For all $l \ge 0$ and for $0 \le \tilde{\tau} = \tilde{\epsilon}t \le 1$, it is true that

$$|||[\mathbf{f}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}^{N+3}h, \quad |||[\mathbf{g}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}^{N+3}h,$$
$$|||[\mathbf{e}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}^{\frac{p+4}{2}}h, \quad |||[\dot{\mathbf{h}}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}^{\frac{p+4}{2}}h, \quad (54)$$
$$|||[\ddot{\mathbf{d}}(0)]^{l}|||_{s} \leq C\tilde{\epsilon}^{\frac{p+2}{2}}h,$$

where the constant C depends on C_0, d, p, s and the norm of V. We have the same estimates for $\hat{\mathbf{e}}$ and $\hat{\mathbf{h}}$ instead of \mathbf{e} and \mathbf{h} provided $||| \cdot |||_s$ is replaced by $||| \cdot |||_{\frac{d+1}{2}}$.

<u>Proof</u> The proof is given in Appendix III.

4.2.6 The numerical solution on short time intervals

In this subsection, the size of the numerical solution u^n on a short time interval of length $\tilde{\epsilon}$ is studied. It is noted that since the considered integrator is implicit, fixed point arguments are considered for EP1 and we rewrite it as the following scheme

$$U^{n+1} = e^{V}u^{n} + h\varphi_{1}(V)\int_{0}^{1} f((1-\sigma)u^{n} + \sigma U^{n+1})d\sigma,$$

$$u^{n+1} = e^{V}u^{n} + h\varphi_{1}(V)\int_{0}^{1} f((1-\sigma)u^{n} + \sigma U^{n+1})d\sigma.$$
(55)

Proposition 8 (The numerical solution on short time intervals.) For $0 \le t_n = nh \le \tilde{\epsilon}^{-1}$ with a sufficiently small $\tilde{\epsilon}$, it is obtained that $||u^n||_s \le 2\tilde{\epsilon}$.

<u>**Proof**</u> This result is proved by induction on n that

$$|u^{n}||_{s} \leq \tilde{\epsilon} + 125Cnh\tilde{\epsilon}^{3} \qquad \text{for} \quad 0 \leq nh \leq \tilde{\epsilon}^{-1}$$

$$\tag{56}$$

and by letting $\tilde{\epsilon}$ be sufficiently small compared to C.

For n = 0 the estimate (56) is clear by considering (30). For n > 0, it follows from the definition of the integrator that

$$\|u^{n}\|_{s} \leq \|u^{n-1}\|_{s} + h \left\| \int_{0}^{1} f((1-\sigma)u^{n-1} + \sigma U^{n}) d\sigma \right\|_{s}$$

$$\leq \|u^{n-1}\|_{s} + h \left(\|u^{n-1}\|_{s} + \|U^{n}\|_{s} \right)^{3},$$
(57)

where (4.9) of [19] is used and U^n is a fixed point of

$$G: U \to e^V u^{n-1} + h\varphi_1(V) \int_0^1 f((1-\sigma)u^{n-1} + \sigma U) d\sigma.$$

For $0 \le nh \le \tilde{\epsilon}^{-1}$, since $\|u^{n-1}\|_s \le 2\tilde{\epsilon} \le 3\tilde{\epsilon}$, the function G maps the ball $\{U : \|U\|_s \le 3\tilde{\epsilon}\}$ to itself. Furthermore, using (4.11) in [19], we obtain

$$\left\| h\varphi_1(V) \int_0^1 f((1-\sigma)u^{n-1} + \sigma U) d\sigma - h\varphi_1(V) \int_0^1 f((1-\sigma)u^{n-1} + \sigma \tilde{U}) d\sigma \right\|_s$$

$$\leq 3C \max\left(\left\| u^{n-1} \right\|_s + \left\| U \right\|_s, \left\| u^{n-1} \right\|_s + \left\| \tilde{U} \right\|_s \right)^2 \left\| U - \tilde{U} \right\|_s.$$

This shows that the map G has a Lipschitz constant smaller than one for sufficiently small $\tilde{\epsilon}$ in the norm $\|\cdot\|_s$ on the ball $\{U : \|U\|_s \leq 3\tilde{\epsilon}\}$. In view of the Banach fixed point theorem, one has $\|U^n\|_s \leq 3\tilde{\epsilon}$ for the fixed point U^n of G. Therefore, (56) can be obtained by the induction hypothesis applied to (57).

4.2.7 The error between the modulated Fourier expansion and the numerical solution

This subsection pays attention to the error $u^n - \tilde{u}(t, x)$ between the numerical solution u^n and the modulated Fourier expansion

$$\tilde{u}(t,x) = \sum_{k} [z_{j(k)}^{k}(\tilde{\epsilon}t)]^{L} \mathrm{e}^{\mathrm{i}(j \cdot x)} \mathrm{e}^{-\mathrm{i}(k \cdot \omega)t},$$

where the iterated modulation functions $z_j^k = [z_j^k]^L$ after L := 2N + 2 iterations replace the exact solution of the modulation system which is not available in fact. For brevity, the index L in the following analysis is omitted.

Proposition 9 (The error between the modulated Fourier expansion and the numerical solution.) For $0 \le t_n = nh \le \tilde{\epsilon}^{-1}$, it is obtained that

$$||u^n - \tilde{u}(t_n, x)||_s \le C\tilde{\epsilon}^{N+2} \tag{58}$$

for $\tilde{\epsilon}$ sufficiently small compared to d, s and the norm of the potential V.

<u>Proof</u> As stated in the previous subsection, fixed point arguments are employed. By the definition of the modulation system (34)-(35) and fixed point arguments, it is arrived at that

$$\tilde{u}(t_n, x) = e^V \tilde{u}(t_{n-1}, x) + h\varphi_1(V) \int_0^1 f((1-\sigma)\tilde{u}(t_{n-1}, x) + \sigma \tilde{U}(t_n, x)) d\sigma + \delta(t_n, x)$$

with the defect $\delta(t,x) = \sum_{k} d_{j(k)}^{k}(\tilde{\epsilon}t) e^{i(j \cdot x)} e^{-i(k \cdot \omega)(t+h)}$. Here we have the following result

$$(1-\sigma)\tilde{u}(t_{n-1},x) + \sigma\tilde{U}(t_n,x) = \sum_{\|k\| \le K} w_{j(k)}^k \left(\tilde{\epsilon}(t+\frac{h}{2}),\sigma\right) \mathrm{e}^{\mathrm{i}(j(k)\cdot x)} \mathrm{e}^{-\mathrm{i}(k\cdot\omega)(t+\frac{h}{2})}$$

It follows from Proposition 7 that $||\delta(t,x)||_s \leq Ch\tilde{\epsilon}^{N+3}$ for $0 \leq t \leq \tilde{\epsilon}^{-1}$, where the constant C depends on C_0, d, N, s and the norm of the potential V.

• Proof of the difference $U^n - \tilde{U}(t_n, x)$.

For the solution U^n appearing in the numerical method (55), we first examine the difference $U^n - \tilde{U}(t_n, x)$. By (34)-(35) and (53), $\tilde{U}(t_n, x)$ is a fixed point of

$$\tilde{G}: \tilde{U} \to e^V \tilde{u}(t_{n-1}, x) + h\varphi_1(V) \int_0^1 f((1-\sigma)\tilde{u}(t_{n-1}, x) + \sigma\tilde{U})d\sigma + \delta(t_{n-1}, x).$$

Obviously, it follows from the proof of Proposition 8 that the fixed point iteration $[U]^l = G([U]^{l-1}), [U]^0 = e^V u^{n-1}$ converges in the norm $\|\cdot\|_s$ to U^n and is bounded in this norm by $3\tilde{\epsilon}$. In what follows, we study the error between $[U]^l$ and $\tilde{U} = \tilde{U}(t_n, x)$, i.e., $[U]^l - \tilde{U}$, for $l = 0, \ldots,$.

On noticing the fact $||U||_s \leq C\tilde{\epsilon}$ by Proposition 6 and the property (4.9) of [19], we obtain the estimate of the defect for l = 0

$$\begin{split} & \left\| [U]^0 - \tilde{U} \right\|_s = \left\| e^V u^{n-1} - \tilde{G}(\tilde{U}) \right\|_s \\ & \leq \left\| u^{n-1} - \tilde{u}(t_{n-1}, x) \right\|_s + h \left\| \int_0^1 f((1-\sigma)\tilde{u}(t_{n-1}, x) + \sigma \tilde{U}) d\sigma \right\|_s + \left\| \delta(t_{n-1}, x) \right\|_s \\ & \leq \left\| u^{n-1} - \tilde{u}(t_{n-1}, x) \right\|_s + Ch\tilde{\epsilon}^3 + Ch\tilde{\epsilon}^{N+3}. \end{split}$$

For l > 0, using (4.11) of [19] gives that

$$\left\| [U]^{l} - \tilde{U} \right\|_{s} = \left\| G([U]^{l-1}) - \tilde{G}(\tilde{U}) \right\|_{s}$$

$$\leq \left\| u^{n-1} - \tilde{u}(t_{n-1}, x) \right\|_{s} + Ch\tilde{\epsilon}^{2} \left\| [U]^{l-1} - \tilde{U} \right\|_{s} + Ch\tilde{\epsilon}^{N+3}$$

with a constant C independent of l. This leads to a recursion on l as follows

$$\left\| [U]^{l} - \tilde{U} \right\|_{s} \leq \left(\left\| u^{n-1} - \tilde{u}(t_{n-1}, x) \right\|_{s} + Ch\tilde{\epsilon}^{N+3} \right) \sum_{j=0}^{l} (Ch\tilde{\epsilon}^{2})^{j} + Ch\tilde{\epsilon}^{3} (Ch\tilde{\epsilon}^{2})^{l}.$$

Considering $l \to \infty$ and $Ch\tilde{\epsilon}^2 \leq \frac{1}{2}$ implies

$$\left\| U^{n} - \tilde{U}(t_{n}, x) \right\|_{s} \le 2 \left\| u^{n} - \tilde{u}(t_{n}, x) \right\|_{s} + 2Ch\tilde{\epsilon}^{N+3}.$$
(59)

• Proof of the difference $u^n - \tilde{u}(t_n, x)$.

We are now in a position to consider $u^n - \tilde{u}(t_n, x)$. When n > 0, using (4.11) of [19] gives

$$\|u^{n} - \tilde{u}(t_{n}, x)\|_{s} \leq \|u^{n-1} - \tilde{u}(t_{n-1}, x)\|_{s} + Ch\tilde{\epsilon}^{2} \|U^{n} - \tilde{U}(t_{n}, x)\|_{s} + Ch\tilde{\epsilon}^{N+3}.$$

Considering again the result (59), we have by induction on n

$$\|u^{n} - \tilde{u}(t_{n}, x)\|_{s} \leq (1 + 2Ch\tilde{\epsilon}^{2})^{n} \left(Cnh\tilde{\epsilon}^{N+3} + \|u^{0} - \tilde{u}(0, x)\|_{s}\right).$$
(60)

On the other hand, by Proposition 7 with the defect $\tilde{\mathbf{d}}$ in the initial condition, we have $\|u^0 - \tilde{u}(0, x)\|_s \le |||[\tilde{\mathbf{d}}(0)]^n|||_s \le C\tilde{\epsilon}^{N+3}$. This result together with (60) guarantees the desired result if $\tilde{\epsilon}$ is sufficiently small.

4.2.8 Almost invariants close to the actions

In what follows, we show an invariant of the modulation system and its relationship with the actions.

Proposition 10 (Almost invariant.) There exits $\tilde{\epsilon} \mathcal{J}_{(j)}(\tilde{\tau})$ such that

$$\sum_{j \in \mathcal{M}} |\omega_j|^s \left| \frac{d}{d\tilde{\tau}} \mathcal{J}_{\langle j \rangle}(\tilde{\tau}) \right| \le Ch \tilde{\epsilon}^{N+3}$$

where $\tilde{\tau} \leq 1$ and C depends on $\max_{j \in \mathcal{M}} \left\{ \frac{1}{\left| \cos(\frac{1}{2}h\omega_j) \right|} \right\}$. Moreover, it is true that

$$\mathcal{J}_{\langle j \rangle}(\tilde{\tau}) = \frac{1}{2} \left| z_j^{\langle j \rangle}(\tilde{\tau}) \right|^2 + \mathcal{O}\left(h \tilde{\epsilon}^2 \right).$$

<u>Proof</u> Let

$$\mathcal{U}(\mathbf{w}) = \sum_{k^1 + k^2 - k^3 - k^4 = 0} \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \int_0^1 w^{k^1} w^{k^2} \overline{w^{k^3} w^{k^4}} d\sigma dx$$

From the above analysis, we can write the defect formula d^k as

$$\tilde{L}^{k} z^{k} = -\mathrm{i}h \sum_{k^{1}+k^{2}-k^{3}=k} \int_{0}^{1} w_{j(k^{1})}^{k^{1}} w_{j(k^{2})}^{k^{2}} \overline{w_{j(k^{3})}^{k^{3}}} d\sigma + d^{k}.$$
(61)

Here we use \tilde{L}^k to denote the truncation of the operator L^k after the $\tilde{\epsilon}^N$ term. The transformation $w^k \to e^{i(k \cdot \mu)\theta} w^k$ for real sequences $\mu = (\mu_l)_{l \ge 0}$ and $\theta \in \mathbb{R}$ and the choice of $k = \langle j \rangle$ leaves \mathcal{U} invariant

$$\begin{split} 0 &= h \frac{d}{d\theta} \mid_{\theta=0} \mathcal{U} \Big((\mathrm{e}^{\mathrm{i}(\langle j \rangle \cdot \mu)\theta} w^{\langle j \rangle})_{\langle j \rangle} \Big) \\ &= -4h \mathrm{Re} \Big(\sum_{j} \mathrm{i}(\langle j \rangle \cdot \mu) \overline{w_{j}^{\langle j \rangle}} \sum_{k^{1}+k^{2}-k^{3}=\langle j \rangle} \int_{0}^{1} w_{j(k^{1})}^{k^{1}} w_{j(k^{2})}^{k^{2}} \overline{w_{j(k^{3})}^{k^{3}}} d\sigma \Big) \\ &= 4 \mathrm{Re} \Big(\sum_{j} (\langle j \rangle \cdot \mu) \overline{w_{j}^{\langle j \rangle}} \big(\tilde{L}^{\langle j \rangle} z_{j}^{\langle j \rangle} - d_{j}^{\langle j \rangle} \big) \Big) \\ &= 4 \mathrm{Re} \Big(\sum_{j} (\langle j \rangle \cdot \mu) \overline{L_{3}^{\langle j \rangle}(\sigma) z_{j}^{\langle j \rangle}} \big(\tilde{L}^{\langle j \rangle} z_{j}^{\langle j \rangle} - d_{j}^{\langle j \rangle} \big) \Big). \end{split}$$

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

$$4\operatorname{Re}\sum_{j}(\langle j\rangle \cdot \mu)\overline{L_{3}^{\langle j\rangle}(1/2)z_{j}^{\langle j\rangle}}\tilde{L}^{\langle j\rangle}z_{j}^{\langle j\rangle} = 4\operatorname{Re}\sum_{j}(\langle j\rangle \cdot \mu)\overline{L_{3}^{\langle j\rangle}(1/2)z_{j}^{\langle j\rangle}}d_{j}^{\langle j\rangle}.$$
(62)

By the expansions of $L_3^{\langle j \rangle}(1/2)$ and $\tilde{L}^{\langle j \rangle}$ and the "magic formulas" on p. 508 of [35], it is known that the left-hand side of (62) is a total derivative of function $\tilde{\epsilon} \mathcal{J}_{\mu}(\tilde{\tau})$. Therefore (62) is identical to

$$\tilde{\epsilon} \frac{d}{d\tilde{\tau}} \mathcal{J}_{\mu} = 4 \operatorname{Re} \sum_{j} (\langle j \rangle \cdot \mu) \overline{L_{3}^{\langle j \rangle}(1/2) z_{j}^{\langle j \rangle}} d_{j}^{\langle j \rangle}.$$

Considering the special case of $\mu = \frac{\operatorname{sinc}(\frac{1}{2}h\omega_j)}{\cos(\frac{1}{2}h\omega_j)}\langle j \rangle$ and for the first result, it needs to prove that

$$\sum_{j \in \mathcal{M}} |\omega_j|^s \left| \frac{\operatorname{sinc}(\frac{1}{2}h\omega_j)}{\cos(\frac{1}{2}h\omega_j)} \right| \left| \overline{L_3^{\langle j \rangle}(1/2) z_j^{\langle j \rangle}} d_j^{\langle j \rangle} \right| \le Ch\tilde{\epsilon}^{N+4}.$$

By the property of L_3 , we have

$$\sum_{j \in \mathcal{M}} \left| \omega_j \right|^s \left| \frac{\operatorname{sinc}(\frac{1}{2}h\omega_j)}{\cos(\frac{1}{2}h\omega_j)} \right| \left| \overline{L_3^{\langle j \rangle}(1/2) z_j^{\langle j \rangle}} d_j^{\langle j \rangle} \right| \le C \sum_{j \in \mathcal{M}} \left| \omega_j \right|^s \left| z_j^{\langle j \rangle} \right| \left| \dot{h}_j^{\langle j \rangle} \right|.$$

Taking advantage of Cauchy-Schwarz inequality, one gets

$$\begin{split} &\sum_{j\in\mathcal{M}} |\omega_j|^s \left| \frac{\operatorname{sinc}(\frac{1}{2}h\omega_j)}{\cos(\frac{1}{2}h\omega_j)} \right| \left| \overline{L_3^{\langle j \rangle}(1/2)z_j^{\langle j \rangle}} d_j^{\langle j \rangle} \right| \\ &\leq C \sqrt{\sum_{j\in\mathcal{M}} \left(|\omega_j|^{\frac{s}{2}} \right)^2 \left| z_j^{\langle j \rangle} \right|^2} \sqrt{\sum_{j\in\mathcal{M}} \left(|\omega_j|^{\frac{s}{2}} \right)^2 \left| \dot{h}_j^{\langle j \rangle} \right|^2} \\ &\leq C \sqrt{\tilde{\epsilon}^2} \sqrt{h^2 \tilde{\epsilon}^{p+4}} = C h \tilde{\epsilon}^{\frac{p}{2}+3} = C h \tilde{\epsilon}^{\frac{L}{2}+3}, \end{split}$$

where the results (52) and (54) are used here. The first statement is immediately obtained by considering L = 2N + 2.

Then, using the Taylor expansions of $L_3^{\langle j \rangle}(1/2)$ and $L^{\langle j \rangle}$ and the "magic formulas" on p. 508 of [35] gives the construction of $\mathcal{J}_{\langle j \rangle}$.

After obtaining the almost invariant, its relationship with the actions is derived below.

Proposition 11 (The relationship between the almost invariant and the actions.) It is true that $\sum_{j \in \mathcal{M}} |\omega_j|^s |\mathcal{J}_{\langle j \rangle}(\tilde{\tau}) - I_j(u^n, \overline{u^n})| \leq C\tilde{\epsilon}^{\frac{7}{2}}$, where $\tilde{\tau} \leq 1$.

<u>Proof</u> This result can be obtained by following the proof of Proposition 6 given in [29].

4.2.9 Near-conservation of actions, density and momentum

According to the analysis stated above, we consider the interface between the modulated Fourier expansions and extend it from short to long time intervals in the same way used in Sects. 4.10-4.11 of [19]. Then the near conservation of actions given in Theorem 4 is obtained. Meanwhile, it follows from the results presented in Sect. 6.4 of [30] and Sect. 4.11 of [19] that the long-time near-conservation of actions implies the long-time near-conservation of density and of momentum. Therefore, the other statements of Theorem 4 are proved.

This concludes the proof of Theorem 4 for the integrator EP1.

4.2.10 **Proof for EP2**

Consider the one-point quadrature formula with $(\tilde{c}_1, \tilde{d}_1)$ and then the scheme of (29) becomes

$$u^{n+1} = e^{V}u^{n} + h\tilde{d}_{1}A_{1,\tilde{c}_{1}}(V)f\Big(C_{\tilde{c}_{1}}(V)u^{n} + A_{\tilde{c}_{1},\tilde{c}_{1}}(V)A_{1,\tilde{c}_{1}}^{-1}(V)(u^{n+1} - e^{V}u^{n})\Big).$$
(63)

Methods	Energy conservation	Optimal convergence	Near conservations
EP1	\checkmark	$\times (h^2)$	\checkmark
EP2	\checkmark	$\sqrt{(\varepsilon h^2)}$	\checkmark
EP3		$\sqrt{(\varepsilon h^3)}$	×

Table 1: Properties of the methods.

In terms of this formula, we can derive the modulation equations for the modulation functions z_j^k as $L^k z_j^k(\tilde{\epsilon}t) = -\mathrm{i}h \sum_{k^1+k^2-k^3=k} z_{j(k^1)}^{k^1}(\tilde{\epsilon}t) z_{j(k^2)}^{k^2}(\tilde{\epsilon}t) \overline{z_{j(k^3)}^{k^3}}(\tilde{\epsilon}t)$ by defining

$$L^k := \left(A_{\tilde{c}_1,\tilde{c}_1}A_{1,\tilde{c}_1}^{-1}(\mathrm{e}^{-\mathrm{i}(k\cdot\omega)h}\mathrm{e}^{\tilde{\epsilon}hD} - \mathrm{e}^{\mathrm{i}h\Omega}) + C_{\tilde{c}_1}\right)^{-1}(\mathrm{e}^{-\mathrm{i}(k\cdot\omega)h}\mathrm{e}^{\tilde{\epsilon}hD} - \mathrm{e}^{\mathrm{i}h\Omega})(\tilde{d}_1B_{\tilde{c}_1})^{-1}.$$

It can be seen that this formula has more concise expression than that of EP1. Then by modifying the nonlinearity and concerning the property of L^k , the analysis given above can be changed accordingly for EP2.

Remark 6 It is noted that the scheme (63) has been analysed in [19]. Under an assumption on the coefficient functions of exponential integrator, long term conservations have been derived there. However, for the coefficients $A_{\tilde{c}_1,\tilde{c}_1}(V)$, $A_{1,\tilde{c}_1}(V)$ of EP2, they do not satisfy that assumption required in [19]. Thus the part 4.2 of the proof given in [19] cannot be used for EP2. Therefor we consider the above approach to proving the result. On the other side, the operator L^k determined by EP3 does not have similar property as (37). Therefore, there is no invariant of the modulation system and the near conservations are not true for EP3.

5 Numerical experiment

For the algorithms presented in this paper, their properties are summarized in Table 1. In order to show their advantages, we choose the second-order explicit exponential integrator which is termed pseudo steady-state approximation which was given in [51] (denoted by EEI) and the fourth-order explicit exponential Runge–Kutta method which was given in [37] (denoted by IEI4). As a numerical experiment, we consider the problem with d = 1 and $\lambda = -2$ and the pseudospectral method with 64 points. In the practical computations, we apply the three-point Gauss-Legendre's rule to the integral in (9) and use a fixed-point iteration with the error tolerance 10^{-16} and the maximum number 100 for each iteration. In order to show the obtained methods behave well for different initial and boundary conditions, we will use various conditions in the experiment.

Energy conservation. The initial value is given by $u^0(x) = 0.5i + 0.025 \cos(\mu x)$ and the periodic boundary condition is u(t, 0) = u(t, L). We consider $L = 4\sqrt{2\pi}$ and integrate this problem on [0, 100] with h = 1/100 for different ε . The conservation of discretised energy is shown in Figures 1. From these results, it can be seen clearly that the EP integrators EP1-EP3 preserve the energy with a very good accuracy, which supports the results of Theorem 1.

Convergence. Following [17], $u^0(x)$ is chosen as $u^0(x) = \cos(x) + \sin(x)$ and the boundary condition is $u(t,0) = u(t,2\pi)$. The long term NSE (17) is solved in $[0,T/\varepsilon]$ with T = 1 and $h = 1/2^i$ for $i = 1, \ldots, 6$. The global errors of our methods measured in L^2 and H^1 for different ε are presented in Figure 2. For comparison, the errors of EEI are also displayed in Figure 2. It

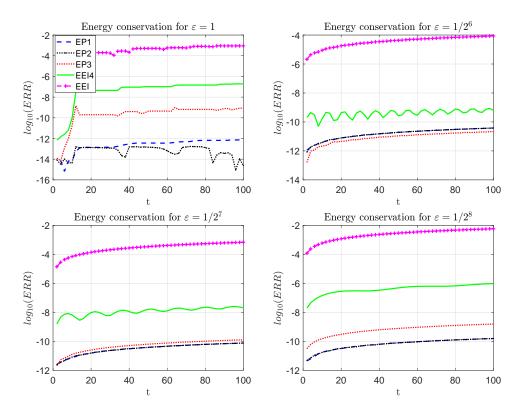


Figure 1: The relative error of discrete energy (EER) against t.

follows that EP1 only has the global error $\mathcal{O}(h^2)$ while EP2 has the error bound $\mathcal{O}(\varepsilon h^2)$ and EP3 shows $\mathcal{O}(\varepsilon h^3)$. This agrees with the results of Theorem 3. It seems here that EP3 has a better convergence than $\mathcal{O}(\varepsilon h^3)$. But after presenting the errors for $\varepsilon = 1$ in Figure 3, it can be observed that EP3 still shows a third-order convergence.

Near-conservations in other aspects. In order to show the near-conservations in other aspects, small initial value is required. Following [19, 30], we change the initial value into $u^0(x) = 0.1(\frac{x}{\pi}-1)^3(\frac{x}{\pi}+1)^2 + i \times 0.1(\frac{x}{\pi}-1)^3(\frac{x}{\pi}+1)^3$ and consider the periodic boundary condition $u(t, -\pi) = u(t, \pi)$. The problem is solved on [0, 10000] with $h = \frac{1}{100}$ and the relative errors of density and momentum are shown in Figures 4-5, respectively ³. It can be observed clearly from these results that the density and momentum are conserved well by EP1-EP2 but not by EP3 over long terms, which supports the results stated in Theorem 4.

Based on the numerical results, we can draw the following observations.

1) The energy-preserving methods EP1-EP3 preserve the energy with a very good accuracy for both regimes of ε , which is much better than the existed exponential integrators EEI and EEI4 (see Figure 1).

2) For the highly oscillatory regime, the integrators EP2-EP3 show improved error bounds while EP1 and EEI do not have the optimal convergence (see Figure 2). For the regime $\varepsilon = 1$, EP1-EP3

³The methods show similar conservation of actions and we omit the corresponding numerical results for brevity.

Systems	Replace $i\mathcal{A}$ by	New f
Hamiltonian system with	$\begin{pmatrix} 0 & I \end{pmatrix}$	$\begin{pmatrix} 0 \end{pmatrix}$
$H(q,p) = \frac{1}{2}p^{T}p + \frac{1}{2}q^{T}\Omega q + U(q)$	$\begin{pmatrix} -\Omega & 0 \end{pmatrix}$	$\left(-\nabla U(q) \right)$
Wave equation	$\begin{pmatrix} 0 & I \end{pmatrix}$	$\begin{pmatrix} 0 \end{pmatrix}$
$u_{tt} - a^2 \Delta u = g(u)$	$\begin{pmatrix} -a^2\Delta & 0 \end{pmatrix}$	$\left(\begin{array}{c} g(u) \end{array} \right)$
Damped Helmholtz-Duffing oscillator	$\begin{pmatrix} 0 & I \end{pmatrix}$	
$q'' + 2\upsilon q' = -Aq - Bq^2 - \varepsilon q^3$	$\begin{pmatrix} 0 & 2v \end{pmatrix}$	$\left(-Aq - Bq^2 - \varepsilon q^3 \right)$
Charged-particle dynamics	$\begin{pmatrix} 0 & I \end{pmatrix}$	$\begin{pmatrix} 0 \end{pmatrix}$
in a constant magnetic field	$\left(\begin{array}{cc} 0 & I \\ 0 & \tilde{B} \end{array}\right)$	$\left(\begin{array}{c} 0\\ F(x) \end{array}\right)$
$x'' = \tilde{B}x' + F(x)$		
First-order ODEs	$\frac{1}{\varepsilon}A$	f(x)
$x' = \frac{1}{\varepsilon}Ax + f(x)$	εΛ	J(x)

Table 2: Some systems which the presented methods can be applied.

show the normal global errors (see Figure 3).

3) The integrators EP1-EP2 have the long term near conservations in the density, momentum and action but the methods EP3, EEI and EEI4 do not show such long time behaviour (see Figures 4-5).

6 Applications and future issues

This is a preliminary research on the long-time behaviour of energy-preserving exponential integrators and it is noted that the algorithms can be extended to the numerical solutions of the following equations (see Table 2) by replacing $i\mathcal{A}$ and f in (6) with the new ones.

We also note that there are some issues which can be further considered.

- The extensions of the methods as well as their analysis in this paper to the logarithmic Schrödinger equation ([4]) and time-dependent Schrödinger equation in semiclassical scaling ([43]) will be researched in future.
- The long term analysis of other kinds of energy-preserving integrators in other PDEs such as Vlasov-Poisson system ([26, 46]) and Maxwell equations will also be considered.
- Another issue for future exploration is the analysis of parareal algorithms of Schrödinger equations.

Appendix

Appendix I. Proof of Proposition 5

• Proof of the first result.

For the case that $(j,k) \in \mathcal{L}_{\tilde{\epsilon},M,h}$, we have $\left|2i\sin\left(\frac{1}{2}h(\omega_j - k \cdot \omega)\right)\right| > \tilde{\epsilon}^{\frac{1}{2}}h$. Then from this it follows that $\left|\frac{\operatorname{sinc}\left(\frac{1}{2}h\omega_j\right)}{2i\sin\left(\frac{1}{2}h(\omega_j - k \cdot \omega)\right)}\right| \leq \frac{1}{\tilde{\epsilon}^{\frac{1}{2}}h}$, which yields $|||\mathbf{\Omega}^{-1}\mathbf{v}|||_s \leq \tilde{\epsilon}^{-\frac{1}{2}}h^{-1}|||\mathbf{v}|||_s$. For other (j,k), the statement is obtained by considering the definition of Ω .

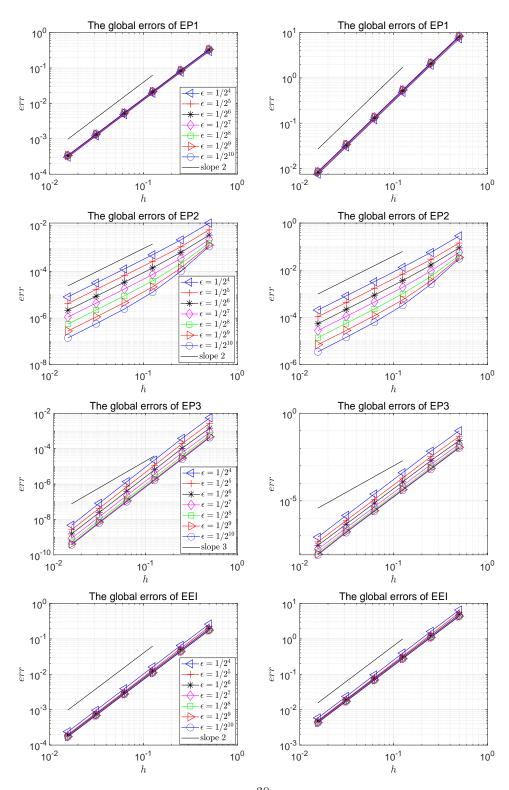


Figure 2: The global error (err) measured in $\overset{30}{L^2}$ (left) and H^1 (right) against the stepsize.

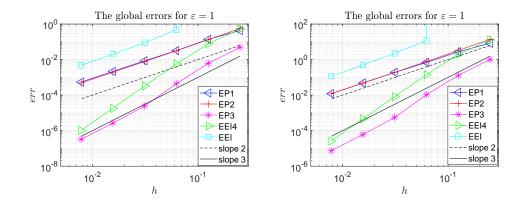


Figure 3: The global error (err) measured in L^2 (left) and H^1 (right) against the stepsize.

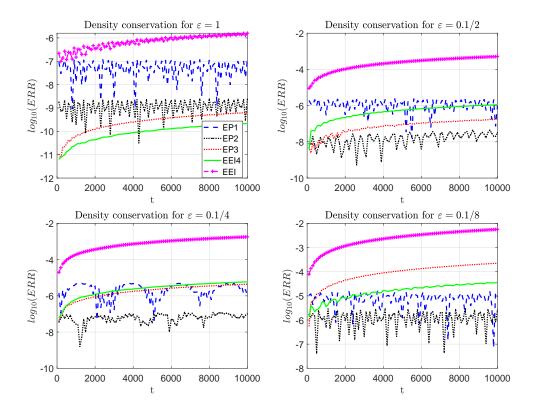


Figure 4: The relative error of density against t.

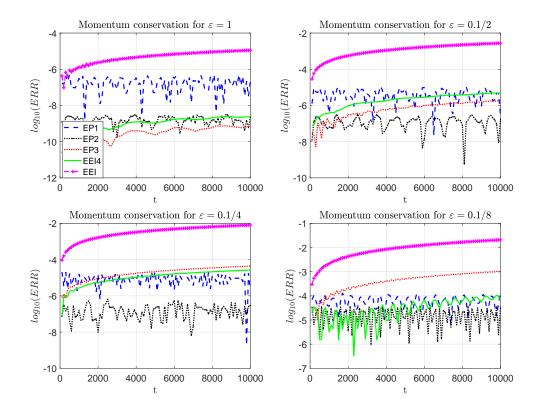


Figure 5: The relative error of momentum against t.

• Proof of the second result.

Taking into account the result proved in [29] $[[k^1]] + [[k^2]] + [[k^3]] \ge \max([[k^1]], 2) + 1)$, one has

$$\begin{split} |||\mathbf{F}(\mathbf{v})|||_{s}^{2} &= \sum_{j} |\omega_{j}|^{s} \left(\sum_{k} \tilde{\epsilon}^{-\max([[k]],2)} \right. \\ &\left. \left. \left. \left. \left| \mathrm{i}h \sum_{k^{1}+k^{2}-k^{3}=k} \int_{0}^{1} \tilde{\epsilon}^{[[k^{1}]]+[[k^{2}]]+[[k^{3}]]} v_{j(k^{1})}^{k^{1}} v_{j(k^{2})}^{k^{2}} \overline{v_{j(k^{3})}^{k^{3}}} d\sigma \right| \right)^{2} \right. \\ &\leq h^{2} \tilde{\epsilon}^{2} \sum_{j} |\omega_{j}|^{s} \sum_{k^{1},k^{2},k^{3}} \left(\left| \int_{0}^{1} v_{j(k^{1})}^{k^{1}} v_{j(k^{2})}^{k^{2}} \overline{v_{j(k^{3})}^{k^{3}}} d\sigma \right| \right)^{2} \\ &= h^{2} \tilde{\epsilon}^{2} \left\| \sum_{k^{1},k^{2},k^{3}} \int_{0}^{1} v_{j(k^{1})}^{k^{1}} v_{j(k^{2})}^{k^{2}} \overline{v_{j(k^{3})}^{k^{3}}} d\sigma \right\|^{2} \leq Ch^{2} \tilde{\epsilon}^{2} (|||\mathbf{\check{v}}|||_{s}^{3})^{2}. \end{split}$$

• Proof of the last result.

According to [29], the following result is true

$$a_1a_2a_3 - b_1b_2b_3 = \sum_{j=1}^3 2^{-j}(a_1 + b_1)\cdots(a_{j-1} + b_{j-1})(a_j + b_j)(a_{j+1}\cdots a_3 + b_{j+1}\cdots b_3).$$

Then from this result and by a similar calculation to that for the second result, the last statement is arrived at.

The same calculation is also true for $\hat{\mathbf{v}}, \hat{\mathbf{F}}$ and $||| \cdot |||_{\frac{d+1}{2}}$ instead of \mathbf{v}, \mathbf{F} and $||| \cdot |||_s$, respectively.

Appendix II. Proof of Proposition 6

• Proof of (50).

In the light of the choice of the initial iteration, we have

$$\begin{aligned} &||| [\mathbf{a}(\tilde{\tau})]^{0} |||_{s} \leq C, \ ||| [\mathbf{a}^{(n)}(\tilde{\tau})]^{0} |||_{s} = 0 \quad \text{for} \quad n \geq 1, \\ &||| [\mathbf{b}^{(n)}(\tilde{\tau})]^{0} |||_{s} = 0 \quad \text{for} \quad n \geq 0. \end{aligned}$$

From the third equality of (48), it follows that

$$||| [\mathbf{a}(0)]^{l+1} |||_{s} = \left(\sum_{j} |\omega_{j}|^{s} \left| [\mathbf{a}_{j}^{\langle j \rangle}(0)]^{l+1} \right|^{2} \right)^{1/2} \leq \tilde{\epsilon}^{-1} \|u(0)\|_{s} + \tilde{\epsilon} \left\| [\mathbf{b}(0)]^{l} \right\|_{s}.$$

According to the first equality of (48), we have

$$\begin{aligned} |||[\mathbf{b}^{(n)}]^{l+1}|||_{s} &\leq |||[\Omega^{-1}\mathbf{B}(\mathbf{b})^{(n)}]^{l}|||_{s} + |||[\Omega^{-1}\mathbf{F}(\mathbf{v}^{l})]^{(n)}|||_{s} \\ &\leq \tilde{\epsilon}^{\frac{1}{2}}|||[\mathbf{b}^{(n+1)}]^{l}|||_{s} + h^{-1}\tilde{\epsilon}^{-\frac{1}{2}}|||[\mathbf{F}(\mathbf{v}^{l})]^{(n)}|||_{s}. \end{aligned}$$

With the second equality of (48), it is deduced that

$$\begin{aligned} |||[\mathbf{a}^{(n+1)}]^{l+1}|||_{s} &\leq |||[\frac{\operatorname{sinc}(\frac{1}{2}h\Omega)}{h\tilde{\epsilon}}\mathbf{A}(\mathbf{a})^{(n)}]^{l}|||_{s} + |||[\frac{\operatorname{sinc}(\frac{1}{2}h\Omega)}{h\tilde{\epsilon}}\mathbf{F}(\mathbf{v}^{l})]^{(n)}|||_{s} \\ &\leq h^{2}\tilde{\epsilon}^{2}|||[\mathbf{a}^{(n+2)}]^{l}|||_{s} + h^{-1}|||[\mathbf{F}(\mathbf{v}^{l})]^{(n)}|||_{s}, \quad l = 0, 1, \dots, \\ &|||[\mathbf{a}]^{l+1}|||_{s} \leq |||[\mathbf{a}(0)]^{l+1}|||_{s} + \sup_{\tilde{\tau}} |||[\dot{\mathbf{a}}(\tilde{\tau})]^{l+1}|||_{s}. \end{aligned}$$

By Proposition 5 and the same analysis as that described in Section 3.6 of [29], the result (50) can be proved.

• Proof of (51).

For $\tilde{u} = [\tilde{u}]^L = \sum_k [z^k]^L e^{-i(k \cdot \omega)t}$ with L the number of ending iterate and by the same calculations as those presented in [29], one has

$$\|\tilde{u}\|_{s}^{2} = \sum_{j} |\omega_{j}|^{s} \left| \sum_{k} [z_{j}^{k}]^{L} \mathrm{e}^{-\mathrm{i}(k \cdot \omega)t} \right|^{2} \leq \tilde{\epsilon}^{2} \sum_{j} |\omega_{j}|^{s} \left(\sum_{k} \left| [c_{j}^{k}]^{L} \right| \right)^{2} = \tilde{\epsilon}^{2} |||[\mathbf{c}]^{L}|||_{s}^{2},$$

which proves (51).

• Proof of (52).

We now turn to the size of the variables $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ in the second rescaling, and we have $|||\hat{\mathbf{a}}|||_{\frac{d+1}{2}} = |||\mathbf{a}|||_s, |||\hat{\mathbf{b}}|||_{\frac{d+1}{2}} = |||\mathbf{b}|||_s$. Then from this fact and the above analysis, (52) is obtained.

Appendix III. Proof of Proposition 7

• Proof of the first result.

In order to estimate \mathbf{f} , the nonresonance condition (32) and Proposition 5 are considered. Under these conditions and for $l = 0, \ldots, L$, one has

$$\begin{split} |||[\mathbf{f}]^{l}|||_{s}^{2} &= \sum_{j} |\omega_{j}|^{s} \left(\sum_{k:(j,k)\in\mathcal{R}_{\bar{\epsilon},M,h}} \left|[f_{j}^{k}]^{l}\right|\right)^{2} \\ &= \sum_{j} |\omega_{j}|^{\frac{d+1}{2}} \left(\sum_{k:(j,k)\in\mathcal{R}_{\bar{\epsilon},M,h}} \frac{|\omega_{j}|^{\frac{2s-d-1}{4}} \tilde{\epsilon}^{\max([[k]],2)}}{\left|\omega^{\frac{2s-d-1}{4}}|k|\right|} \left|[\hat{\mathbf{F}}(\hat{\mathbf{u}})_{j}^{k}]^{l}\right|\right)^{2} \\ &\leq |||[[\hat{\mathbf{F}}(\hat{\mathbf{u}})]^{n}|||_{\frac{d+1}{2}}^{2} \sup_{(j,k)\in\mathcal{R}_{\bar{\epsilon},M,h}} \left(\frac{|\omega_{j}|^{\frac{2s-d-1}{4}}}{\left|\omega^{\frac{2s-d-1}{4}}|k|\right|} \tilde{\epsilon}^{[[k]]}\right)^{2} \\ &\leq C(h\tilde{\epsilon})^{2} \tilde{\epsilon}^{2N+4} = Ch^{2} (\tilde{\epsilon}^{N+3})^{2}. \end{split}$$

• Proof of the second result.

From ||k|| > K, it follows that $[[k]] \ge (K+2)/2 = N+2$. With the same arguments as those

given in the proof of Proposition 5, we obtain

$$\begin{split} & \left\| \sum_{\|k\| > K} [g^k]^l \right\|_s \\ = \left\| \sum_{\|k\| > K} \tilde{\epsilon}^{[[k]]} \left[\tilde{\epsilon}^{-[[k]]} \sum_{k^1 + k^2 - k^3 = k} \int_0^1 \tilde{\epsilon}^{[[k^1]] + [[k^2]] + [[k^3]]} w_{j(k^1)}^{k^1} w_{j(k^2)}^{k^2} \overline{w_{j(k^3)}^{k^3}} d\sigma \right] \right\|_s \\ \leq C \tilde{\epsilon}^{\frac{K+2}{2}} h \tilde{\epsilon} = C \tilde{\epsilon}^{N+3} h. \end{split}$$

• Proof of the third and fourth results.

The off-diagonal part \mathbf{e} and the diagonal part \mathbf{h} of the defect can be expressed respectively by

$$[e_j^k]^l = \tilde{\epsilon}^{[[k]]} \big([(\mathbf{\Omega}\mathbf{b})_j^k]^l - [(\mathbf{\Omega}\mathbf{b})_j^k]^{l+1} \big), \quad [h_j^k]^l = \tilde{\epsilon}^{3/2} \big([(\mathbf{\Omega}\mathbf{a})_j^k]^l - [(\mathbf{\Omega}\mathbf{a})_j^k]^{l+1} \big).$$

Using a Lipschitz estimate given in Proposition 5 for the nonlinearity and by an analysis of the iteration used as in Sect. 5.7 of [30], it is obtained that

$$\begin{aligned} |||[\mathbf{h}(\tilde{\tau})]^{l}|||_{s} &\leq C\tilde{\epsilon}\frac{p+4}{2}h, \ |||[\mathbf{h}^{(n)}(\tilde{\tau})]^{l}|||_{s} \leq C\tilde{\epsilon}\frac{p+4}{2}h, \ l \geq 1, \\ |||[\mathbf{e}^{(n)}(\tilde{\tau})]^{l}|||_{s} &\leq C\tilde{\epsilon}\frac{p+4}{2}h, \ l \geq 0 \end{aligned}$$

for $0 \leq \tilde{\tau} \leq 1$.

• Proof of the last result.

The last result can follows from the same arguments as the description of (29) in [30].

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