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Hamiltonian Interpolation of Splitting Approximations for Nonlinear PDEs

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Abstract We consider a wide class of semilinear Hamiltonian partial differential equations and their approximation by time splitting methods. We assume that the nonlinearity is polynomial, and that the numerical trajectory remains at least uniformly integrable with respect to an eigenbasis of the linear operator (typically the Fourier basis). We show the existence of a modified interpolated Hamiltonian equation whose exact solution coincides with the discrete flow at each time step over a long time. While for standard splitting or implicit–explicit schemes, this long time depends on a cut-off condition in the high frequencies (CFL condition), we show that it can be made exponentially large with respect to the step size for a class of modified splitting schemes.

Keywords Hamiltonian interpolation · Backward error analysis · Splitting integrators · Nonlinear Schrödinger equation · Nonlinear wave equation · Long-time behavior

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1 Introduction

The *Hamiltonian interpolation* of a symplectic map which is a perturbation of the identity is a central problem both in the study of Hamiltonian systems and in their discretization by numerical methods. This question actually goes back to Moser [26] who interpreted such a map as the exact flow of a Hamiltonian system in the finite-dimensional context. Such a result was later refined and extended by Benettin and Giorgilli [5] to the analysis of symplectic numerical methods, and leads to the seminal backward error analysis results of Hairer, Lubich [17] and Reich [27] for numerical integrators applied to ordinary differential equations. These results constitute now a cornerstone of the *geometric numerical integration theory* [19, 23].

In the finite-dimensional case, the situation can be described as follows: if $(p,q)\mapsto\Psi^h(p,q)$ is a symplectic map from the phase space $\mathbb{R}^{2d}$ into itself, and if this map is a perturbation of the identity, $\Psi^h=\mathrm{Id}+\mathcal{O}(h)$, then there exists a Hamiltonian function $H_h(p,q)$ such that Ψ^h can be interpreted as the flow at time $t=h$ of the Hamiltonian system associated with H_h. If Ψ^h is analytic, such results hold up to an error that is exponentially small with respect to the small parameter h, and for (p,q) in a compact set of the phase space. In applications to numerical analysis, the map $\Psi^h(p,q)\simeq\Phi_H^h(p,q)$ is a numerical approximation of the exact flow associated with a given Hamiltonian H. As a consequence, the modified Hamiltonian H_h, which turns out to be a perturbation of the initial Hamiltonian H, is preserved along the numerical solution, $(p_n,q_n)=(\Psi^h)^n(p_0,q_0)$, $n\in\mathbb{N}$. More precisely, we have

$$(p_n,q_n)=\big(\Psi^h\big)^n(p_0,q_0)=\big(\Phi_{H_h}^{nh}\big)(p_0,q_0)+nh\exp\big(-1/(ch)\big) \tag{1.1}$$

under the *a priori* assumption that the sequence $(p_n,q_n)_{n\in\mathbb{N}}$ remains in a compact set used to derive the analytic estimates. Here the constant c depends on the eigenvalues of the quadratic part of the Hamiltonian H (i.e., the linear part of the associated ODE). As a consequence the qualitative behavior of the discrete dynamics associated with the map Ψ^h over exponentially long times can be pretty well understood through the analysis of the continuous system associated with H_h.

The extension of such results to Hamiltonian partial differential equations (PDE) faces the principal difficulty that the Hamiltonian function involves operators with unbounded eigenvalues making the constant c in the previous estimate blow up. The goal of this work is to overcome this difficulty and to give Hamiltonian interpolation results for splitting methods applied to semilinear Hamiltonian PDEs.

We consider a class of Hamiltonian PDEs associated with a Hamiltonian H that can be split into a quadratic functional H_0 associated with an unbounded linear operator having a discrete spectrum and a nonlinearity P which is a polynomial functional and at least cubic:

$$H=H_0+P.$$

Typical examples are given by the nonlinear Schrödinger equation (NLS)

$$\mathrm{i}\partial_t u=\Delta u+f(u,\bar{u}) \tag{1.2}$$

or the nonlinear wave equation (NLW)

$$\partial_{tt} u - \Delta u = g(u) \tag{1.3}$$

set on the torus $\mathbb{T}^d$. Here f and g are polynomials having a zero of order at least three at the origin, for instance $f(u, \bar{u}) = |u|^2 u$ for the cubic defocussing NLS and $g(u) = u^3$ for the classical NLW.

To approximate such equations, splitting methods are widely used: They consist in decomposing the exact flow Φ_H^h at a small time step h as compositions of the flows $\Phi_{H_0}^h$ and Φ_P^h. The Lie–Trotter splitting methods

$$u(nh, x) \sim u^n(x) := \left(\Phi_{H_0}^h \circ \Phi_P^h\right)^n u_0(x) \quad \text{or} \quad u^n(x) := \left(\Phi_P^h \circ \Phi_{H_0}^h\right)^n u_0(x) \tag{1.4}$$

are known to be order 1 approximation schemes in time, when the solution is *smooth*. Here *smooth* means that the numerical solution belongs to some Sobolev space H^s, $s > 1$, uniformly in time; see [20, 22] for the linear case and [25] for the nonlinear Schrödinger equation.

These schemes are all symplectic, preserve the L^2 norm if H_0 and P do, and can be easily implemented in practice. For instance, in the cases of NLS or NLW just above, we can diagonalize the linear part and integrate it by using the fast Fourier transform and integrate the nonlinear part explicitly (it is an ordinary differential equation). More generally, instead of the fast Fourier transform, pseudo spectral methods are used if the spectrum of H_0 is known and available.

The Hamiltonian interpolation problem described above can be formulated here as follows: is it possible to find a *modified energy* (or modified Hamiltonian function) H_h depending on H_0, P and on the chosen stepsize, such that

$$\Phi_P^h \circ \Phi_{H_0}^h \simeq \Phi_{H_h}^h ? \tag{1.5}$$

Formally, this question corresponds to the classical Baker–Campbell–Hausdorff (BCH) formula (see [2, 21]) for which the modified Hamiltonian H_h is expressed as iterated Poisson brackets between the two Hamiltonian P and H_0. Hence we observe that the validity of such representation *a priori* depends on the smoothness of the discrete solution u^n. But this is not fair, as there is no reason for u^n to be, *a priori*, uniformly smooth over a long time. Actually, it is well known that this assumption is not satisfied in general and we illustrate this in Sect. 6 by numerical examples in the case of the simulation of a solitary wave for NLS.

In this work, we establish backward error analysis results in the spirit of [5, 17, 27] for the Lie–Trotter splitting methods. We follow a general approach recently developed in [9] for linear PDEs. In this linear context, Debussche and Faou proved a formula of the form (1.5) by considering smoothed schemes, namely schemes where $\Phi_{H_0}^h$ is replaced by the midpoint approximation of the unbounded part H_0. This yields schemes of the form

$$\Phi_P^h \circ \Phi_{A_0}^1 \quad \text{or} \quad \Phi_{A_0}^1 \circ \Phi_P^h, \tag{1.6}$$

where A_0 depends on h, and is an approximation of the operator hH_0 when $h \to 0$.

In the present work we consider the context of nonlinear PDEs (P is at least cubic). Let us focus in the introduction on the NLS equation on the torus $\mathbb{T}^d$ (a more general setting is consider in Sect. 2). The quadratic part reads $H_0(u) = \sum_{k\in\mathbb{Z}^d} |k|^2|\hat{u}_k|^2$ and corresponds to the unbounded linear operator $-\Delta$. We approximate hH_0 by A_0 defined by

$$A_0(u) = \sum_{k\in\mathbb{Z}^d} \lambda_k|\hat{u}_k|^2, \quad \lambda_k = \alpha_h\bigl(h|k|^2\bigr), \tag{1.7}$$

where α_h is a *filter* function satisfying $\alpha_h(x) \simeq x$ for small x. It turns out that under such an assumption, (1.6) remains an order one approximation of the continuous solution, provided that the numerical solution is smooth. This general setting contains the *standard* splitting method (1.4) which corresponds to the choice $\alpha_h(x) = x$ for all x, and the midpoint approximation of the linear flow which corresponds to the function [9] $\alpha_h(x) = 2\arctan(x/2)$.

Our principal result can be described as follows:

We assume that, in the Fourier variables, the numerical trajectory remains bounded in the space[1] ℓ^1 (the Wiener algebra). Then we construct a Hamiltonian H_h such that

$$\bigl\|\Phi_P^h \circ \Phi_{A_0}^1(z) - \Phi_{H_h}^h(z)\bigr\|_{\ell^1} \le h^{N+1}(CN)^N \tag{1.8}$$

uniformly for z in a fixed ball of ℓ^1 and for some constant C depending on P. The number N depends on a sort of regularization condition satisfied by the eigenvalues λ_k of A_0:

$$\forall j = 1,\dots,r, \forall(k_1,\dots,k_j) \quad |\lambda_{k_1} \pm \cdots \pm \lambda_{k_j}| < 2\pi. \tag{1.9}$$

If it is satisfied for some $r \ge 2$, then we can take in the previous estimate

$$N = (r-2)/(r_0-2),$$

where r_0 is the degree of the polynomial P. Actually Theorem 4.2 is more general since estimate (1.8) is obtained in ℓ_s^1, the space of sequences $(z_k)_{k\in\mathbb{Z}^d}$ such that $\sum |k|^s|z_k| < \infty$.

For numerical schemes associated with a filter function

$$\alpha_h(x) = \sqrt{h}\arctan\bigl(x/\sqrt{h}\bigr), \tag{1.10}$$

we can actually prove that the regularization condition (1.9) is satisfied for $r \simeq 1/\sqrt{h}$. The analytic estimate (1.8) then yields an exponentially small error at each step. The choice (1.10) typically induces a stronger regularization in the high frequencies than the midpoint rule, without breaking the order of approximation of the method.

For the other classical schemes (standard splitting, implicit–explicit schemes), the regularization condition (1.9) is in general not satisfied unless a Courant–Friedrichs–Lewy (CFL) condition is imposed [8], depending on the desired approximation level N in (1.8) (see Sect. 5 for details and other examples).

[1] This implies that the numerical trajectory remains bounded in $L^\infty(\mathbb{T}^d)$ uniformly in time. This is actually the standard assumption is the finite-dimensional case: no blow up in finite time.

We can make precise in which sense the estimate (1.8) induces a better control of the numerical solution. Actually, the modified Hamiltonian reads $A_0/h + \widetilde{P}$ where $\widetilde{P}$ is a modified polynomial. This modified energy will be close to the original energy only if u is smooth, something that is not guaranteed by the present analysis. However, in Corollary 5.3 we prove that the preservation of this modified energy implies the control of the H^1 norm of low modes of the numerical solution, and of the L^2 norm of high modes, as in [9], over a very long time. Using this analysis, it is possible to prove the almost global existence in H^1 of small *fully discrete* numerical solutions of NLS in dimension 1. Indeed in this case the H^1 norm controls the ℓ^1 norm making possible the use of a bootstrap argument: see [11, Chap. 6]. In a similar direction, the existence of this modified energy allows one to prove the stability of numerical solitons: see [4] and the numerical experiments performed in Sect. 2.

The relative question of persistence of smoothness of the numerical solution has recently seen many progresses: see [7, 10, 12–15, 18]. However, in all these works non-resonance conditions are imposed on the stepsize and/or on the frequencies of the original PDE. In the nonlinear case, such analysis holds only when the linear operators in (1.2) or (1.3) are slightly perturbed by a smooth potential, see also [3, 16]. Here we do not need any non-resonance assumption on the original frequencies, and the smoothing condition (1.9) is sufficient to ensure the absence of *numerical resonances* (see [12, 13] for a similar discussion).

2 Abstract Hamiltonian Formalism

In this section we consider Hamiltonian PDEs whose linear part has a discrete spectrum. The solution of the PDE under study is decomposed in the eigenbasis of the linear part:

$$\psi(t,x) = \sum \xi_k(t)\phi_k(x)$$

and we observe the PDE in the Fourier-like variables $\xi = (\xi_k)$.

The main difference with the presentation in [12, 13, 16] lies in the choice of the phase space. We consider Fourier variables ξ belonging to ℓ^1_s spaces, based on the Wiener algebra, and not to ℓ^2_s, the classical weighted ℓ^2 spaces (Sobolev spaces).

2.1 Setting and Notations

We denote $\mathcal{N} = \mathbb{Z}^d$ or $\mathbb{N}^d$ (depending on the concrete application) for some $d \geq 1$. For $a = (a_1, \dots, a_d) \in \mathcal{N}$, we set $|a|^2 = \max(1, a_1^2 + \cdots + a_d^2)$. We consider the set of variables $(\xi_a, \eta_b) \in \mathbb{C}^{\mathcal{N}} \times \mathbb{C}^{\mathcal{N}}$ equipped with the symplectic structure

$$\mathrm{i} \sum_{a\in\mathcal{N}} \mathrm{d}\xi_a \wedge \mathrm{d}\eta_a. \tag{2.1}$$

We define the set $\mathcal{Z} = \mathcal{N} \times \{\pm 1\}$. For $j = (a, \delta) \in \mathcal{Z}$, we define $|j| = |a|$ and we denote by $\overline{j}$ the index $(a, -\delta)$. We will identify a couple $(\xi, \eta) \in \mathbb{C}^{\mathcal{N}} \times \mathbb{C}^{\mathcal{N}}$ with

$(z_j)_{j\in\mathcal{Z}} \in \mathbb{C}^{\mathcal{Z}}$ via the formula

$$j=(a,\delta)\in\mathcal{Z} \quad \Longrightarrow \quad \begin{cases} z_j=\xi_a & \text{if } \delta=1,\\ z_j=\eta_a & \text{if } \delta=-1. \end{cases}$$

By a slight abuse of notation, we often write $z=(\xi,\eta)$ to denote such an element.

Example 2.1 In the case where $H_0=-\Delta$ on the torus $\mathbb{T}^d$, the eigenbasis is the Fourier basis, $\mathcal{N}=\mathbb{Z}^d$ and ξ is the sequence associated with a function ψ while η is the Fourier sequence associated with a function ϕ via the formula

$$\psi(x)=\sum_{a\in\mathcal{N}}\xi_a \mathrm{e}^{\mathrm{i}a.x} \quad \text{and} \quad \phi(x)=\sum_{a\in\mathcal{N}}\eta_a \mathrm{e}^{-\mathrm{i}a.x}.$$

For a given $s\geq 0$, we consider the Banach space $\ell^1_s := \ell^1_s(\mathcal{Z},\mathbb{C})$ made of elements $z\in\mathbb{C}^{\mathcal{Z}}$ such that

$$\|z\|_{\ell^1_s} := \sum_{j\in\mathcal{Z}} |j|^s |z_j| < \infty,$$

and equipped with the symplectic form (2.1). We will often write simply $\ell^1=\ell^1_0$. We moreover define for $s>1$ the Sobolev norms

$$\|z\|_{H^s}=\left(\sum_{j\in\mathcal{Z}}|j|^{2s}|z_j|^2\right)^{1/2}.$$

For a function F of $\mathcal{C}^1(\ell^1_s,\mathbb{C})$, we define its gradient by

$$\nabla F(z)=\left(\frac{\partial F}{\partial z_j}\right)_{j\in\mathcal{Z}}, \quad \text{where for } j=(a,\delta),\ \frac{\partial F}{\partial z_j}=\begin{cases} \frac{\partial F}{\partial \xi_a} & \text{if } \delta=1,\\ \frac{\partial F}{\partial \eta_a} & \text{if } \delta=-1. \end{cases}$$

Let $H(z)$ be a function defined on ℓ^1_s. If H is smooth enough, we can associate with this function the Hamiltonian vector field $X_H(z)$ defined by

$$X_H(z)=J\nabla H(z),$$

where J is the symplectic operator on ℓ^1_s induced by the symplectic form (2.1).

For two functions F and G, the Poisson Bracket is (formally) defined as

$$\{F,G\}=\nabla F^T J\nabla G = \mathrm{i}\sum_{a\in\mathcal{N}} \frac{\partial F}{\partial \eta_j}\frac{\partial G}{\partial \xi_j}-\frac{\partial F}{\partial \xi_j}\frac{\partial G}{\partial \eta_j}. \tag{2.2}$$

We say that $z\in\ell^1_s$ is *real* when $z_{\bar{j}}=\overline{z_j}$ for any $j\in\mathcal{Z}$. In this case, we write $z=(\xi,\bar{\xi})$ for some $\xi\in\mathbb{C}^{\mathcal{N}}$. Furthermore, we say that a Hamiltonian function H is *real* if $H(z)$ is real for all real z.

Example 2.2 Following Example 2.1, a real z corresponds to the relation $\phi = \bar{\psi}$ and a typical real Hamiltonian reads $H(z) = \int_{\mathbb{T}^d} h(\psi(x), \phi(x))\,\mathrm{d}x$ where h is a regular function from $\mathbb{C}^2$ to $\mathbb{C}$ satisfying $h(\zeta, \bar{\zeta}) \in \mathbb{R}$ for all $\zeta \in \mathbb{C}$.

Definition 2.3 For a given $s \geq 0$, we denote by $\mathcal{H}_s$ the space of real Hamiltonians P satisfying

$$P \in \mathcal{C}^1(\ell_s^1, \mathbb{C}) \quad \text{and} \quad X_P \in \mathcal{C}^1(\ell_s^1, \ell_s^1).$$

Notice that for F and G in $\mathcal{H}_s$ the formula (2.2) is well defined.

We will verify later (see Example 2.6) that the typical real Hamiltonians given in Example 2.2 belong to the class $\mathcal{H}_s$. Actually the proof is not totally trivial, because the Fourier transform is not well adapted to the ℓ_s^1 space.

With a given Hamiltonian function $H \in \mathcal{H}_s$, we associate the Hamiltonian system

$$\dot{z} = J\nabla H(z)$$

which can be written

$$\begin{cases} \dot{\xi}_a = -\mathrm{i}\frac{\partial H}{\partial \eta_a}(\xi, \eta), & a \in \mathcal{N}, \\ \dot{\eta}_a = \mathrm{i}\frac{\partial H}{\partial \xi_a}(\xi, \eta), & a \in \mathcal{N}. \end{cases} \tag{2.3}$$

In this situation, we define the flow $\Phi_H^t(z)$ associated with the previous system (for an interval of times $t \geq 0$ depending *a priori* on the initial condition z). Note that if $z = (\xi, \bar{\xi})$ and if H is real, the flow $(\xi^t, \eta^t) = \Phi_H^t(z)$ is also real for all time t where the flow is defined: $\xi^t = \bar{\eta}^t$. When H is real, it may be useful to introduce the real variables p_a and q_a given by

$$\xi_a = \frac{1}{\sqrt{2}}(p_a + \mathrm{i}q_a) \quad \text{and} \quad \bar{\xi}_a = \frac{1}{\sqrt{2}}(p_a - \mathrm{i}q_a),$$

the system (2.3) is then equivalent to the system

$$\begin{cases} \dot{p}_a = -\frac{\partial H}{\partial q_a}(q, p), & a \in \mathcal{N}, \\ \dot{q}_a = \frac{\partial H}{\partial p_a}(q, p), & a \in \mathcal{N}, \end{cases}$$

where by a slight abuse of notation we still denote the Hamiltonian with the same letter: $H(q, p) = H(\xi, \bar{\xi})$.

We now describe the hypothesis needed on the Hamiltonian nonlinearity P.

Let $\ell \geq 2$. We consider $\boldsymbol{j} = (j_1, \ldots, j_\ell) \in \mathcal{Z}^\ell$, and we set for all $i = 1, \ldots, \ell$, $j_i = (a_i, \delta_i)$ where $a_i \in \mathcal{N}$ and $\delta_i \in \{\pm 1\}$. We define

$$\overline{\boldsymbol{j}} = (\overline{j}_1, \ldots, \overline{j}_\ell) \quad \text{with } \overline{j}_i = (a_i, -\delta_i), i = 1, \ldots, \ell.$$

We also use the notation

$$z_{\boldsymbol{j}} = z_{j_1} \cdots z_{j_\ell}.$$

We define the momentum $\mathcal{M}(\boldsymbol{j})$ of the multi-index $\boldsymbol{j}$ by

$$\mathcal{M}(\boldsymbol{j}) = a_1\delta_1 + \cdots + a_\ell\delta_\ell. \tag{2.4}$$

We then define the set of indices with zero momentum

$$\mathcal{I}_\ell = \{\boldsymbol{j} = (j_1, \ldots, j_\ell) \in \mathcal{Z}^\ell, \text{with } \mathcal{M}(\boldsymbol{j}) = 0\}. \tag{2.5}$$

We can now define precisely the type of polynomial nonlinearities we consider:

Definition 2.4 We say that a polynomial Hamiltonian $P \in \mathcal{P}_k$ if P is real, of degree k, has a zero of order at least 2 in $z = 0$, if

- P contains only monomials $a_{\boldsymbol{j}} z_{\boldsymbol{j}}$ having zero momentum, i.e. such that $\mathcal{M}(\boldsymbol{j}) = 0$ when $a_{\boldsymbol{j}} \neq 0$ and thus P formally reads

$$P(z) = \sum_{\ell=2}^{k} \sum_{\boldsymbol{j} \in \mathcal{I}_\ell} a_{\boldsymbol{j}} z_{\boldsymbol{j}} \tag{2.6}$$

  with the relation $a_{\bar{\boldsymbol{j}}} = \bar{a}_{\boldsymbol{j}}$.
- The coefficients $a_{\boldsymbol{j}}$ are bounded, i.e. satisfy

$$\forall \ell = 2, \ldots, k, \forall \boldsymbol{j} = (j_1, \ldots, j_\ell) \in \mathcal{I}_\ell \quad |a_{\boldsymbol{j}}| \le C.$$

  In the following, we set

$$\|P\| = \sum_{\ell=2}^{k} \sup_{\boldsymbol{j} \in \mathcal{I}_\ell} |a_{\boldsymbol{j}}|. \tag{2.7}$$

Definition 2.5 We say that $P \in \mathcal{SP}_k$ if $P \in \mathcal{P}_k$ has coefficients $a_{\boldsymbol{j}}$ such that $a_{\boldsymbol{j}} \neq 0$ implies that $\boldsymbol{j}$ contains the same numbers of positive and negative indices:

$$\sharp\{i \mid j_i = (a_i, +1)\} = \sharp\{i \mid j_i = (a_i, -1)\}.$$

In other words, P contains only monomials with the same numbers of ξ_i and η_i. Note that this implies that k is even.

Example 2.6 Following Example 2.2, $P(z) = \int_{\mathbb{T}^d} p(\psi(x), \phi(x))\,\mathrm{d}x$, where p is a polynomial of degree k in $\mathbb{C}[X, Y]$ satisfying $p(\zeta, \bar{\zeta}) \in \mathbb{R}$ and having a zero of order at least 2 at the origin, defines a Hamiltonian in $\mathcal{P}_k$.

An example of a polynomial Hamiltonian in $\mathcal{SP}_{2k}$ is given by $P = \int |\psi|^{2k}\,\mathrm{d}x$.

The zero momentum assumption in Definition 2.4 is crucial in order to obtain the following proposition:

Proposition 2.7 *Let $k \ge 2$ and $s \ge 0$; then we have $\mathcal{P}_k \subset \mathcal{H}_s$, and for $P \in \mathcal{P}_k$, we have the estimates*

$$|P(z)| \le \|P\| \Big(\max_{n=2,\ldots,k} \|z\|^n_{\ell^1_s} \Big) \tag{2.8}$$

and

$$\forall z \in \ell_s^1, \quad \left\|X_P(z)\right\|_{\ell_s^1} \le 2k(k-1)^s \|P\| \, \|z\|_{\ell_s^1} \Big(\max_{n=1,\dots,k-2} \|z\|_{\ell^1}^n \Big). \tag{2.9}$$

Moreover, for z and y in ℓ_s^1, we have

$$\left\|X_P(z) - X_P(y)\right\|_{\ell_s^1} \le 4k(k-1)^s \|P\| \Big(\max_{n=1,\dots,k-2} \big(\|y\|_{\ell_s^1}^n, \|z\|_{\ell_s^1}^n \big) \Big) \|z-y\|_{\ell_s^1}. \tag{2.10}$$

Therefore, for $P \in \mathcal{P}_k$ and $Q \in \mathcal{P}_\ell$, we have $\{P, Q\} \in \mathcal{P}_{k+\ell-2}$ and we have the estimate

$$\left\|\{P, Q\}\right\| \le 2k\ell \|P\| \, \|Q\|. \tag{2.11}$$

If now $P \in \mathcal{SP}_k$ and $Q \in \mathcal{SP}_k$, then $\{P, Q\} \in \mathcal{SP}_{k+\ell-2}$.

Remark 2.8 The estimate (2.9) is a sort of tame estimate. The same estimate with ℓ_s^1 replaced by ℓ_s^2 is proved in [16] under the assumption of decreasing coefficients of the polynomial P. Actually the present proof is much simpler.

Proof Assume that P is given by (2.6), and denote by P_i the homogeneous component of degree i of P, i.e.

$$P_i(z) = \sum_{\boldsymbol{j} \in \mathcal{I}_i} a_{\boldsymbol{j}} z_{\boldsymbol{j}}, \quad i = 2, \dots, k.$$

We have for all z

$$\left|P_i(z)\right| \le \|P_i\| \, \|z\|_{\ell^1}^i \le \|P_i\| \, \|z\|_{\ell_s^1}^i.$$

The first inequality (2.8) is then a consequence of the fact that

$$\|P\| = \sum_{i=2}^k \|P_i\|. \tag{2.12}$$

Now let $j = (a, \epsilon) \in \mathcal{Z}$ be fixed. The derivative of a given monomial $z_{\boldsymbol{j}} = z_{j_1} \cdots z_{j_i}$ with respect to z_j vanishes except if $j \subset \boldsymbol{j}$. Assume for instance that $j = j_i$. Then the zero momentum condition implies that $\mathcal{M}(j_1, \dots, j_{i-1}) = -\epsilon a$ and we can write

$$|j|^s \left|\frac{\partial P_i}{\partial z_j}\right| \le i \|P_i\| \sum_{\boldsymbol{j} \in \mathcal{Z}^{i-1}, \mathcal{M}(\boldsymbol{j}) = -\epsilon a} |j|^s |z_{j_1} \cdots z_{j_{i-1}}|. \tag{2.13}$$

Now in this formula, for a fixed multi-index $\boldsymbol{j}$, the zero momentum condition implies that

$$|j|^s \le \big(|j_1| + \cdots + |j_{i-1}|\big)^s \le (i-1)^s \max_{n=1,\dots,i-1} |j_n|^s. \tag{2.14}$$

Therefore, after summing over a and ϵ we get

$$\begin{aligned}\left\|X_{P_i}(z)\right\|_{\ell_s^1} &\le 2i(i-1)^s\|P_i\| \sum_{\boldsymbol{j}\in\mathcal{Z}^{i-1}} \max_{n=1,\dots,i-1} |j_n|^s|z_{j_1}|\cdots|z_{j_{i-1}}| \\ &\le 2i(i-1)^s\|P_i\|\,\|z\|_{\ell^1}\,\|z\|_{\ell_s^1}^{i-2} \qquad (2.15)\end{aligned}$$

which yields (2.9) after summing over $i=2,\dots,k$.

Now for z and y in ℓ_s^1, we have, with the previous notation,

$$|j|^s\left|\frac{\partial P_i}{\partial z_j}(z)-\frac{\partial P_i}{\partial z_j}(y)\right| \le \sum_{q\in\mathcal{Z}}|j|^s\left|\int_0^1 \frac{\partial P_i}{\partial z_j\partial z_q}\big(ty+(1-t)z\big)\,\mathrm{d}t\right||z_q-y_q|.$$

But we have for fixed $j=(\epsilon,a)$ and $q=(\delta,b)$ in $\mathcal{Z}$, and for all $u\in\ell_s^1$

$$|j|^s\left|\frac{\partial P_i}{\partial z_j\partial z_q}(u)\right| \le i\|P_i\| \sum_{\boldsymbol{j}\in\mathcal{Z}^{i-2},\mathcal{M}(\boldsymbol{j})=-\epsilon a-\delta b} |j|^s|u_{j_1}\cdots u_{j_{i-2}}|.$$

In the previous sum, we necessarily have $\mathcal{M}(\boldsymbol{j},j,k)=0$, and hence as before

$$|j|^s \le \big(|j_1|+\cdots+|j_{i-2}|+|q|\big)^s \le (i-1)^s|q|^s\prod_{n=1}^{i-2}|j_n|^s.$$

Let $u(t)=ty+(1-t)z$; we have for all $t\in[0,1]$ with the previous estimates

$$\begin{aligned}&|j|^s\left|\int_0^1\frac{\partial P_i}{\partial z_j\partial z_q}\big(u(t)\big)\,\mathrm{d}t\right| \\ &\quad\le i(i-1)^s|q|^s\|P_i\|\int_0^1 \sum_{\boldsymbol{j}\in\mathcal{Z}^{i-2},\mathcal{M}(\boldsymbol{j})=-\epsilon a-\delta b} |j_1|^s\big|u_{j_1}(t)\big|\cdots|j_2|^s\big|u_{j_{i-2}}(t)\big|\,\mathrm{d}t.\end{aligned}$$

Multiplying by (z_q-y_q) and summing over k and j, we obtain

$$\left\|Z_{P_i}(z)-X_{P_i}(y)\right\|_{\ell_s^1} \le 4i(i-1)^s\|P_i\|\left(\int_0^1\left\|u(t)\right\|_{\ell_s^1}^{i-2}\,\mathrm{d}t\right)\|z-y\|_{\ell_s^1}.$$

Hence we obtain the result after summing over i, using the fact that

$$\left\|ty+(1-t)z\right\|_{\ell_s^1} \le \max\big(\|y\|_{\ell_s^1},\|z\|_{\ell_s^1}\big).$$

Assume now that P and Q are homogeneous polynomials of degrees k and ℓ, respectively, and with coefficients $a_{\boldsymbol{k}}$, $\boldsymbol{k}\in\mathcal{I}_k$ and $b_{\boldsymbol{\ell}}$, $\boldsymbol{\ell}\in\mathcal{I}_\ell$. It is clear that $\{P,Q\}$ is a monomial of degree $k+\ell-2$ satisfying the zero momentum condition. Furthermore, writing

$$\{P,Q\}(z)=\sum_{\boldsymbol{j}\in\mathcal{I}_{k+\ell-2}} c_{\boldsymbol{j}}z_{\boldsymbol{j}},$$

$c_{\boldsymbol{j}}$ is expressed as a sum of coefficients $a_{\boldsymbol{k}}b_{\boldsymbol{\ell}}$ for which there exists an $a \in \mathcal{N}$ and $\epsilon \in \{\pm 1\}$ such that

$$(a,\epsilon) \subset \boldsymbol{k} \in \mathcal{I}_k \quad \text{and} \quad (a,-\epsilon) \subset \boldsymbol{\ell} \in \mathcal{I}_\ell,$$

and such that if for instance $(a,\epsilon) = k_1$ and $(a,-\epsilon) = \ell_1$, we necessarily have $(k_2,\dots,k_k,\ell_2,\dots,\ell_\ell) = \boldsymbol{j}$. Hence for a given $\boldsymbol{j}$, the zero momentum condition on $\boldsymbol{k}$ and on $\boldsymbol{\ell}$ determines the value of ϵa, which in turn determines the value of (ϵ, a) when $\mathcal{N} = \mathbb{N}^d$ and determines two possible values of (ϵ, a) when $\mathcal{N} = \mathbb{Z}^d$.

This proves (2.11) for monomials. If

$$P = \sum_{i=2}^{k} P_j \quad \text{and} \quad Q = \sum_{j=2}^{\ell} Q_j,$$

where P_i and Q_j are homogeneous polynomials of degree i and j, respectively, then we have

$$\{P,Q\} = \sum_{n=2}^{k+\ell-2} \sum_{i+j-2=n} \{P_i, Q_j\}.$$

Hence by definition of $\|P\|$ (see (2.7)) and the fact that all the polynomials $\{P_i, Q_j\}$ in the sum are homogeneous of degree $i+j-2$, we have by the previous calculations

$$\begin{aligned}
\|\{P,Q\}\| &= \sum_{n=2}^{k+\ell-2} \Bigg\| \sum_{i+j-2=n} \{P_i, Q_j\} \Bigg\| \\
&\le 2 \sum_{n=2}^{k+\ell-2} \sum_{i+j-2=n} ij \|P_i\| \, \|Q_j\| \\
&\le 2k\ell \left(\sum_{i=2}^{k} \|P_i\| \right) \left(\sum_{j=2}^{\ell} \|Q_j\| \right) = 2k\ell \|P\| \, \|Q\|,
\end{aligned}$$

where we used (2.12) for the last equality.

The last assertion, as well as the fact that the Poisson bracket of two real Hamiltonian is real, follow immediately from the definition of the Poisson bracket. □

With the previous notation, we consider the following Hamiltonian functions:

$$H(z) = H_0(z) + P(z) = \sum_{a \in \mathcal{N}} \omega_a I_a(z) + P(z), \tag{2.16}$$

where for all $a \in \mathcal{N}$, $I_a(z) = \xi_a \eta_a$ are the *actions* and $\omega_a \in \mathbb{R}$ are the associated frequencies. We assume

$$\forall a \in \mathcal{N}, \quad |\omega_a| \le C|a|^m \tag{2.17}$$

for some constants $C > 0$ and $m > 0$. The Hamiltonian system (2.3) then reads

$$\begin{cases} \dot{\xi}_a = -\mathrm{i}\omega_a \xi_a - \mathrm{i}\frac{\partial P}{\partial \eta_a}(\xi, \eta), & a \in \mathcal{N}, \\ \dot{\eta}_a = \mathrm{i}\omega_a \eta_a + \mathrm{i}\frac{\partial P}{\partial \xi_a}(\xi, \eta), & a \in \mathcal{N}. \end{cases} \tag{2.18}$$

2.2 Examples

2.2.1 Nonlinear Schrödinger Equation

We first consider nonlinear Schrödinger equations of the form

$$\mathrm{i}\partial_t \psi = -\Delta\psi + \partial_2 g(\psi, \bar{\psi}), \quad x \in \mathbb{T}^d, \tag{2.19}$$

where $g : \mathbb{C}^2 \to \mathbb{C}$ is a polynomial of order r_0. We assume that $g(z, \bar{z}) \in \mathbb{R}$, and that $g(z, \bar{z}) = \mathcal{O}(|z|^3)$ is a polynomial with a zero of order at least 3 at the origin. The corresponding Hamiltonian functional is given by

$$H(\psi, \bar{\psi}) = \int_{\mathbb{T}^d} \big(|\nabla\psi|^2 + g(\psi, \bar{\psi})\big)\, \mathrm{d}x.$$

Let $\phi_a(x) = \mathrm{e}^{\mathrm{i}a\cdot x}$, $a \in \mathbb{Z}^d$ be the Fourier basis on $L^2(\mathbb{T}^d)$. With the notation

$$\psi = \left(\frac{1}{2\pi}\right)^{d/2} \sum_{a\in\mathbb{Z}^d} \xi_a \phi_a(x) \quad \text{and} \quad \bar{\psi} = \left(\frac{1}{2\pi}\right)^{d/2} \sum_{a\in\mathbb{Z}^d} \eta_a \bar{\phi}_a(x),$$

the Hamiltonian associated with (2.19) can (formally) be written

$$H(\xi, \eta) = \sum_{a\in\mathbb{Z}^d} \omega_a \xi_a \eta_a + \sum_{r=3}^{r_0} \sum_{\boldsymbol{a},\boldsymbol{b}} P_{\boldsymbol{a}\boldsymbol{b}} \xi_{a_1} \cdots \xi_{a_p} \eta_{b_1} \cdots \eta_{b_q}. \tag{2.20}$$

Here $\omega_a = |a|^2$ satisfying (2.17) with $m = 2$ are the eigenvalues of the Laplace operator $-\Delta$. As previously seen in Examples 2.1, 2.2, 2.6, the nonlinearity $P = \int_{\mathbb{T}^d} g(\psi(x), \phi(x))\, \mathrm{d}x$ is real, satisfies the zero momentum condition and belongs to $\mathcal{H}_s$ (as g is polynomial).

In this situation, working in the space ℓ^1 for ξ corresponds to working in a subspace of bounded functions $\psi(x)$. Similarly the control of the ℓ^1_s norm of ξ for $s \geq 0$ leads to a control of $\|\nabla^s \psi\|_{L^\infty}$.

2.2.2 Nonlinear Wave Equation

As a second concrete example we consider a 1-d nonlinear wave equation

$$u_{tt} - u_{xx} = g(u), \quad x \in (0, \pi), t \in \mathbb{R}, \tag{2.21}$$

with Dirichlet boundary condition: $u(0, t) = u(\pi, t) = 0$ for any t. We assume that $g : \mathbb{R} \to \mathbb{R}$ is polynomial of order $r_0 - 1$ with a zero of order two at $u = 0$. Defining

$v = u_t$, (2.21) reads

$$\partial_t \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} v \\ u_{xx} + g(u) \end{pmatrix}.$$

Furthermore, let $H : H^1(0,\pi) \times L^2(0,\pi) \mapsto \mathbb{R}$ be defined by

$$H(u,v) = \int_{S^1} \left(\frac{1}{2} v^2 + \frac{1}{2} u_x^2 + G(u) \right) \mathrm{d}x, \tag{2.22}$$

where G such that $\partial_u G = -g$ is a polynomial of degree r_0; then (2.21) can be expressed as a Hamiltonian system

$$\begin{aligned} \partial_t \begin{pmatrix} u \\ v \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -u_{xx} + \partial_u G \\ v \end{pmatrix} \\ &= J \nabla_{u,v} H(u,v), \end{aligned} \tag{2.23}$$

where $J = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ represents the symplectic structure and where $\nabla_{u,v} = \left(\begin{smallmatrix} \nabla_u \\ \nabla_v \end{smallmatrix}\right)$ with ∇_u and ∇_v denoting the L^2 gradient with respect to u and v, respectively.

Let $-\Delta_D$ be the Laplace operator with Dirichlet boundary conditions. Let $A = (-\Delta_D)^{1/2}$. We introduce the variables (p,q) given by

$$q := A^{1/2} u \quad \text{and} \quad p := A^{-1/2} v.$$

Then, on $H^s(0,\pi) \times H^s(0,\pi)$ with $s \geq 1/2$, the Hamiltonian (2.22) takes the form $H_0 + P$ with

$$H_0(q,p) = \frac{1}{2} \big(\langle Ap, p \rangle_{L^2} + \langle Aq, q \rangle_{L^2} \big) \tag{2.24}$$

and

$$P(q,p) = \int_{S^1} G\big(A^{-1/2} q\big) \, \mathrm{d}x. \tag{2.25}$$

In this context $\mathcal{N} = \mathbb{N} \setminus \{0\}$, $\omega_a = a$, $a \in \mathcal{N}$ are the eigenvalues of A and $\phi_a = \sin ax$, $a \in \mathcal{N}$, the associated eigenfunctions.

Substituting the decompositions

$$q(x) = \sum_{a \in \mathcal{N}} q_a \phi_a(x) \quad \text{and} \quad p(x) = \sum_{a \in \mathcal{N}} p_a \phi_a(x)$$

into the Hamiltonian functional, we see that it takes the form

$$H = \sum_{a \in \mathcal{N}} \omega_a \frac{p_a^2 + q_a^2}{2} + P,$$

where P is a function of the variables q_a. Using the complex coordinates

$$\xi_a = \frac{1}{\sqrt{2}} (q_a + \mathrm{i} p_a) \quad \text{and} \quad \eta_a = \frac{1}{\sqrt{2}} (q_a - \mathrm{i} p_a)$$

the Hamiltonian function can be written in the form (2.20) with a nonlinearity depending on G. In this case, the space ℓ^1 for $z=(\xi,\eta)$ corresponds to functions $u(x)$ such that the Fourier transform $\widehat{u}(a)=\frac{1}{\pi}\int_0^\pi u(x)\sin(ax)\,\mathrm{d}x$ satisfies $(a\widehat{u}(a))_{a\in\mathcal{N}}\in\ell^1(\mathcal{N})$ and $(a^{-1}\widehat{u}(a))_{a\in\mathcal{N}}\in\ell^1(\mathcal{N})$. This implies in particular a control of $u(x)$ and $\partial_x u(x)$ in $L^\infty(0,\pi)$. More generally, with a z in some ℓ^1_s space, $s\in\mathbb{N}$, there is associated a function $u(x)$ such that $\partial_x^k u(x)\in L^\infty(0,\pi)$ for $k=0,\dots,s+1$.

2.3 Splitting Schemes

The standard Lie–Trotter splitting methods for the PDE associated with the Hamiltonian H_0+P consists in replacing the flow generated by H during the time h (the small time step) by the composition of the flows generated by H_0 and P during the same time, namely

$$\Phi^h_{H_0}\circ\Phi^h_P \quad \text{and} \quad \Phi^h_P\circ\Phi^h_{H_0}.$$

As explained in the introduction, it turns out that it is convenient to consider more general splitting methods including in particular a regularization in the high modes of the linear part. Thus we replace the operator hH_0 by a more general Hamiltonian A_0. Precisely, let $\alpha_h(x)$ be a real function, depending on the stepsize h, satisfying $\alpha_h(0)=0$ and $\alpha_h(x)\simeq x$ for small x. We define the diagonal operator A_0 by the relation

$$\forall j=(a,\delta)\in\mathcal{Z},\quad A_0 z_j=\delta\alpha_h(h\omega_a)z_j. \tag{2.26}$$

For $a\in\mathcal{N}$, we set $\lambda_a=\alpha_h(h\omega_a)$. We consider the splitting methods

$$\Phi^h_P\circ\Phi^1_{A_0} \quad \text{and} \quad \Phi^1_{A_0}\circ\Phi^h_P, \tag{2.27}$$

where Φ^h_P is the exact flow associated with the Hamiltonian P, and where $\Phi^1_{A_0}$ is defined by the relation

$$\forall j=(a,\delta)\in\mathcal{Z},\quad \big(\Phi^1_{A_0}(z)\big)_j=\exp(\mathrm{i}\delta\lambda_a)z_j.$$

We will mainly consider the cases listed in the Table 1 below.

Table 1 Splitting schemes

Method	$\alpha_h(x)$
Splitting	$\alpha_h(x)=x$
Splitting + CFL	$\alpha_h(x)=x\mathbb{1}_{x<c}(x)$
Mid-split	$\alpha_h(x)=2\arctan(x/2)$
Mid-split + CFL	$\alpha_h(x)=2\arctan(x/2)\mathbb{1}_{x<c}(x)$
New scheme (I)	$\alpha_h(x)=h^\beta\arctan(h^{-\beta}x)$
New scheme (II)	$\alpha_h(x)=\frac{x+x^2/h^\beta}{1+x/h^\beta+x^2/h^{2\beta}}$

Let us comment on these choices. The "mid-split" cases correspond to the approximation of the system

$$\begin{cases} \dot{\xi}_a = -\mathrm{i}\omega_a \xi_a, & a \in \mathcal{N}, \\ \dot{\eta}_a = \mathrm{i}\omega_a \eta_a, & a \in \mathcal{N}, \end{cases}$$

by the midpoint rule [1, 28]. Starting from a given point (ξ_a^0, η_a^0) we have by definition for the first equation

$$\xi_a^1 = \left(\frac{1 - \mathrm{i}h\omega_a/2}{1 + \mathrm{i}h\omega_a/2}\right)\xi_a^0 = \exp\bigl(-2\mathrm{i}\arctan(h\omega_a/2)\bigr)\xi_a^0$$

which is the solution at time 1 of the system

$$\begin{cases} \dot{\xi}_a = -\mathrm{i}2\arctan(h\omega_a/2)\xi_a, & a \in \mathcal{N}, \\ \dot{\eta}_a = \mathrm{i}2\arctan(h\omega_a/2)\eta_a, & a \in \mathcal{N}. \end{cases}$$

Thus in this case the Hamiltonian A_0 is given by

$$A_0(\xi, \eta) = \sum_{a \in \mathcal{Z}} 2\arctan(h\omega_a/2)\xi_a \eta_a.$$

Note that using the relation

$$\forall y \in \mathbb{R}, \quad \bigl|\arctan(y) - y\bigr| \le \frac{|y|^3}{3} \tag{2.28}$$

we obtain, for all $a \in \mathcal{N}$,

$$\bigl|\exp(-\mathrm{i}h\omega_a) - \exp\bigl(-2\mathrm{i}\arctan(h\omega_a/2)\bigr)\bigr| \le Ch^3\omega_a^3$$

for some constant C independent of a. Using the bound (2.17), we get for all z,

$$\bigl\|\Phi_{H_0}^h(z) - \Phi_{A_0}^1(z)\bigr\|_{L^2} \le Ch^3\|z\|_{H^{3m}}.$$

More generally, we have the following approximation result:

Lemma 2.9 *Assume that the function $\alpha_h(x)$ satisfies*

$$\forall x > 0, \quad \bigl|\alpha_h(x) - x\bigr| \le Ch^{-\sigma}x^\gamma \tag{2.29}$$

for some constants $C > 0$, $\sigma \ge 0$ and $\gamma \ge 2$. Then we have

$$\bigl\|\Phi_{H_0}^h(z) - \Phi_{A_0}^1(z)\bigr\|_{L^2} \le Ch^{\gamma-\sigma}\|z\|_{H^{\gamma m}}. \tag{2.30}$$

Proof For a given $a \in \mathcal{N}$, we have

$$\bigl|\alpha_h(h\omega) - h\omega_a\bigr| \le Ch^{\gamma-\sigma}\omega_a^\gamma.$$

Hence owing to the fact that $|e^{ix} - e^{iy}| \leq |x - y|$ for real x and y, we obtain

$$|\exp(-\mathrm{i}h\omega_a) - \exp(-\mathrm{i}\alpha_h(h\omega_a)| \leq Ch^{\gamma-\sigma}\omega_a^{\gamma},$$

and this yields the result. □

Commentary 2.10 Under the assumption that P acts on sufficiently high index Sobolev spaces H^s, the previous result can be combined with standard convergence analysis to show that the splitting methods (2.27) yield consistent approximation of the exact solution Φ_H^h provided the initial solution is smooth enough (depending on m). The condition $\gamma - \sigma = 2$ guarantees a local order 2 in (2.30) that will be of the same order of the error made by the splitting decomposition after one step. Such a local error propagates to a global error of order 1, which means that for a give finite time T, the error with the exact solution after n iteration with $nh = T$ will be of order $n \times h^2 \simeq h$ up to constants depending on T, and under the assumption that the numerical solution remains smooth. To give more precise results would be out of the scope of this paper, and we refer to [25] for the case of NLS.

Let us consider the function

$$\alpha_h(x) = h^{\beta} \arctan\bigl(h^{-\beta}x\bigr) \tag{2.31}$$

for $1 > \beta \geq 0$. It satisfies (2.29) with $C = 1/3$, $\sigma = 2\beta$ and $\gamma = 3$ (see (2.28)). Hence for $\beta = 1/2$, the estimate (2.30) shows a local error of order $\gamma - \sigma = 2$, and hence the splitting schemes (2.27) remains of local order 2 (though with more smoothness required than with the midpoint approximation) which means that the error made after one step is of order h^2. Of course, when $\beta = 1$, the approximation is not consistent (local error of order 1).

The second example

$$\alpha_h(x) = \frac{x + x^2/h^{\beta}}{1 + x/h^{\beta} + x^2/h^{2\beta}} \tag{2.32}$$

exhibits similar properties. Note that the simple choice

$$\alpha_h(x) = \frac{x}{1 + x/h^{\beta}} \tag{2.33}$$

ensures only a local error of order $h^{2-\beta}$ ($\gamma = 2$ and $\sigma = \beta$ in (2.30)). Hence the corresponding splitting schemes (2.27) are of global order $1 - \beta$ (hence $1/2$ in the case where $\beta = 1/2$).

All these "new" schemes have the particularity that $\alpha_h(x) \simeq x$ when x is small, but when $x \to \infty$, we have $\alpha_h(x) \simeq h^{\beta}$. Their use thus leads to a stronger regularization effect in the high modes than the midpoint approximation, without breaking the order of approximation for smooth functions. We will see in Sects. 3 and 4 that this property allows us to construct a modified equation over exponentially long times for all these schemes.

Note that, in practice, the implementation of the schemes associated with the filter functions (2.31) or (2.32) *a priori* requires the knowledge of a spectral decomposition of H_0. This will be the case for NLS on the torus, or NLW with Dirichlet boundary conditions, where the switch from the x-space (to calculate Φ_P^h) to the Fourier space (to calculate $\Phi_{A_0}^1$) can be easily implemented using the fast Fourier transform.

3 Recursive Equations

In this section we explain the strategy in order to prove the existence of a modified energy. We will see that it leads us to solve by induction a sort of homological equation in the spirit of normal form theory (see for instance [16]). For simplicity, we consider only the splitting method $\Phi_P^h \circ \Phi_{A_0}^1$. The second Lie splitting $\Phi_{A_0}^1 \circ \Phi_P^h$ can be treated similarly.

We look for a real Hamiltonian function $Z(t, \xi, \eta)$ such that for all $t \le h$ we have

$$\Phi_P^t \circ \Phi_{A_0}^1 = \Phi_{Z(t)}^1 \tag{3.1}$$

and such that $Z(0) = A_0$.

For a given Hamiltonian $K \in \mathcal{H}_s$, we denote by $\mathcal{L}_K$ the Lie differential operator associated with the Hamiltonian vector field X_K: for a given function g acting on ℓ_s^1, $s \ge 0$, and taking values on $\mathbb{C}$ or ℓ_s^1, we have

$$\mathcal{L}_K(g) = \sum_{j\in\mathcal{Z}} (X_K)_j \frac{\partial g}{\partial z_j}.$$

Denoting by $z(t)$ the flow generated by X_K starting from $z \in \ell_s^1$, i.e. $z(t) = \Phi_K^t(z)$, we have (if K is in $\mathcal{H}_s$)

$$z^{(k)}(t) = \mathcal{L}_K^k[I]\big(z(t)\big), \qquad \text{for all } k \in \mathbb{N},$$

where I defines the identity vector field: $I(z)_j = z_j$. Thus we can write, at least formally,

$$\Phi_K^1 = \exp(\mathcal{L}_K)[I]. \tag{3.2}$$

Differentiating the exponential map we calculate as in [19, Sect. III.4.1]

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_{Z(t)}^1 = X_{Q(t)} \circ \Phi_{Z(t)}^1,$$

where the differential operator associated with $Q(t)$ is given by

$$\mathcal{L}_{Q(t)} = \sum_{k\ge 0} \frac{1}{(k+1)!} \mathrm{Ad}^k_{\mathcal{L}_{Z(t)}}(\mathcal{L}_{Z't)})$$

with

$$\mathrm{Ad}_{\mathcal{L}_A}(\mathcal{L}_H) = [\mathcal{L}_A, \mathcal{L}_H]$$

being the commutator of two vector fields.

As the vector fields are Hamiltonian, we have

$$[\mathcal{L}_A, \mathcal{L}_H] = \mathcal{L}_{\{A,H\}},$$

where

$$\mathrm{ad}_K(G) = \{K, G\}.$$

Hence we obtain the formal series equation for Q:

$$Q(t) = \sum_{k\geq 0} \frac{1}{(k+1)!} \mathrm{ad}^k_{Z(t)} Z'(t), \tag{3.3}$$

where $Z'(t)$ denotes the derivative with respect to t of the Hamiltonian function $Z(t)$.

Therefore taking the derivative of (3.1), we obtain

$$X_P \circ \Phi^t_P \circ \Phi^1_{A_0} = X_{Q(t)} \circ \Phi^1_{Z(t)}$$

and hence the equation to be satisfied by $Z(t)$ reads

$$\sum_{k\geq 0} \frac{1}{(k+1)!} \mathrm{ad}^k_{Z(t)} Z'(t) = P. \tag{3.4}$$

Notice that the series $\sum_{k\geq 0} \frac{1}{(k+1)!} z^k = \frac{e^z - 1}{z}$ is invertible in the open disc $|z| < 2\pi$ with inverse given by $\sum_{k\geq 0} \frac{B_k}{k!} z^k$ where B_k are the Bernoulli numbers. So formally, (3.4) is equivalent to the formal series equation (see also [9], Eqn. (3.1))

$$Z'(t) = \sum_{k\geq 0} \frac{B_k}{k!} \mathrm{ad}^k_{Z(t)} P. \tag{3.5}$$

Substituting an Ansatz expansion $Z(t) = \sum_{\ell\geq 0} t^\ell Z_\ell$ into this equation, we get $Z_0 = A_0$ and for $n \geq 0$

$$(n+1) Z_{n+1} = \sum_{k\geq 0} \frac{B_k}{k!} \sum_{\ell_1+\cdots+\ell_k = n} \mathrm{ad}_{Z_{\ell_1}} \cdots \mathrm{ad}_{Z_{\ell_k}} P. \tag{3.6}$$

Commentary 3.1 The analysis made to obtain this recursive equation is formal. To obtain our main result, we will verify that the series we manipulate are in fact convergent series in $\mathcal{H}_s$ uniformly on balls of ℓ^1_s that contain the different flows involved in the formulas (see in particular Lemma 4.3 below).

For instance, (3.2) holds true as soon as $z(t)$ remains in a ball $B^s_M := \{z \in \ell^1_s \mid \|z\|_{\ell^1_s} \leq M\}$ for $0 \leq t \leq 1$, and the series $\sum \frac{\mathcal{L}^k_K[I](z)}{k!}$ is uniformly convergent on B^s_M. Notice that this in turn implies that $t \mapsto z(t)$ is analytic on the complex disc of radius 1.

Commentary 3.2 In the case of Strang splitting methods of the form

$$\Phi^{h/2}_P \circ \Phi^1_{A_0} \circ \Phi^{h/2}_P$$

we can apply the same strategy and look for a Hamiltonian $Z(t)$ satisfying, for all $t \leq h$,

$$\Phi^1_{Z(t)} = \Phi^{t/2}_P \circ \Phi^1_{A_0} \circ \Phi^{t/2}_P$$

and this yields equations similar to (3.6). We do not give the details here, as the analysis will be very similar.

The key lemma in order to prove that the previous series converge (and thus to justify the previous formal analysis) is the following one (whose proof is straightforward calculus):

Lemma 3.3 *Assume that*

$$Q(z) = \sum_{j \in \mathcal{Z}} a_{\boldsymbol{j}} z_{\boldsymbol{j}}$$

is a polynomial. Then

$$\mathrm{ad}_{Z_0}(Q) = \sum_{j \in \mathcal{Z}} \mathrm{i}\Lambda(\boldsymbol{j}) a_{\boldsymbol{j}} z_{\boldsymbol{j}},$$

where for a multi-index $\boldsymbol{j} = (j_1, \dots, j_r)$ *with for* $i = 1, \dots, r$, $j_i = (a_i, \delta_i) \in \mathcal{N} \times \{\pm 1\}$, *we denote*

$$\Lambda(\boldsymbol{j}) = \delta_1 \lambda_{a_1} + \cdots + \delta_r \lambda_{a_r}.$$

Hence we see that if $|\Lambda(\boldsymbol{j})| < 2\pi$ we will be able to define at least the first term Z_1 by summing the series in k in the formula (3.6).

4 Analytic Estimates

We assume in this section that α_h and h satisfy the following condition: there exist r and a constant $\delta < 2\pi$ such that

$$\forall n \leq r, \forall \boldsymbol{j} \in \mathcal{I}_n \quad \left|\Lambda(\boldsymbol{j})\right| \leq 2\pi - \delta. \tag{4.1}$$

Using Lemma 3.3, this condition implies that for any polynomial $Q \in \mathcal{P}_r$, we have the estimate

$$\left\|\mathrm{ad}_{Z_0} Q\right\| \leq (2\pi - \delta)\|Q\| \tag{4.2}$$

as, for homogeneous polynomials, the degree of $\mathrm{ad}_{Z_0} Q$ is the same as the degree of Q.

Theorem 4.1 *Let* $r_0 \geq 3$. *Assume that* $P \in \mathcal{P}_{r_0}$ *and that the condition* (4.1) *is fulfilled for some constants* δ *and* r. *Then for* $n \leq N := \frac{r-2}{r_0-2}$ *we can define polynomials* $Z_n \in \mathcal{P}_{n(r_0-2)+2}$ *satisfying* (3.6) *up to the order* n, *and satisfying the estimates* $\|Z_1\| \leq c$ *and for* $2 \leq n \leq N$,

$$\|Z_n\| \leq c(Cn)^{n-2} \tag{4.3}$$

for some constants c and C depending only on $\|P\|$, r_0 and δ. If, moreover, $P \in \mathcal{SP}_{r_0}$ then $Z_n \in \mathcal{SP}_{n(r_0-2)+2}$.

Proof Let

$$P(z) = \sum_{\ell=2}^{r_0} \sum_{\boldsymbol{j}\in\mathcal{I}_\ell} a_{\boldsymbol{j}} z_{\boldsymbol{j}}.$$

First we prove the existence of the Z_k for $k \le N$. Equation (3.6) for $n = 0$ reads

$$Z_1 = \sum_{k\ge 0} \frac{B_k}{k!} \mathrm{ad}_{Z_0}^k P.$$

The previous lemma and the condition (4.1) show that Z_1 exists and is given by

$$Z_1 = \sum_{\ell=2}^{r_0} \sum_{\boldsymbol{j}\in\mathcal{I}_\ell} \frac{\mathrm{i}\Lambda(\boldsymbol{j})}{\exp(\mathrm{i}\Lambda(\boldsymbol{j}))-1} a_{\boldsymbol{j}} z_{\boldsymbol{j}}.$$

Furthermore, we deduce immediately that Z_1 is real and satisfies $\|Z_1\| \le c_\delta \|P\|$ for some constant c_δ.

Assume now that the Z_k are constructed for $0 \le k \le n$, $n \ge 1$ and are such that Z_k is a polynomial of degree $k(r_0-2)+2$. Formally, Z_{n+1} is defined as a series

$$Z_{n+1} = \frac{1}{n+1} \sum_{k\ge 0} \frac{B_k}{k!} A_k,$$

where

$$A_k = \sum_{\ell_1+\cdots+\ell_k=n} \mathrm{ad}_{Z_{\ell_1}} \cdots \mathrm{ad}_{Z_{\ell_k}} P.$$

Let us prove that this series converges absolutely. In the previous sum, we separate the number of indices j for which $\ell_j = 0$. For them, we can use (4.2). Only for the other indices, we will use the estimates of Proposition 2.7 by taking into account that the right-hand side is a sum of terms that are all real polynomials of degree $(\ell_1+\cdots+\ell_k)(r_0-2)+r_0 = (n+1)(r_0-2)+2 \le (n+1)r_0$ and hence the inequality of Proposition 2.7 is only used with polynomials of order less than $(n+1)r_0$. Thus we write for $k \ge n$

$$\begin{aligned}\|A_k\| &:= \Big\| \sum_{\ell_1+\cdots+\ell_k=n} \mathrm{ad}_{Z_{\ell_1}} \cdots \mathrm{ad}_{Z_{\ell_k}} P \Big\| \\ &\le \sum_{i=1}^{n} \frac{k!\,(2\pi-\delta)^{k-i}}{(k-i)!\,i!} \sum_{\ell_1+\cdots+\ell_i=n \mid \ell_j>0} (n+1)^{i-1} 2^i r_0^{2i} \ell_1 \|Z_{\ell_1}\| \cdots \ell_i \|Z_{\ell_i}\| \, \|P\| \\ &\le (2\pi-\delta)^{k-n} k^n \sum_{i=1}^{n} \sum_{\ell_1+\cdots+\ell_i=n \mid \ell_j>0} (n+1)^{i-1} 2^i r_0^{2i} \ell_1 \|Z_{\ell_1}\| \cdots \ell_i \|Z_{\ell_i}\| \, \|P\|,\end{aligned}$$

and thus $\sum_{k\ge 0} \frac{B_k}{k!} A_k$ converges and Z_{n+1} is well defined up to $n+1 \le N$.

Further, as the right-hand side of (3.6) is a sum of terms that are all real polynomials of degree $(n+1)(r_0-2)+2$, Z_{n+1} is a polynomial of degree $(n+1)(r_0-2)+2$.

Now we have to prove the estimate (4.2). Following the previous calculation we get

$$(n+1)\|Z_{n+1}\| \le \sum_{i=1}^{n} \sum_{\ell_1+\cdots+\ell_i=n|\ell_j>0} \sum_{k\ge i} \frac{B_k}{i!\,(k-i)!}(2\pi-\delta)^{k-i}(n+1)^{i-1}2^i r_0^{2i} \\ \times \ell_1\|Z_{\ell_1}\|\cdots\ell_i\|Z_{\ell_i}\|\,\|P\|.$$

On the other hand, the entire series $f(z) := \sum_{k\ge1} \frac{B_k}{k!}z^k$ defines an analytic function on the disc $|z|<2\pi$. Thus its ith derivative $\sum_{k\ge i}\frac{B_k}{(k-i)!}z^{k-i}$ also defines an analytic function on the same disc and, by Cauchy estimates, there exists a constant $C_\delta = \sup_{|z|\le 2\pi-\delta/2}|f(x)|$ such that

$$\sum_{k\ge i}\frac{B_k}{(k-i)!}(2\pi-\delta)^{k-i} \le C_\delta i!\left(\frac{2}{\delta}\right)^i.$$

We then define for $n\ge1$

$$\zeta_n = nr_0\|Z_n\|.$$

These numbers satisfy the estimates, for $n\ge0$,

$$\zeta_{n+1} \le \delta_n^0 r_0 c_\delta\|P\| + C_\delta r_0\|P\|\sum_{i=1}^{n}\sum_{\ell_1+\cdots+\ell_i=n|\ell_j>0}(n+1)^{i-1}\left(4\delta^{-1}r_0\right)^i\zeta_{\ell_1}\cdots\zeta_{\ell_i}.$$

Let us fix $N\ge1$. We have for $n=0,\dots,N$

$$\begin{aligned}
&4\delta^{-1}r_0(N+1)\zeta_{n+1} \\
&\quad\le 4\delta^{-1}r_0(N+1)\delta_n^0 r_0 c_\delta\|P\| \\
&\qquad + C_\delta 4\delta^{-1}r_0^2\|P\|\sum_{i=1}^{n}\sum_{\ell_1+\cdots+\ell_i=n|\ell_j>0}(N+1)^i\left(4\delta^{-1}r_0\right)^i\zeta_{\ell_1}\cdots\zeta_{\ell_i}.
\end{aligned}$$

Let β_j, $j=0,\dots,N$ be the sequence satisfying

$$\beta_{n+1} = \delta_n^0 C_1 + C_2\sum_{i=1}^{n}\sum_{\ell_1+\cdots+\ell_i=n|\ell_j>0}\beta_{\ell_1}\cdots\beta_{\ell_i} \tag{4.4}$$

where

$$C_1 = 4(N+1)r_0^2 c_\delta\,\delta^{-1}\|P\| \quad\text{and}\quad C_2 = \frac{4C_\delta}{\delta}r_0^2\|P\|.$$

By induction, we see that for all $n=0,\dots,N$,

$$(N+1)\frac{4r_0}{\delta}\zeta_n \le \beta_n.$$

Multiplying (4.4) by t^{n+1} and summing over $n \geq 0$ we see that the formal series $\beta(t) = \sum_{j\geq 1} t^j \beta_j$ satisfies the relation

$$\beta(t) = tC_1 + tC_2\left(\frac{1}{1-\beta(t)} - 1\right).$$

This yields

$$\bigl(1-\beta(t)\bigr)\bigl(\beta(t) - tC_1\bigr) = tC_2\beta(t)$$

or equivalently

$$\beta(t)^2 - \beta(t)\bigl(1 + t(C_1 - C_2)\bigr) + tC_1 = 0.$$

The discriminant of this equation is

$$\bigl(1 + t(C_1 - C_2)\bigr)^2 - 4tC_1 = 1 - 2t(C_1 + C_2) + t^2(C_1 - C_2)^2$$

and hence, for $t \leq 1/2(C_1 + C_2)$, we find, using $\beta(0) = 0$,

$$2\beta = 1 + t(C_1 - C_2) - \bigl(1 - 2t(C_1 + C_2) + t^2(C_1 - C_2)^2\bigr)^{1/2}.$$

We verify that for $t \leq 1/2(C_1 - C_2)$ we have

$$2\beta \leq \frac{3}{2}.$$

By analytic estimate, we obtain for all $n \geq 0$

$$\beta_n = \frac{\beta^{(n)}(0)}{n!} \leq \frac{3}{2}\bigl(2(C_1 - C_2)\bigr)^n.$$

For $n = N$, this yields

$$\beta_N \leq \bigl(CN\|P\|\bigr)^N$$

for some constant C depending on r_0 and δ. We deduce the claimed result from the expression of ζ_N. □

For $s \geq 0$, we define

$$B_M^s = \bigl\{z \in \ell_s^1 \mid \|z\|_{\ell_s^1} \leq M\bigr\},$$

and we will use the notation $B_M = B_M^0$.

Theorem 4.2 *Let $r_0 \geq 3$, $s \geq 0$ and $M \geq 1$ be fixed. We assume that $P \in \mathcal{P}_{r_0}$ and that the condition (4.1) is fulfilled for some constants δ and $r \geq r_0$ and we denote by N the largest integer smaller than $\frac{r-2}{r_0-2}$. Then there exist constants c_0 and C depending on r_0, s, δ, $\|P\|$ and M such that, for all $hN \leq c_0$, there exists a real Hamiltonian polynomial $H_h \in \mathcal{P}_{N(r_0-2)+2}$ such that, for all $z \in B_M^s$, we have*

$$\bigl\|\Phi_P^h \circ \Phi_{A_0}^1(z) - \Phi_{H_h}^h(z)\bigr\|_{\ell_s^1} \leq h^{N+1}(CN)^N. \tag{4.5}$$

Moreover, assuming that

$$P(z)=\sum_{\ell=1}^{r_0}\sum_{\boldsymbol{j}\in\mathcal{I}_\ell}a_{\boldsymbol{j}}z_{\boldsymbol{j}}$$

for $z\in B^s_M$ *we have*

$$\left|H_h(z)-H_h^{(1)}(z)\right|\le Ch \tag{4.6}$$

where

$$H_h^{(1)}(z)=\sum_{a\in\mathcal{N}}\frac{1}{h}\alpha_h(h\omega_a)\xi_a\eta_a+\sum_{\ell=1}^{r_0}\sum_{\boldsymbol{j}\in\mathcal{I}_\ell}\frac{\mathrm{i}\Lambda(\boldsymbol{j})}{\exp(\mathrm{i}\Lambda(\boldsymbol{j}))-1}a_{\boldsymbol{j}}z_{\boldsymbol{j}}. \tag{4.7}$$

If finally, $P\in\mathcal{SP}_{r_0}$, *then* $H_h\in\mathcal{SP}_{N(r_0-2)+2}$.

Proof We define the real Hamiltonian $H_h=\frac{Z_h(h)}{h}$, where

$$Z_h(t)=\sum_{j=0}^{N}t^jZ_j,$$

and where, for $j=0,\dots,N$, the polynomials Z_j are defined in Theorem 4.1. Notice that N depends on r and thus on h via the condition (4.1).

By definition, $Z_h(t)(z)$ is a polynomial of order $N(r_0-2)+2\le Nr_0$ and using Theorem 4.1 we get

$$\left\|Z_h(t)\right\|\le c_1\left(1+\sum_{j=2}^{N}(Ctj)^{j-2}\right)<\infty$$

for some constant c_1 depending on δ and $\|P\|$. Thus $Z_h\in\mathcal{P}_{N(r_0-2)+2}$ (and in $\mathcal{SP}_{N(r_0-2)+2}$ if $P\in\mathcal{SP}_{r_0}$).

We will use the fact that for all s, there exists a constant c_s such that, for all $j\ge1$,

$$j^s\le(c_s)^j. \tag{4.8}$$

Now, as for all j, Z_j is a polynomial of order $j(r_0-2)+2\le jr_0$ with a zero of order at least 2 in the origin, we have, using Proposition 2.7 and Theorem 4.1, for $z\in B^s_{9M}$ and $j\ge1$

$$\left\|X_{Z_j}(z)\right\|_{\ell^1}\le 2c(jr_0)^{s+1}(Cj)^{j-1}\Big(\sup_{k=1,\dots,jr_0-1}\|z\|^k_{\ell^1}\Big)\le M\big(2Cc_sr_0^{s+1}cj(9M)^{r_0}\big)^j,$$

where the constants c and C are given by estimate (4.3). On the other hand we have, using Lemma 3.3 and (4.1),

$$\left\|X_{Z_0}(z)\right\|_{\ell^1}\le2\pi\|z\|_{\ell^1}\le2\pi M.$$

Hence, for $t \le (4NCc_s r_0^{s+1}c)^{-1}(9M)^{-r_0}$ we have

$$\|X_{Z_h(t)}(z)\|_{\ell^1} \le 2\pi M + M\sum_{j=1}^{N}\big(t2Cc_s r_0^{s+1}cN(9M)^{r_0}\big)^j < (2\pi+1)M < 8M. \quad (4.9)$$

Therefore by a classical bootstrap argument, the time 1 flow $\Phi^1_{Z_h(t)}$ maps B^s_M into B^s_{9M} provided that $t \le (4NCc_s r_0^{s+1}c)^{-1}(9M)^{-r_0}$.

On the other hand, $\Phi^1_{A_0}$ is an isometry of ℓ^1_s and hence maps B^s_M into itself; while using again Proposition 2.7, we see that Φ^t_P maps B^s_M into B^s_{9M} as long as $t \le (4r_0^{s+1}\|P\|M^{(r_0-1)})^{-1}$. We then define

$$\begin{aligned} T &\equiv T\big(N, M, r_0, s, \delta, \|P\|\big) \\ &:= \min\big\{\big(4r_0^{s+1}\|P\|M^{(r_0-1)}\big)^{-1}, \big(4NCc_s r_0^{s+1}c\big)^{-1}(9M)^{-r_0}\big\} \end{aligned} \quad (4.10)$$

and we assume in the sequel that $0 \le t \le T$ in such a way that all the flows remain in the ball B_{9M}.

Let $u(t) = \Phi^t_P \circ \Phi^1_{A_0}(z) - \Phi^1_{Z_h(t)}(z)$ and denote by $Q_h(t)$ the Hamiltonian defined by

$$Q_h(t) = \sum_{k\ge 0}\frac{1}{(k+1)!}\mathrm{ad}^k_{Z_h(t)} Z'_h(t).$$

Lemma 4.3 *For $t \le T$ given in (4.10), the Hamiltonian $Q_h(t) \in \mathcal{H}_s$ and satisfies for $z \in B^s_M$*

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi^1_{Z_h(t)}(z) = X_{Q_h(t)} \circ \Phi^1_{Z_h(t)}(z). \quad (4.11)$$

We postpone the proof of this lemma to the end of this section.

Using this result, as $u(0) = 0$, we get for $t \le T$ given in (4.10)

$$\begin{aligned} \|u(t)\|_{\ell^1_s} &\le \int_0^t \big\|X_P\big(\Phi^s_P \circ \Phi^1_{A_0}(z)\big) - X_{Q_h(s)}\big(\Phi^1_{Z_h(s)}(z)\big)\big\|_{\ell^1_s}\,\mathrm{d}s \\ &\le \int_0^t \big\|X_P\big(\Phi^1_{Z_h(s)}(z)\big) - X_{Q_h(s)}\big(\Phi^1_{Z_h(s)}(z)\big)\big\|_{\ell^1_s}\,\mathrm{d}s \\ &\quad + \int_0^t \big\|X_P\big(\Phi^s_P \circ \Phi^1_{A_0}(z)\big) - X_P\big(\Phi^1_{Z_h(s)}(z)\big)\big\|_{\ell^1_s}\,\mathrm{d}s. \end{aligned}$$

Therefore for $t \le T$

$$\|u(t)\|_{\ell^1_s} \le \int_0^t \sup_{z\in B_{9M}}\big\|X_P(z) - X_{Q_h(s)}(z)\big\|_{\ell^1_s}\,\mathrm{d}s + L_P\int_0^t \|u(s)\|_{\ell^1_s}\,\mathrm{d}s \quad (4.12)$$

where, using (2.10) in Proposition 2.7, we can take

$$L_P = 4r_0^{s+1}\|P\|(9M)^{r_0-2}.$$

So it remains to estimate $\sup_{z\in B_{9M}}\|X_P(z) - X_{Q_h(t)}(z)\|_{\ell^1_s}$ for $z \in B_{9M}$ and $t \le T$.

Now by the definition of $Q_h(t)$ and using Lemma 4.3 we have

$$Z_h'(t) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{Z_h(t)}^k Q_h(t),$$

where the right-hand side actually defines a convergent series by the argument used in the proof of Theorem 4.1. By construction (cf. Sect. 3), we have

$$\sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{Z_h(t)}^k \big(Q_h(t) - P\big) = \mathcal{O}\big(t^N\big)$$

in the sense of the Hamiltonian in the space $\mathcal{H}_s$. Taking the inverse of the series, we see

$$Q_h(t) - P = \sum_{n \geq N} K_n, \tag{4.13}$$

where we have the explicit expressions

$$K_n = \sum_{\ell+m=n|\ m<N} (m+1) \sum_{k\geq 0} \frac{1}{(k+1)!} \sum_{\ell_1+\cdots+\ell_k=\ell|\ell_j\leq N} \mathrm{ad}_{Z_{\ell_1}} \cdots \mathrm{ad}_{Z_{\ell_k}} Z_{m+1}. \tag{4.14}$$

Estimates similar to the one in the proof of Theorem 4.1 lead to

$$\begin{aligned} \|K_n\| \leq & \sum_{\ell+m=n|m<N} (m+1) \sum_{i=0}^{\ell} 2^i r_0^{2i} (n+1)^i \sum_{k\geq i} \frac{(2\pi - \delta)^{(k-i)}}{i!\,(k-i)!} \\ & \times \sum_{\ell_1+\cdots+\ell_i=\ell|0<\ell_j\leq N} \ell_1 \|Z_{\ell_1}\| \cdots \ell_{i-1} \|Z_{\ell_{i-1}}\| \ell_i \|Z_{\ell_i}\|\, \|Z_{m+1}\| \end{aligned}$$

and hence, after summing over k,

$$\begin{aligned} \|K_n\| \leq C_1 & \sum_{\ell+m=n\,|\,m<N} (m+1) \sum_{i=0}^{\ell} \frac{2^i r_0^{2i} (n+1)^i}{i!} \\ & \times \sum_{\ell_1+\cdots+\ell_i=\ell|0<\ell_j\leq N} \ell_1 \|Z_{\ell_1}\| \cdots \ell_{i-1} \|Z_{\ell_{i-1}}\| \ell_i \|Z_{\ell_i}\|\, \|Z_{m+1}\| \end{aligned}$$

for some constant C_1 depending on δ. Using the estimates in Theorem 4.1, we have for $\ell_j > 0$ and $\ell_j \leq N$,

$$\ell_j \|Z_{\ell_j}\| \leq c(C\ell_j)^{\ell_j - 1} \leq c(CN)^{\ell_j - 1}.$$

Using, moreover, $\|Z_{m+1}\| \le c(CN)^m$, and as the number of integers $\ell_1, \dots, \ell_i$ strictly positive such that $\ell_1 + \cdots + \ell_i = \ell$ is bounded by $2^{2\ell}$, we obtain

$$\begin{aligned}\|K_n\| &\le cC_1 \sum_{\ell+m=n\ m<N} (m+1) \sum_{i=0}^{\ell} \frac{(2c)^i r_0^{2i} (n+1)^i}{i!} \\ &\quad\times \sum_{\ell_1+\cdots+\ell_i=\ell | 0<\ell_j\le N} (CN)^{\ell_1+\cdots+\ell_i+m-i} \\ &\le cC_1 (CN)^n \sum_{\ell+m=n} 2^{2\ell} \sum_{i=0}^{\ell} \frac{(2c)^i r_0^{2i} (n+1)^{i+1}}{i!}.\end{aligned}$$

Therefore, there exists a constant D depending on r_0 and $\|P\|$ such that

$$\forall n \ge N \quad \|K_n\| \le (DN)^n.$$

As K_n is a polynomial of order at most $r_0 n$, we deduce from the previous estimate and Proposition 2.7 that, for $z \in B^s_{9M}$,

$$\|X_{K_n}(z)\|_{\ell^1_s} \le 2(nr_0)^{s+1}(DN)^n (9M)^{nr_0} \le \left(2c_s r_0^{s+1} DN (9M)^{r_0}\right)^n,$$

where the constant c_s is defined in (4.8). Hence the series $\sum_{n\ge 0} t^n X_{K_n}(z)$ converges for $t \le (4c_s r_0^{s+1} DN(9M)^{r_0})^{-1}$. Furthermore, again for $z \in B^s_{9M}$ and $t \le (4c_s r_0^{s+1} DN(9M)^{r_0})^{-1}$, we get, using (4.13) and the previous bound,

$$\|X_{Q_h(t)}(z) - X_P(z)\|_{\ell^1_s} \le \sum_{n\ge N} t^n \|X_{K_n}(z)\|_{\ell^1_s} \le (N+1)t^N (BN)^N$$

for some constant B depending on $\|P\|$, s, δ and r_0.

Let us set

$$\begin{aligned}c_0(M, r_0, \delta, s, \|P\|) := \min\Big\{&\left(4r_0^{s+1} \,|\, \|P\| M^{(r_0-1)}\right)^{-1}, \left(4Cc_s r_0^{s+1} c\right)^{-1} (9M)^{-r_0}, \\ &\left(4c_s r_0^{s+1} D (9M)^{r_0}\right)^{-1}\Big\}.\end{aligned}$$

For $t \le c_0(M, r_0, \delta, s, \|P\|)N^{-1}$, inserting the last estimate in (4.12) we get

$$\|u(t)\|_{\ell^1_s} \le t^{N+1}(BN)^N + L_P \int_0^t \|u(s)\|_{\ell^1_s} \mathrm{d}s,$$

and this leads to

$$\|u(t)\|_{\ell^1_s} \le t^{N+1}\left(\tilde{B}N\right)^N$$

for some constant $\tilde{B}$ depending on r_0, δ, s, $\|P\|$ and M. This implies (4.5) defining $H_h = Z_h(h)/h$ for $h \le c_0(M, r_0, \delta, s, \|P\|)N^{-1}$.

The second assertion of the theorem is just a calculus defining

$$H_h^{(1)} = \frac{1}{h} Z_0 + Z_1.$$

Using the previous bounds and the first inequality in Proposition 2.7, we then calculate that for $z \in B_M^s$

$$\begin{aligned}
\left\| H_h(z) - H_h^{(1)}(z) \right\|_{\ell_s^1} &\le \sum_{j=2}^{N} h^{j-1} \| Z_j(z) \|_{\ell_s^1} \\
&\le hcM^{2r_0} \sum_{j=2}^{N} h^{j-2} (CjM^{r_0})^{j-2} \\
&\le hcM^{2r_0} \sum_{j=2}^{N} \left(\frac{j}{2N} \right)^{j-2} \le 2hM^{2r_0}
\end{aligned}$$

by definition of $c_0(M, r_0, \delta, s, \|P\|)$. □

Proof of Lemma 4.3 With the previous notations, we have

$$Q_h(t) = \sum_{n \ge 0} t^n K_n,$$

where K_n is given by (4.14) and the bounds obtained show that $Q_h(t)(z)$ and $X_{Q_h(t)}(z)$ are well defined on B_{9M}. Now let us consider the flow $\Phi^1_{Z_h(t)}$. As previously mentioned, it acts from B_M^s to B_{9M}^s. Now we can write formally

$$\begin{aligned}
\Phi^1_{Z_h(t)}(z) &= \sum_{k \ge 0} \frac{1}{k!} (\mathcal{L}_{Z_h(t)})^k \\
&= \sum_{n \ge 0} t^n \sum_{k \ge 0} \frac{1}{k!} \sum_{\ell_1 + \cdots + \ell_k = n | \ell_i \le N} \mathcal{L}_{Z_{\ell_1}} \circ \cdots \circ \mathcal{L}_{Z_{\ell_l}} [I](z) \\
&= \sum_{n \ge 0} t^n \Psi_n(z). \qquad (4.15)
\end{aligned}$$

We are going to show that this series converges uniformly for $z \in B_M^s$ and $t \le T$.

Let K be a fixed polynomial of degree k, and $G(z) = (G_j(z))_{j \in \mathcal{Z}}$ a function acting on ℓ_s^1, and taking values in ℓ_s^1, such that the entries $G_j(z)$ are all polynomials of degree ℓ. By definition, we have

$$(\mathcal{L}_K \circ G)_j = \sum_{i \in \mathcal{Z}} (X_K)_i \frac{\partial G_j}{\partial z_i} = \{K, G_j\}.$$

Now using the relation (2.11) of Proposition 2.7, we see that $(\mathcal{L}_K \circ G)_j$ is a polynomial of degree $k + \ell - 2$ and of norm smaller that $2k\ell \|K\| \, \|G_j\|$. Now if $K = Z_0$, this bound can be refined in $\|(\mathcal{L}_{Z_0} \circ G)_j\| \le (2\pi - \delta)\|G_j\|$ using (4.2).

For a given $z \in B^s_M$, the jth component of $\mathcal{L}_{Z_{\ell_1}} \circ \cdots \circ \mathcal{L}_{Z_{\ell_l}}(I)(z)$ is a polynomial of order $n(r_0-2)+2$ and involves terms of momentum $\mathcal{M}(\boldsymbol{j}) = -\epsilon a$ if $j=(a,\epsilon)$ (see (2.13)). Hence summing over j, and separating as before the indices m for which $\ell_m = 0$ in the sum, we obtain for a given n and $z \in B^s_M$,

$$\begin{aligned}\left\|\Psi_n(z)\right\|_{\ell^1_s} &\leq 2(nr_0)^{s+1}M^{r_0 n}\\ &\quad\times \sum_{i=1}^{n}\sum_{k\geq i}\sum_{\ell_1+\cdots+\ell_i=n|\ell_n\leq N}\frac{(2\pi-\delta)^{k-i}}{(k-i)!i!}\left(2nr_0^2\right)^i \ell_1\|Z_{\ell_1}\|\cdots\ell_i\|Z_{\ell_i}\|\end{aligned}$$

and we conclude as before that this series is convergent for $t \leq T$ given in (4.10) with K depending on r_0, M, $\|P\|$, s and δ.

Now writing down the same argument for the series (in $k \geq 0$ and t^n, $n \geq 0$) defining $\frac{\mathrm{d}}{\mathrm{d}t}\Phi^1_{Z_h(t)}$ and $X_{Q_h(t)} \circ \Phi^1_{Z_h(t)}$, we see that this series is again convergent, which justifies the relation (4.11). □

5 Applications

In this section we analyze the consequences of the analytic estimates obtained in the previous section. We first show that, for the "new schemes" in Table 1, we obtain exponential estimates. We then show that for general splitting schemes, we obtain results under an additional CFL condition.

5.1 Exponential Estimates

We consider the following splitting scheme $\Phi^h_P \circ \Phi^1_{A_0}$ where the operator A_0 is associated with a function $\alpha_h(x)$ (see (2.26)) satisfying

$$\forall x \in \mathbb{R} \quad \left|\alpha_h(x)\right| \leq \gamma h^\beta \tag{5.1}$$

for some $\beta \in (0,1)$ and some $\gamma > 0$. Examples of such methods, preserving the global order 1 approximation property for smooth functions, are given in Table 1. For such a scheme, we obtain an exponentially close modified energy.

Theorem 5.1 *Let $r_0 \geq 3$ $s \geq 0$ and $M \geq 1$ be fixed. Assume that $P \in \mathcal{P}_{r_0}$ and that α_h satisfies the condition (5.1) for some constants γ and β. Then there exists a constant h_0 depending on r_0, $\|P\|$, s, M and γ such that for all $h \leq h_0$, there exists a real polynomial Hamiltonian H_h such that, for all $z \in B^s_M$, we have*

$$\left\|\Phi^h_P \circ \Phi^1_{A_0}(z) - \Phi^h_{H_h}(z)\right\|_{\ell^1_s} \leq h\exp\left(-(h_0/h)^\beta\right). \tag{5.2}$$

Proof The hypothesis (5.1) implies that the eigenvalues λ_a of the operator A_0 are bounded by γh^β. Hence for a multi-index $\boldsymbol{j} = (j_1,\ldots,j_r)$ we have

$$\left|\Lambda(\boldsymbol{j})\right| \leq r\gamma h^\beta$$

and the condition $|\Lambda(\boldsymbol{j})| \le \pi$ will be satisfied as long as $r \le (\pi/\gamma)h^{-\beta}$. Taking r_1 such that $r_1 \le (\pi/\gamma)h^{-\beta} < r_1 + 1$ and defining $N = (r_1 - 1)/(r_0 - 1)$, we get $b_1 h^{-\beta} \le N \le b_2 h^{-\beta}$ for some positive constants b_1 and b_2, depending on γ and r_0. Now the estimate (4.5) in Theorem 4.2 for this N yields

$$\big\| \Phi_P^h \circ \Phi_{A_0}^1(z) - \Phi_{H_h}^h(z) \big\|_{\ell_s^1} \le h^{N+1}(CN)^N \le h\big(Cb_2 h^{1-\beta}\big)^N,$$

as long as $hN \le c_0$. Thus defining $h_0 = \min\{(c_0 b_1^{-1})^{1/(1-\beta)}, (eCb_2)^{-1/(1-\beta)}, b_1^{1/\beta}\}$, we have for $0 < h \le h_0$

$$\big\| \Phi_P^h \circ \Phi_{A_0}^1(z) - \Phi_{H_h}^h(z) \big\|_{\ell_s^1} \le h e^{-N} \le h e^{-b_1 h^{-\beta}} \le h \exp\big(-(h_0/h)^\beta\big). \qquad \square$$

The dynamical consequences for the associated numerical scheme are given in the following corollaries. We first assume that the numerical solution remains *a priori* in ℓ^1 *only* over an arbitrarily long time.

Corollary 5.2 *Under the hypothesis of the previous Theorem, let* $z^0 = (\xi^0, \bar{\xi}^0) \in \ell^1$ *and the sequence* z^n *be defined by*

$$z^{n+1} = \Phi_P^h \circ \Phi_{A_0}^1(z^n), \quad n \ge 0. \tag{5.3}$$

Assume that, for all n, *the numerical solution* z^n *remains in a ball* B_M *of* ℓ^1 *for a given* $M > 0$. *Then there exist constants* h_0 *and* c *such that for all* $h \le h_0$, *there exists a polynomial Hamiltonian* H_h *such that*

$$H_h\big(z^n\big) = H_h\big(z^0\big) + \mathcal{O}\big(\exp\big(-ch^{-\beta}\big)\big)$$

for $nh \le \exp(ch^{-\beta})$. *Moreover, with the Hamiltonian* $H_h^{(1)}$ *defined in* (4.7) *we have*

$$H_h^{(1)}\big(z^n\big) = H_h^{(1)}\big(z^0\big) + \mathcal{O}(h) \tag{5.4}$$

over exponentially long times $nh \le \exp(ch^{-\beta})$.

This means that the modified energy remains exponentially close to its initial value during exponentially long times. Or more practically (since $H_h^{(1)}$ is explicit) the first modified energy is almost conserved during exponentially long times.

Proof As all the Hamiltonian functions considered are real, we have for all n, $z^n = (\xi^n, \bar{\xi}^n)$, i.e. z^n is real. Hence for all n, $H_h(z^n) \in \mathbb{R}$. Note, moreover, that we can always assume that $M \ge 1$.

We use the notations of the previous theorems and we notice that $H_h(z)$ is a conserved quantity by the flow generated by H_h. Therefore, we have

$$H_h\big(z^{n+1}\big) - H_h\big(z^n\big) = H_h\big(\Phi_P^h \circ \Phi_{A_0}^1\big(z^n\big)\big) - H_h\big(\Phi_{H_h}^h\big(z^n\big)\big)$$

and hence

$$\big|H_h\big(z^{n+1}\big) - H_h\big(z^n\big)\big| \le \Big(\sup_{z \in B_{2M}} \big\|\nabla H_h(z)\big\|_{\ell^\infty}\Big) \big\| \Phi_P^h \circ \Phi_{A_0}^1\big(z^n\big) - \Phi_{H_h}^h\big(z^n\big)\big\|_{\ell^1}.$$

Now using (4.9) and (5.2) we obtain for all n

$$\left|H_h\left(z^{n+1}\right)-H_h\left(z^n\right)\right|\le 4\pi Mh\exp\left(-(h_0/h)^\beta\right)$$

and hence

$$\left|H_h\left(z^n\right)-H_h\left(z^0\right)\right|\le (nh)\exp\left(-2ch^{-\beta}\right)$$

for some constant c, provided h_0 is small enough. This implies the result. The second estimate is then a clear consequence of (4.6). □

The preservation of the Hamiltonian $H_h^{(1)}$ over a long time induces, for $z^n=(\xi^n,\eta^n)$,

$$\sum_{a\in\mathcal{N}}\frac{1}{h}\alpha_h(h\omega_a)\xi_a^n\eta_a^n$$

to be bounded over a long time, provided z^0 is smooth. For the functions α_h given in Table 1, this yields $H^{m/2}$ bounds for low modes, while the L^2 norm of high modes remains small (see [9, Corollary 2.4] for similar results in the linear case). We detail here the result in the specific situation where $\alpha_h(x)$ is given by (1.10).

Corollary 5.3 *Let $r_0\ge 3$, $P\in\mathcal{P}_{r_0}$ and $\alpha_h(x)=\sqrt{h}\arctan(x/\sqrt{h})$. We assume that there exists a constant $b\ge 1$ such that*

$$\forall a\in\mathcal{N}\quad \frac{1}{b}|a|^m\le\omega_a\le b|a|^m. \tag{5.5}$$

Let z^n be the sequence defined by (5.3). We assume that $z^0=(\xi^0,\bar{\xi}^0)\in H^{m/2}$ and that the sequence z^n remains bounded in ℓ^1. Then there exist constants C, α and β such that

$$\sum_{|j|<\alpha h^{-1/2m}}|j|^m\left|z_j^n\right|^2+\frac{1}{\sqrt{h}}\sum_{|j|\ge\alpha h^{-1/2m}}\left|z_j^n\right|^2\le C$$

over exponentially long times $nh\le\exp(ch^{-\beta})$.

Proof The almost conservation of the Hamiltonian $H_h^{(1)}$ (cf. (5.4)) shows that, for all n such that $nh\le\exp(ch^{-\beta})$, we have

$$\begin{aligned}&\sum_{a\in\mathcal{N}}\frac{1}{\sqrt{h}}\arctan\left(\sqrt{h}\omega_a\right)\left|\xi_a^n\right|^2\\&\quad\le\left|P_h^{(1)}\left(z^0\right)-P_h^{(1)}\left(z^n\right)\right|+\sum_{a\in\mathcal{N}}\frac{1}{\sqrt{h}}\arctan\left(\sqrt{h}\omega_a\right)\left|\xi_a^0\right|^2+Ch\end{aligned}$$

for some constant C, where $P_h^{(1)}(z)$ is the nonlinear Hamiltonian of (4.7). As z^n remains bounded in ℓ^1, we see that $|P_h^{(1)}(z^0)-P_h^{(1)}(z^n)|$ is uniformly bounded. Now we have for all a

$$\frac{1}{\sqrt{h}}\arctan\big(\sqrt{h}\omega_a\big) \le \omega_a$$

and we deduce, using (5.5),

$$\sum_{a\in\mathcal{N}} \frac{1}{\sqrt{h}}\arctan\big(\sqrt{h}\omega_a\big)\big|\xi_a^0\big|^2 \le C\|z\|_{H^{m/2}}.$$

Hence we have

$$\sum_{a\in\mathcal{N}} \frac{1}{\sqrt{h}}\arctan\big(\sqrt{h}\omega_a\big)\big|\xi_a^n\big|^2 \le C$$

for some constant C depending on M and $\|z\|_{H^{m/2}}$. We conclude by using

$$x > 1 \quad \Longrightarrow \quad \arctan x > \arctan(1) \quad \text{and} \quad x \le 1 \quad \Longrightarrow \quad \arctan x > \frac{x}{2}$$

and the bounds (5.5) on ω_a. □

5.2 Results Under a CFL Condition

We now consider cases where α_h does not depend on h and thus does not satisfy (5.1). We focus on schemes such that

$$\alpha_h(x) = \beta(x)\mathbb{1}_{x<c}(x) \tag{5.6}$$

i.e. schemes associated with a filter function β and a CFL condition with CFL number c. We mainly have in mind the two applications (see Table 1)

$$\beta(x) = x \quad \text{and} \quad \beta(x) = 2\arctan(x/2)$$

corresponding to standard and implicit–explicit splitting schemes. Now, for such a scheme and for all multi-indices $\boldsymbol{j} = (j_1, \dots, j_r)$, we have at most

$$\big|\Lambda(\boldsymbol{j})\big| \le r\beta(c).$$

Hence if we define

$$c_r = \beta^{-1}\left(\frac{2\pi}{r}\right),$$

the condition (4.1) will be satisfied for some δ if $c < c_r$. Now considering a fixed order of approximation N, the construction of the modified energy of Theorem 4.2 can be performed up to $r = (r_0 - 2)N + 2$. The following result is then an easy consequence of Theorem 4.2.

Theorem 5.4 *Let $r_0 \ge 3$, N, $s \ge 0$ and $M > 0$ be fixed. Assume that $P \in \mathcal{P}_{r_0}$ and that α_h is of the form (5.6) for some constants c. Assume that*

$$c < \beta^{-1}\left(\frac{2\pi}{(r_0 - 2)N + 2}\right);$$

then there exist constants h_0 and C_N such that for all $h \le h_0$, there exists a real polynomial Hamiltonian H_h such that, for all $z \in B^s_M$, we have

$$\left\| \Phi^h_P \circ \Phi^1_{A_0}(z) - \Phi^h_{H_h}(z) \right\|_{\ell^1_s} \le C_N h^{N+1}. \tag{5.7}$$

If moreover $P \in \mathcal{SP}_{r_0}$, and if for all $a \in \mathcal{N}$, $\omega_a \ge 0$, then the same results holds under the condition

$$c < \beta^{-1}\left(\frac{4\pi}{(r_0 - 2)N + 2}\right). \tag{5.8}$$

Proof The former part of the theorem is a consequence of the previous estimates. The latter assertion comes from the fact that all the λ_a are positive. Hence for a given r and a given monomial of $\mathcal{SP}_r$ associated with a symmetric multi-index $\boldsymbol{j} = (j_1, \dots, j_{r/2}, k_1, \dots, k_{r/2})$ with $j_i = (a_i, +1)$ and $k_i = (b_i, -1)$, a_i and $b_i \in \mathcal{N}$, we have

$$\lambda(\boldsymbol{j}) = \lambda_{a_1} + \cdots + \lambda_{a_{r/2}} - \lambda_{b_1} - \cdots - \lambda_{b_{r/2}} \le \frac{r\beta(c)}{2}$$

and this yields the bound (5.8) for $r < (r_0 - 2)N + 2$. □

This result implies the preservation of the Hamiltonian over long times of order h^{-N}, as in Corollary 5.2. Similarly, Corollary 5.3 extends to the case of the mid-split scheme (i.e. the case $\beta(x) = 2\arctan(x/2)$) leading to $H^{m/2}$ control of the frequencies smaller than $c_r h^{-1/m}$, over long times of order h^{-N}, namely

$$\sum_{|j| < c_r h^{-1/m}} |j|^m \left|z^n_j\right|^2 \le C$$

for $n \le h^{-N}$. As the proof is completely similar, we do not give the details here. Note, however, that the high frequency cut-off does not give a control of the L^2 for high modes unless considering a fully discrete system where the high modes are by definition not present (see [11, Chap. 6]).

In Table 2, we give the expression of the CFL constant c in (5.8) required to obtain a given precision of order h^{N+1} in the estimate (5.7) in the two cases where $\beta(x) = x$ and $\beta(x) = 2\arctan(x/2)$ and in the special case of the cubic nonlinear Schrödinger equation for which the nonlinearity belongs to $\mathcal{SP}_4$. In this situation, we have $r_0 = 4$. The required CFL number c is then calculated using the formula (5.8).

6 Numerical Example

The goal of this last section is to illustrate the link between the features of the numerical integrator (CFL number, use of an implicit solver) and the preservation of the energy and regularity of the solution. In particular, we show that the preservation of the regularity of the numerical solution over long times depends on the CFL number

Table 2 CFL conditions for cubic NLS

h^{N+1}	$\beta(x) = x$	$\beta(x) = 2\arctan(x/2)$
h^2	3.14	∞
h^3	2.10	3.46
h^4	1.57	2.00
h^5	1.27	1.45
h^6	1.05	1.15
h^7	0.90	0.96
h^8	0.80	0.83
h^9	0.70	0.73
h^{10}	0.63	0.65

or the type of the integrator (explicit, implicit), making in general the *a priori* mathematical assumption irrelevant that the numerical solution remains smooth over a long time.

We consider the cubic nonlinear Schrödinger equation

$$\mathrm{i}\partial_t u(t,x) = -\partial_{xx}u(t,x) - \left|u(t,x)\right|^2 u(t,x), \quad u(t,x) = u^0(x)$$

set on the real line, $x \in \mathbb{R}$. Here, we aim at approximating the particular ground state solution

$$u(t,x) = \frac{\sqrt{2}\mathrm{e}^{\mathrm{i}t}}{\cosh(x)},$$

for which long time stability results can be proved (see for instance [6] and the references therein). We introduce a large window $[-\pi/L, \pi/L]$ where L is a small parameter, and we use a Fourier pseudospectral collocation method (see for instance [24] and the reference therein). In this scaled situation the CFL number is given by

$$\mathsf{cfl} = hL^2\left(\frac{K}{2}\right)^2.$$

We take $K = 256$, $L = 0.11$ and $h = 0.1$ ($\mathsf{cfl} = 19.8$), $h = 0.05$ ($\mathsf{cfl} = 9.9$) and $h = 0.01$ ($\mathsf{cfl} = 1.9$). As time integrator, we consider splitting schemes of the form (1.6). We first consider the case where A_0 in (1.7) is associated with the eigenvalues $\lambda_k = hk^2L^{-2}$, $k = -K/2, \dots, K/2 - 1$ (standard explicit splitting method). In Fig. 1, we plot the evolution of the discrete approximation of the energy

$$H(u,\bar{u}) = \int_{\mathbb{R}} \left|\partial_x u(x)\right|^2 - \frac{1}{2}\left|u(x)\right|^4 \mathrm{d}x$$

along the numerical solution, with respect to the time. We see that in the two cases $\mathsf{cfl} = 19.8$ and $\mathsf{cfl} = 9.9$, there is a serious drift, while in the case $\mathsf{cfl} = 1.9$, we observe a good preservation of the energy.

In Fig. 2, we plot the absolute value of the numerical solution $|u^n(x)|$ at time $t = nh$. In the case where $\mathsf{cfl} = 19.8$ we observe a deterioration at time $t = 300$ where the

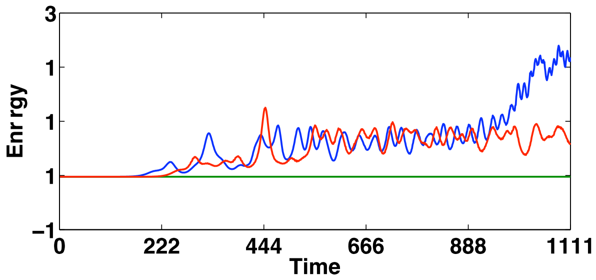

Fig. 1 Evolution of the energy for the Strang splitting with cfl $= 19.8$ (*blue*), 9.9 (*red*) and 1.9 (*green*)

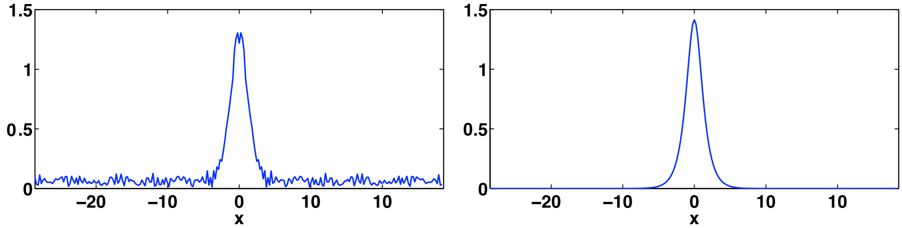

Fig. 2 $|u^n(x)|$ for the Strang splitting with cfl $= 19.8$ at time $t = 300$ (*left*) and cfl $= 1.9$ at time $t = 10{,}000$ (*right*)

smoothness of the initial solution seems to be lost. The right figure is obtained with a CFL number cfl $= 1.9$ and we observe that the numerical solution is particularly stable. The profile of the solution is almost the same as for the initial solution. This picture is drawn at time $t = 10{,}000$.

We then repeat the same experiments for implicit–explicit integrator, where A_0 corresponds to the midpoint rule applied to the free Schrödinger equation: $\lambda_k = 2\arctan(hk^2L^{-2}/2)$ [9]. In this situation, the energy is well preserved, independently of the CFL condition, and the shape of the soliton is stable for a very long time.

Hence we see that for the classical explicit splitting method, the preservation of the energy relies on the use of a CFL condition, as expected from the analysis developed in the previous sections. Moreover, we see that we cannot *a priori* assume that the solution remains smooth for all time independently of the space discretization. For the existence and stability of the numerical soliton with the help of the modified energy constructed in this paper, we refer to a forthcoming paper [4].

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