Birkhoff normal form for splitting methods applied to semi linear Hamiltonian PDEs. Part I: Finite dimensional discretization.

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Abstract

We consider *discretized* Hamiltonian PDEs associated with a Hamiltonian function that can be split into a linear unbounded operator and a regular nonlinear part. We consider splitting methods associated with this decomposition. Using a finite dimensional Birkhoff normal form result, we show the almost preservation of the *actions* of the numerical solution associated with the splitting method over arbitrary long time and for asymptotically large level of space approximation, provided the Sobolev norm of the initial data is small enough. This result holds under *generic* non-resonance conditions on the frequencies of the linear operator and on the step size. We apply these results to nonlinear Schrödinger equations as well as the nonlinear wave equation.

Contents

1 Introduction

In this work, we consider a class of Hamiltonian partial differential equations whose Hamiltonian functionals $H = H_0 + P$ can be divided into a linear unbounded operator H_0 with discrete spectrum and a nonlinear function P having a zero of order at least 3 at the origin of the phase space. Typical examples are given by the nonlinear wave equation on a segment with Dirichlet boundary conditions or the nonlinear Schrödinger equation on the torus. We consider discretizations of these PDEs and denote by $H^{(K)} = H_0^{(K)} + P^{(K)}$ the corresponding discrete Hamiltonian, where K is a discretization parameter. Typically, K denotes a spectral parameter in a collocation method.

Amongst all the numerical schemes that can be applied to these Hamiltonian PDEs, splitting methods entail many advantages, as they provide symplectic and explicit schemes, and can be easily implemented using fast Fourier transform if the spectrum of H_0 simply expresses in Fourier basis. Generally speaking, a splitting scheme is based on the approximation

$$\varphi^h_{H^{(K)}} \simeq \varphi^h_{H_0^{(K)}} \circ \varphi^h_{P^{(K)}} \tag{1.1}$$

for small time h, and where φ^t_Q denotes the exact flow of the Hamiltonian system associated with the Hamiltonian function Q. For a given time $t = nh$, $n \in \mathbb{N}$, the solution starting at some initial value z^0 is then approximated by

$$\varphi^t_{H^{(K)}}(z^0) \simeq z^n = \left(\varphi^h_{H_0^{(K)}} \circ \varphi^h_{P^{(K)}}\right)^n (z^0). \tag{1.2}$$

The understanding of the long-time behavior of splitting methods for Hamiltonian PDEs is a fundamental ongoing challenge in the field of geometric integration, as the classical arguments of *backward error analysis* (see for instance [20]) do not apply in this situation, where the frequencies of the system are arbitrary large, and where resonances phenomena are known to occur for some values of the step size. For example, considering the case of the Schrödinger equation on the one dimensional torus, the eigenvalues of $H_0^{(K)}$ range from 1 to K^2 and the assumption $hK^2 << 1$ used in the finite dimensional situation becomes drastically restrictive in practice.

Recently, many progresses have been made in the understanding of the long time behaviour of numerical methods applied to Hamiltonian PDEs. A first result using normal form techniques was given by Dujardin & Faou in [11] for the case of splitting methods applied to the linear Schrödinger equation with small potential. More recently DEBUSSCHE & FAOU showed in [9] the existence of a modified energy for implicit-explicit split-step methods applied to the linear Schrödinger equation. Concerning the nonlinear case, results exist by COHEN, HAIRER & LUBICH, see [19, 8], for the wave equation and GAUCKLER & LUBICH, see [14, 15], for the nonlinear Schrödinger equation using the technique of modulated Fourier expansion.

Typically time discretizations of Hamiltonian PDE introduce *numerical* resonances. Such effects are not physical and do not come from the structure of the spectrum of the linear operator H_0. They are induced by interactions between the time stepsize h and the frequencies of H_0. In the case where a CFL condition is satisfied, such phenomenon will not be observed. We refer to FAOU & GRÉBERT [12] for results in this direction. In section 4.2.1 we give a numerical example of resonances effects due to a resonant step size *outside* the CFL regime. To go beyond this CFL condition, one has to rely on a non resonance assumption mixing the frequencies of H_0 and the time step size h, and being satisfied for a large set of h and frequencies.

Normal form techniques have proven to be one of the most important tools for the understanding of the long time behavior of Hamiltonian PDEs (see [1, 4, 17, 2, 3, 18]). Roughly speaking, the dynamical consequences of such results are the following: starting with a small initial value of size ε in a Sobolev space H^s, then the solution remains small in the same norm over long time, namely for time $t \leq C_r\varepsilon^{-r}$ for arbitrary r (with a constant C_r depending on r). Such results hold under *generic* non-resonance conditions on the frequencies of the underlying linear operator H_0 associated with the Hamiltonian PDE, that are valid in a wide number of situations (nonlinear Schrödinger equation on a torus of dimension d or with Dirichlet boundary conditions, nonlinear wave equation with periodic or Dirichlet conditions in dimension 1 [4], Klein Gordon equation on spheres or Zoll manifolds [3] or nonlinear quantum harmonic oscillator on $\mathbb{R}^d$ [18]).

This work is the first of a series of two.

In this paper, we consider full discretizations of the Hamiltonian PDE, with a spectral discretization parameter K and consider the exact splitting method. In this case, we show that under the hypothesis $K \leq \varepsilon^{-\sigma}$ for some constant σ then the *actions* of the initial value are almost preserved over a very large number of iterations $n \leq C_r\varepsilon^{-r}$, provided the initial solution is small (of order ε) in L^2 norm. The constant σ depends on the precision degree r (and of course decreases with r). These actions can be interpreted as the oscillatory energies corresponding to an eigenvalue of $H_0^{(K)}$. Moreover, the L^2 norm of this numerical solution remains small for this large number of iterations.

The method used in this situation is by essence (for fixed K) a finite dimensional Birkhoff normal form result (explaining why we work here essentially with the L^2 norm). Using a *generic* non-resonance condition on the step size that turns out to be valid for many equations and that is *independent of* K, we mainly show that we can take K asymptotically large (i.e. of order $\varepsilon^{-\sigma}$) without altering the nature of the classical result. Our main result is given by Theorem 4.1.

Roughly speaking, the method consists in applying techniques that are now standard in normal form theory, by tracking the dependence in K of the constants appearing in the estimates. The use of a non-resonance condition that is independent of K is however crucial, and reflects the infinite dimensional nature of the initial continuous problem without space approximation.

For each fixed K our normal form result could be deduced from existing normal form results for a close to linear symplectic map (see for instance [5, 6, 21]). Nevertheless, in these works, it is not clear how to track the dependence in the dimension K and in the step size h (in particular in the non-resonance condition) which is crucial for the dynamical consequences on the numerical scheme. That is the reason why we prefer to present a new proof using the underlying infinite dimensional structure given by the PDE that we are discretizing.

In some sense, the second paper [13] studies the case where $K > \varepsilon^{-\sigma}$ by considering the splitting method where no discretization in space is made (i.e. $K = +\infty$). The techniques used involve the abstract framework developed in [4, 17, 2]. However, instead of being valid for the (exact) abstract splitting (1.1), we have to consider *rounded* splitting methods (see [13] for definition and comments on this concept). On the contrary, in the present article we deal with the true splitting algorithm, in the regime $K \leq \varepsilon^{-\sigma}$.

Finally we notice that, in this present form, our results apply only to non resonant Hamiltonian PDEs (see section 4.2). However they could be extended to the finitely resonant case, i.e. when the frequencies are finitely degenerated. This could be done for the periodic nonlinear wave equation in the the spirit of [4], for the Klein Gordon equation on the sphere in the spirit of [3] or for the nonlinear quantum harmonic oscillator on $\mathbb{R}^d$ (see [18]).

2 Description of the method

Before going on into the precise statements and proofs of this work, we would like to give tentative explanations of the restrictions observed in comparison with the continuous case.

In [4], in order to prove the long-time conservation of Sobolev norms for small initial data, the authors consider a Hamiltonian $H = H_0 + P$ depending on an infinite number of complex variable (ξ_j, η_k), $j, k \in \mathbb{N}$ endowed with the symplectic form $\sum_j d\xi_j \wedge d\eta_j$, where H_0 is the infinite dimensional harmonic oscillator:

$$H_0 = \sum_{j\in\mathbb{N}} \omega_j \xi_j \eta_j,$$

and P is a nonlinearity of order at least 3. Typically, ξ_j and η_j represent the conjugate components of the solution of the PDE in an orthonormal eigenbasis of the operator H_0 and the Hamiltonian is assumed to be *real* which means that $H(\xi,\eta) \in \mathbb{R}$ when $\xi_j = \bar{\eta}_j$.

Then for a fixed number r, they construct a hamiltonian transformation τ close to the identity and such that, in the new variables, the Hamiltonian can be written

$$H_0 + Z + R \tag{2.1}$$

where Z is a real Hamiltonian depending only on the actions $I_j = \xi_j \eta_j$ and R a real Hamiltonian having a zero of order r.

The key for this construction is an induction process with, at each step, the resolution of an homological equation of the form

$$\{H_0, \chi\} + Z = G \tag{2.2}$$

where G is a given homogeneous polynomial of order n, and where Z, depending only on the actions, and χ are unknown. Assume that the polynomial G has the form

$$G = G_{\boldsymbol{jk}}\, \xi_{j_1} \cdots \xi_{j_p} \eta_{k_1} \cdots \eta_{k_q}$$

where $G_{\boldsymbol{jk}}$ is a coefficient, $\boldsymbol{j} = (j_1, \ldots, j_p) \in \mathbb{N}^p$ and $\boldsymbol{k} = (k_1, \ldots, k_q) \in \mathbb{N}^q$. Then it is easy to see that the equation (2.2) can be written

$$\Omega(\boldsymbol{j},\boldsymbol{k})\chi_{\boldsymbol{jk}} + Z_{\boldsymbol{jk}} = G_{\boldsymbol{jk}} \tag{2.3}$$

where

$$\Omega(\boldsymbol{j},\boldsymbol{k}) = \omega_{j_1} + \cdots + \omega_{j_p} - \omega_{k_1} - \cdots - \omega_{k_q}$$

and $Z_{\boldsymbol{jk}}$ and $\chi_{\boldsymbol{jk}}$ are unknown coefficients.

It is clear that for $\boldsymbol{j} = \boldsymbol{k}$ (up to a permutation), we have $\Omega(\boldsymbol{j},\boldsymbol{k}) = 0$ which imposes $Z_{\boldsymbol{jk}} = G_{\boldsymbol{jk}}$. When $\boldsymbol{j} \neq \boldsymbol{k}$ (taking into account the permutation), the solution of (2.3) relies on a non-resonance conditions on the small divisors $\Omega(\boldsymbol{j},\boldsymbol{k})^{-1}$.

In [4], Bambusi & Grébert use a non-resonance condition of the form

$$\forall\, \boldsymbol{j} \neq \boldsymbol{k}, \quad |\Omega(\boldsymbol{j},\boldsymbol{k})| \geq \gamma\mu(\boldsymbol{j},\boldsymbol{k})^{-\alpha} \tag{2.4}$$

where $\mu(\boldsymbol{j},\boldsymbol{k})$ denotes the third largest integer amongst $|j_1|, \ldots, |k_q|$. They moreover show that such a condition is guaranteed in a large number of situations (see [4], [17] or [2] for precise results).

Considering now the splitting method $\varphi_{H_0}^h \circ \varphi_P^h$, we see that we cannot work directly at the level of the Hamiltonian. To avoid this difficulty, we embed the splitting into the family of applications

$$[0,1] \ni \lambda \mapsto \varphi_{H_0}^h \circ \varphi_{hP}^\lambda$$

and we take the derivative of this expression with respect to λ, in order to work in the tangent space, where it is much easier to identify real Hamiltonian than unitary flows.

This explains why in contrast with [4] we deal here with time-dependent Hamiltonians. Note that we do not expand the operator $\varphi_{H_0}^h$ in powers of h, as this would yields positive powers of the unbounded operator H_0 appearing in the series. Unless a drastic CFL condition is employed, this method does not give the desired results (and does not explain the resonance effects observed for some specific values of h, see the numerical example in section 4.2.1).

Now, instead of (2.2), the homological equation appearing for the splitting methods is given in a discrete form

$$\chi \circ \varphi_{H_0}^h - \chi + Z = G. \tag{2.5}$$

In terms of coefficients, this equations yields

$$(e^{ih\Omega(\boldsymbol{j},\boldsymbol{k})} - 1)\chi_{\boldsymbol{jk}} + Z_{\boldsymbol{jk}} = G_{\boldsymbol{jk}}.$$

The main difference with (2.3) is that we have to avoid not only the indices $(\boldsymbol{j},\boldsymbol{k})$ so that $\Omega(\boldsymbol{j},\boldsymbol{k}) = 0$, but all of those for which $h\Omega(\boldsymbol{j},\boldsymbol{k}) = 2m\pi$ for some (unbounded) integer m.

In the case of a fully discretized system for which $\nabla_{z_j} P \equiv 0$ for $|j| > K$, then under a CFL-like condition of the form $hK^m \leq C$ where m depends on the growth of the eigenvalues of H_0 and C depends on r, then we have $|h\Omega(\boldsymbol{j},\boldsymbol{k})| \leq \pi$, and hence

$$|e^{ih\Omega(\boldsymbol{j},\boldsymbol{k})} - 1| \geq h\gamma\mu(\boldsymbol{j},\boldsymbol{k})^{-\alpha} \tag{2.6}$$

is then a consequence of (2.4). Under this assumption, we can apply the same techniques used in [4] and draw the same conclusions.

The problem with (2.6) is that it is non generic in h outside the CFL regime. For example, in the case of the Schrödinger equation, the frequencies of the operator H_0 are such that $\omega_j \simeq j^2$. Hence, for large N, if $(j_1,\dots,j_p,k_1,\dots,k_q)$ is such that $j_1 = N+1$, $k_1 = N$ and all the other ones are of order 1 (N is large here), we have $\Omega(\boldsymbol{j},\boldsymbol{k}) \simeq (N+1)^2 - N^2 \simeq 2N$. Hence,

$$|e^{ih\Omega(\boldsymbol{j},\boldsymbol{k})} - 1| \simeq |e^{2ihN} - 1|$$

cannot be assumed to be greater than $h\gamma\mu(\boldsymbol{j},\boldsymbol{k})^{-\alpha} \simeq h$ for all (large) N. Note that a generic hypothesis on h would be here that this small divisor is greater than $h\gamma N^{-\alpha}$ for some constants γ and α: see Hypothesis 3.4 and Lemma 3.6 below. This example shows that we cannot control the small divisors $|e^{ih\Omega(\boldsymbol{j},\boldsymbol{k})}-1|$ associated with the splitting scheme by the *third largest* integer in the multi index (which is actually of order 1 in this case), but only by the *largest*.

A numerical example of resonances effect due to a resonant step size outside CFL regime is given in section 4.2.1. Actually h is chosen such that $h(\omega_7-\omega_1) = 2\pi$ which implies an exact resonance $|e^{ih(\omega_7-\omega_1)}-1| = 0$ in the numerical scheme while this resonance does not exist for the continuous model since $\omega_7 - \omega_1 \neq 0$.

The fact that the control of the small denominators involves the largest index makes impossible a direct application of the method used for instance in [4]. In our case, for a given frequency cut-off N, the homological equation can only be solved for muti-indices with all indices smaller than N. As usual in such procedure (see [1, 4]), it turns out that this frequency cut-off N can be taken of order $\varepsilon^{-\sigma}$. Now two situations can be distinguished:

- In the case of a full discretization of the Hamiltonian PDE with a spectral discretization parameter $K \leq N \simeq \varepsilon^{-\sigma}$, then no frequencies higher than N are present in the problem and the homological equation can be solved for *all* frequencies (up to the actions terms). As a consequence the normal form term Z actually depends only on the actions and long time preservation consequences can be drawn as in the continuous case. This is essentially the result of the first part of this paper.
- In the case where $K > \varepsilon^{-\sigma}$, the normal form term Z is now made of terms depending only of the actions *and* additional terms containing frequencies greater than $N \simeq \varepsilon^{-\sigma}$. As a consequence, we do not obtain preservation results for the exact splitting but only for rounded splitting methods (see [13] for precise statements). Moreover, we use a zero momentum condition to ensure the presence of at least *two* large indices in the normal form. This is the result given in the second part [13] of this work.

3 Setting of the problem

3.1 Hamiltonian formalism

We set $\mathcal{N} = \mathbb{Z}^d$ or $\mathbb{N}^d$. For $a = (a_1, \dots, a_d) \in \mathcal{N}$, we set

$$|a| = \max_{i=1,\dots,d} |a_i|.$$

Let $K \in \mathbb{N}$, and let $\mathcal{N}_K$ a finite subset of $\mathcal{N}$, included in the ball $\{a \in \mathcal{N} \mid |a| \leq K\}$. Typically, we can take $\mathcal{N}_K$ of the form $[-K, \dots, K]^d \subset \mathbb{Z}^d$ or $[0, \dots, K]^d \subset \mathbb{N}^d$ or a sparse set of the form (see for instance [16, 22])

$$\mathcal{N}_K = \{\, a = (a_1, \dots, a_d) \in \mathbb{Z}^d \mid (1+|a_1|)\cdots(1+|a_d|) \leq K \,\} \subset \mathbb{Z}^d.$$

We consider the set of variables $(\xi_a, \eta_b) \in \mathbb{C}^{\mathcal{N}_K} \times \mathbb{C}^{\mathcal{N}_K}$ equipped with the symplectic structure

$$i \sum_{a\in\mathcal{N}_K} \mathrm{d}\xi_a \wedge \mathrm{d}\eta_a. \tag{3.1}$$

We define the set $\mathcal{Z}_K = \mathcal{N}_K \times \{\pm 1\}$. For $j = (a, \delta) \in \mathcal{Z}_K$, we define $|j| = |a|$ and we denote by $\bar{j}$ the index $(a, -\delta)$.

We then define the variables $(z_j)_{j\in\mathcal{Z}_K} \in \mathbb{C}^{\mathcal{Z}_K}$ by the formula

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

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

We set

$$\|z\|^2 := \sum_{j\in\mathcal{Z}_K} |z_j|^2$$

and for any $\rho > 0$,

$$B_K(\rho) = \{\, z \in \mathbb{C}^{\mathcal{Z}_K} \mid \|z\| \leq \rho \,\}.$$

Note that in the case where $K = +\infty$, we set by convention $\mathcal{Z}_K = \mathcal{Z} = \mathcal{N} \times \{\pm 1\}$ and the previous norm defines a Hilbert structure on $\ell^2_{\mathcal{Z}}$. We denote by

$$\Pi_K : \ell^2_{\mathcal{Z}} \to \left(\mathbb{C}^{\mathcal{Z}_K}, \|\cdot\|\,\right)$$

the natural projection.

Let $\mathcal{U}_K$ be a an open set of $\mathbb{C}^{\mathcal{Z}_K}$. For a function F in $\mathcal{C}^1(\mathcal{U}_K, \mathbb{C})$, we define its gradient as

$$\nabla F(z) = \left(\frac{\partial F}{\partial z_j}\right)_{j\in\mathcal{Z}_K}$$

where by definition, we set for $j = (a, \delta) \in \mathcal{N}_K \times \{\pm 1\}$,

$$\frac{\partial F}{\partial z_j} = \begin{cases} \dfrac{\partial F}{\partial \xi_a} & \text{if} \quad \delta = 1, \\ \dfrac{\partial F}{\partial \eta_a} & \text{if} \quad \delta = -1. \end{cases}$$

Let $H(z)$ be a function defined on $\mathcal{U}_K$. If H is smooth enough, we can associate with this function the Hamiltonian vector field $X_H(z)$ defined as

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

where J is the symplectic operator induced by the symplectic form (3.1).

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

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

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

With a given function $H \in \mathcal{C}^\infty(\mathcal{U}_K, \mathbb{C})$, we associate the Hamiltonian system

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

which can be written

$$\begin{cases} \dot{\xi}_a &= -i\dfrac{\partial H}{\partial \eta_a}(\xi,\eta) \quad a \in \mathcal{N}_K \\ \dot{\eta}_a &= i\dfrac{\partial H}{\partial \xi_a}(\xi,\eta) \quad\quad a \in \mathcal{N}_K. \end{cases} \tag{3.2}$$

In this situation, we define the flow $\varphi_H^t(z)$ associated with the previous system (for times $t \geq 0$ depending on $z \in \mathcal{U}_K$). Note that if $z = (\xi, \bar{\xi})$ and H is real, the flow $(\xi^t, \eta^t) = \varphi_H^t(z)$, for all time where it is defined, satisfies the relation $\xi^t = \bar{\eta}^t$, where ξ^t is solution of the equation

$$\dot{\xi}_a = -i\frac{\partial H}{\partial \eta_a}(\xi, \bar{\xi}), \quad a \in \mathcal{N}_K. \tag{3.3}$$

In this situation, introducing the real variables p_a and q_a such that

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

the system (3.3) is equivalent to the system

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

where $\tilde{H}(q,p) = H(\xi, \bar{\xi})$.

Note that the flow $\tau^t = \varphi_\chi^t$ of a real Hamiltonian χ defines a symplectic map, i.e. satisfies for all time t and all point z where it is defined

$$(D_z\tau^t)_z^T J (D_z\tau^t)_z = J \tag{3.4}$$

where D_z denotes the derivative with respect to the initial conditions.

The following result is classical:

Lemma 3.1 *Let $\mathcal{U}_K$ and $\mathcal{W}_K$ be two domains of $\mathbb{C}^{\mathcal{Z}_K}$, and let $\tau = \varphi^1_\chi \in \mathcal{C}^\infty(\mathcal{U}_K, \mathcal{W}_K)$ be the flow of the real smooth Hamiltonian χ. Then for $H \in \mathcal{C}^\infty(\mathcal{W}_K, \mathbb{C})$, we have*

$$\forall\, z \in \mathcal{U} \quad X_{H\circ\tau}(z) = (D_z\tau(z))^{-1} X_H(\tau(z)).$$

Moreover, if H is a real Hamiltonian, $H \circ \tau$ is a real Hamiltonian.

3.2 Hypothesis

We describe now the hypothesis needed on the Hamiltonian H.

In the following, we consider an infinite set of frequencies $(\omega_a)_{a\in\mathcal{N}}$ satisfying

$$\forall\, a \in \mathcal{N}, \quad |\omega_a| \leq C|a|^m \tag{3.5}$$

for some constants $C > 0$ and $m > 0$.

Let $\mathcal{U}$ be an open domain of $\ell^2(\mathbb{C}^{\mathcal{Z}})$ containing the origin, and let $\mathcal{U}_K = \Pi_K \mathcal{U}$ its projection onto $\mathbb{C}^{\mathcal{Z}_K}$.

We consider the collection of Hamiltonian functions

$$H^{(K)} = H_0^{(K)} + P^{(K)}, \quad K \geq 0, \tag{3.6}$$

with

$$H_0^{(K)} = \sum_{a\in\mathcal{N}_K} \omega_a I_a(z)$$

where for all $a \in \mathcal{N}_K$,

$$I_a(z) = \xi_a \eta_a \tag{3.7}$$

are the *actions* associated with $a \in \mathcal{N}_K$. Note that if $z = (\xi, \bar{\xi})$, then $I_a(z) = |\xi_a|^2$.

We moreover assume that the functions $P^{(K)} \in \mathcal{C}^\infty(\mathcal{U}_K, \mathbb{C})$ are *real*, of *order at least 3*, and satisfy the following: For all $\ell > 1$, there exists constants $C(\ell) \geq 0$ and $\beta(\ell) \geq 0$ such that for all $K \geq 1$, $(j_1, \cdots, j_\ell) \in \mathcal{Z}_K^\ell$ and $z \in \mathcal{U}_K$, the following estimate holds:

$$\left| \frac{\partial P^{(K)}}{\partial z_{j_1} \cdots \partial z_{j_\ell}}(z) \right| \leq C(\ell) K^{\beta(\ell)}. \tag{3.8}$$

The Hamiltonian system (3.2) can hence be written

$$\left\{ \begin{array}{rcll} \dot{\xi}_a &=& -i\omega_a \xi_a - i\dfrac{\partial P^{(K)}}{\partial \eta_a}(\xi, \eta) & a \in \mathcal{N}_K \\ \dot{\eta}_a &=& i\omega_a \eta_a + i\dfrac{\partial P^{(K)}}{\partial \xi_a}(\xi, \eta) & a \in \mathcal{N}_K. \end{array} \right. \tag{3.9}$$

Denoting by φ_Q^t the exact flow of a Hamiltonian flow, splitting methods are based on the approximation

$$\varphi^h_{H^{(K)}} \simeq \varphi^h_{H_0^{(K)}} \circ \varphi^h_{P^{(K)}}$$

for a small time step $h > 0$. Note that in this case, the exact flow of $H_0^{(K)}$ is explicit and given by

$$\varphi^h_{H_0^{(K)}}(\xi, \eta) = (e^{-i\omega_a h}\xi_a, e^{i\omega_a h}\eta_a)_{a\in\mathcal{N}_K}$$

while the calculation of $\varphi^h_{P^{(K)}}$ requires the solution of an ordinary differential equation, whose solution is often given explicitely (see the examples below).

The goal of this paper is the study of the long-time behavior of the numerical solution z^n given by (1.2) for large number n of iterations.

Remark 3.2 *Note that no hypothesis is made here concerning the preservation of the L^2 norm by the flow of* (3.9).

3.3 Non-resonance condition

In the following, for $\boldsymbol{j} = (j_1, \ldots, j_r) \in \mathcal{Z}_K^r$ with $r \geq 1$, we use the notation

$$z_{\boldsymbol{j}} = z_{j_1} \cdots z_{j_r}.$$

Moreover, for $\boldsymbol{j} = (j_1, \ldots, j_r) \in \mathcal{Z}_K^r$ with $j_i = (a_i, \delta_i) \in \mathcal{N}_K \times \{\pm 1\}$ for $i = 1, \ldots, r$, we set

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

and we define

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

We say that $\boldsymbol{j} \in \mathcal{Z}_K^r$ is resonant and we write $\boldsymbol{j} \in \mathcal{A}_K^r$ if r is even and if we can write (up to a permutation of the indices)

$$\forall\, i = 1, \ldots r/2, \quad j_i = (a_i, 1), \quad \text{and} \quad j_{i+r/2} = (a_i, -1)$$

for some $a_i \in \mathcal{N}_K$. For odd r, $\mathcal{A}_r$ is the empty set.

Associated with this resonant set we define the notion of polynomial in normal form:

Definition 3.3 *A polynomial Z on $\mathbb{C}^{\mathcal{Z}_K}$ is said to be in normal form if we can write it*

$$Z = \sum_{\ell=3}^{r} \sum_{\boldsymbol{j}\in\mathcal{A}_K^\ell} Z_{\boldsymbol{j}} z_{\boldsymbol{j}}.$$

Note that if $\boldsymbol{j} \in \mathcal{A}_K^r$ then

$$\begin{aligned} z_{\boldsymbol{j}} = z_{j_1} \cdots z_{j_r} &= \xi_{a_1}\eta_{a_1} \cdots \xi_{a_{r/2}}\eta_{a_{r/2}} \\ &= I_{a_1}(z) \cdots I_{a_{r/2}}(z) \end{aligned}$$

where for all $a \in \mathcal{N}_K$, $I_a(z)$ denote the actions associated with a (see (3.7)). Thus a polynomial in normal form is a polynomial that depends only of the actions. As a consequence, the actions are invariant by the hamiltonian flow of a polynomial in normal form.

We will assume now that the step size h satisfies the following property:

Hypothesis 3.4 *For all $r \in \mathbb{N}$, there exist constants γ^* and α^* such that for all $K \in \mathbb{N}^*$,*

$$(j_1, \ldots, j_r) \in \mathcal{Z}_K^r \backslash \mathcal{A}_K^r \quad \Longrightarrow \quad |1 - e^{ih\Omega(\boldsymbol{j})}| \geq \frac{h\gamma^*}{K^{\alpha^*}}. \tag{3.10}$$

The following Lemma 3.6 (see [20, 23] for similar statements) shows that condition (3.10) is *generic* in the sense that it is satisfied for a large set of $h \leq h_0$ (and in particular *independently of* K), provided that the frequencies ω_a satisfy a non-resonance condition that we state now:

Hypothesis 3.5 *For all $r \in \mathbb{N}$, there exist constants $\gamma(r)$ and $\alpha(r)$ such that $\forall\, K \in \mathbb{N}^*$,*

$$(j_1, \ldots, j_r) \in \mathcal{Z}_K^r \backslash \mathcal{A}_K^r \quad \Longrightarrow |\Omega(\boldsymbol{j})| \geq \frac{\gamma}{K^{\alpha}}. \tag{3.11}$$

In the next section, we will check this condition in different concrete cases.

Lemma 3.6 *Assume that Hypothesis 3.5 holds, and let h_0 and r be given numbers. Let γ and α be such that (3.11) holds and assume that $\gamma^* \leq (2/\pi)\gamma$, $\alpha^* \geq \alpha + m\tau + r$ with $\tau > 1$ and m the constant appearing in (3.5), then we have*

$$\text{meas}\{\, h < h_0 \,|\, h \textit{ does not satisfy } (3.10)\,\} \leq C\frac{\gamma^*}{\gamma} h_0^{1+\tau}$$

where C depends on τ and r. As a consequence the set

$$Z(h_0) = \{\, h < h_0 \,|\, h \textit{ satisfies Hypothesis } 3.4\,\}$$

is a dense open subset of $(0, h_0)$.

Proof. Denote

$$\mathsf{R}(h_0, \gamma^*, \alpha^*) = \{\, h < h_0 \,|\, h \text{ does not satisfy } (3.10)\}.$$

Assume that $h \in \mathsf{R}(h_0, \gamma^*, \alpha^*)$. There exist $K > 1$ and $\boldsymbol{j} \notin \mathcal{A}_K^r$ such that

$$|j_1|, \ldots, |j_r| \leq K \quad \text{and} \quad |1 - e^{ih\Omega(\boldsymbol{j})}| < \frac{h\gamma^*}{K^{\alpha^*}}.$$

For this $\boldsymbol{j}$, there exist an $\ell \in \mathbb{Z}$ such that

$$|1 - e^{ih\Omega(\boldsymbol{j})}| \geq \frac{2}{\pi}|2\pi\ell - h\Omega(\boldsymbol{j})|. \tag{3.12}$$

If $\ell = 0$, the previous inequality and (3.11) imply

$$|1 - e^{ih\Omega(\boldsymbol{j})}| \geq \frac{2}{\pi} h \frac{\gamma}{K^\alpha}$$

which is impossible with the assumptions on γ^* and α^*. Hence, we can assume $\ell \neq 0$. Eqn. (3.12) implies

$$\frac{2|\Omega(\boldsymbol{j})|}{\pi}\Big|\frac{2\pi\ell}{\Omega(\boldsymbol{j})} - h\Big| < \frac{h\gamma^*}{K^{\alpha^*}}$$

and using (3.11)

$$\Big|\frac{2\pi\ell}{\Omega(\boldsymbol{j})} - h| \leq \frac{h\pi\gamma^*}{2\gamma}\frac{1}{K^{\alpha^*-\alpha}}.$$

Moreover, we have for this ℓ

$$|2\pi\ell - h\Omega(\boldsymbol{j})| \leq \pi$$

whence using (3.5)

$$2\pi|\ell| \leq \pi + Ch_0K^m$$

where C is a constant depending on r. This implies

$$|\ell| - \frac{1}{2} \leq \frac{C}{2\pi}h_0K^m.$$

Hence, $\mathsf{R}(h_0, \gamma^*, \alpha^*)$ is included in the union of balls of center

$$\frac{2\pi\ell}{\Omega(\boldsymbol{j})}, \quad \text{with} \quad |j_1|, \dots, |j_r| \leq K, \quad |\ell| - \frac{1}{2} \leq \frac{C}{2\pi}h_0K^m, \quad \ell \neq 0$$

and radius

$$\frac{h_0\pi\gamma^*}{2\gamma}\frac{1}{K^{\alpha^*-\alpha}}$$

Hence, we have for $\tau > 1$

$$\begin{aligned}
\text{meas}(\mathsf{R}(h_0, \gamma^*, \alpha^*)) &\leq \sum_{|j_i| \leq K} \sum_{|\ell| - \frac{1}{2} \leq \frac{C}{2\pi}h_0K^m} \frac{h_0\pi\gamma^*}{2\gamma}\frac{1}{K^{\alpha^*-\alpha}} \\
&\leq \sum_{|j_i| \leq K} \sum_{\ell \in \mathbb{Z}^*} \Big(\frac{1}{|\ell| - \frac{1}{2}}\Big)^\tau \frac{h_0\pi\gamma^*}{2\gamma}\frac{1}{K^{\alpha^*-\alpha-m\tau}}\Big(\frac{Ch_0}{2\pi}\Big)^\tau. \\
&\leq C\frac{\gamma^*}{\gamma}h_0^{1+\tau}\frac{1}{K^{\alpha^*-\alpha-m\tau-r}}.
\end{aligned}$$

Furthermore

$$\text{meas}(\cap_{\gamma^*>0}\mathsf{R}(h_0, \gamma^*, \alpha^*)) = 0$$

and thus $Z(h_0)$ has full measure. ■

4 Statement of the result and applications

4.1 Main results

Theorem 4.1 *Assume that $P^{(K)}$, the frequencies and $h < h_0$ satisfy the previous hypothesis (cf. (3.8) and (3.10)). Let $r \in \mathbb{N}^*$ be fixed. There exist positive constants σ, C and ε_0 depending only on r, h_0 and the constants $\beta(\ell)$ and $C(\ell)$, $\ell = 0, \dots r$ in (3.8), such that the following holds: For all $\varepsilon < \varepsilon_0$ and $K \leq \varepsilon^{-\sigma}$, and for all z^0 real such that*

$$\|z^0\| \leq \varepsilon$$

if we define

$$z^n = \big(\varphi^h_{H_0^{(K)}} \circ \varphi^h_{P^{(K)}}\big)^n (z^0) \tag{4.1}$$

then for all n, z^n is still real, and moreover

$$\|z^n\| \leq 2\varepsilon \quad \text{for} \quad n \leq \frac{1}{\varepsilon^{r-1}}, \tag{4.2}$$

and

$$\forall\, a \in \mathcal{N}_K, \quad |I_a(z^n) - I_a(z^0)| \leq C\varepsilon^{5/2} \quad \text{for} \quad n \leq \frac{1}{\varepsilon^{r-2}} \tag{4.3}$$

The proof of this result relies on the following Birkhoff normal form result, whose proof is postponed to Section 5:

Theorem 4.2 *Assume that $P^{(K)}$, the frequencies and $h < h_0$ satisfy hypothesis (3.8) and (3.10). Let $r \in \mathbb{N}^*$ be fixed. Then there exist constants β and C depending on r, h_0, $\beta(\ell)$ and $C(\ell)$, $\ell = 0, \dots r$ in (3.8) and a canonical transformation τ_K from $B_K(\rho)$ into $B_K(2\rho)$ with $\rho = (CK)^{-\beta}$ satisfying for all $z \in B_K(\rho)$,*

$$\|\tau_K(z) - z\| \leq (CK)^\beta \|z\|^2 \quad \text{and} \quad \|\tau_K^{-1}(z) - z\| \leq (CK)^\beta \|z\|^2, \tag{4.4}$$

satisfying the following result: For all $z \in B_K(\rho)$,

$$\tau_K^{-1} \circ \varphi^h_{H_0^{(k)}} \circ \varphi^h_{P^{(K)}} \circ \tau_K(z) = \varphi^h_{H_0^{(K)}} \circ \psi_K(z)$$

where ψ_K satisfies:

- *$\psi_K(z)$ is real if z is real,*
- *For all $z \in B_K(\rho)$,*

$$\|\psi_K(z) - z\| \leq (CK)^\beta \|z\|^2, \tag{4.5}$$

- *For all $z \in B_K(\rho)$,*

$$|I_a(\psi_K(z)) - I_a(z)| \le (CK)^\beta \|z\|^{r+1}. \tag{4.6}$$

Proof of Theorem 4.1. First, let us note that as the Hamiltonian functions $H_0^{(K)}$ and $P^{(K)}$ are real Hamiltonians, it is clear that there exist $\xi^n \in \mathbb{C}^{\mathcal{N}}$ such that for all n, we have $z^n = (\xi^n, \bar{\xi}^n)$, that is z^n is real.
Let β given by Theorem 4.2 and let $\sigma = 1/(2\beta)$. We have for $K \le \varepsilon^{-\sigma}$,

$$(CK)^\beta \le C^\beta \varepsilon^{-1/2}.$$

Let τ_K be defined by Theorem 4.2, and let $y^n = \tau_K^{-1}(z^n)$. Using the property of τ_K, we see that y^n is real, i.e. we have $y^n = (\zeta^n, \bar{\zeta}^n)$ for all n. By definition, we have

$$\forall\, n \ge 0, \quad y^{n+1} = \big(\varphi^h_{H_0^{(K)}} \circ \psi_K\big)(y^n). \tag{4.7}$$

Using the fact that $K \le \varepsilon^{-\sigma}$ and (4.4), the transformation τ_K in the previous Theorem satisfies the following: For all z such that $\|z\| \le 2\varepsilon$,

$$\|\tau_K^{-1}(z) - z\| \le C^\beta \varepsilon^{-1/2} \|z\|^2 \le 4C^\beta \varepsilon^{3/2} \le \tfrac{1}{4}\varepsilon \tag{4.8}$$

provided ε_0 is sufficiently small. Hence we have $\|y^0\| = \|\tau_K^{-1}(z^0)\| \le \frac{5}{4}\varepsilon$.
Note that we have $\rho = (CK)^{-\beta} \ge C^{-\beta}\varepsilon^{1/2} \ge 2\varepsilon$ provided that ε_0 is small enough. Using (4.5) we get that as long as $\|y^n\| \le 2\varepsilon$, we have

$$\|y^{n+1}\| \le \|y^n\| + (CK)^\beta \|y^n\|^r \le \|y^n\| + 2^r C^\beta \varepsilon^{r-1/2}$$

By induction, we thus see that for

$$n \le 2^{-r-1} C^{-\beta} \varepsilon^{3/2-r}$$

we have $\|y^n\| \le \frac{7}{4}\varepsilon \le 2\varepsilon$. Assuming that ε_0 is such that $2^{-r-1}C^{-\beta}\varepsilon_0^{1/2} \le 1$, this shows that for $n \le \varepsilon^{1-r}$ we have $\|y^n\| \le \frac{7}{4}\varepsilon$. Using (4.4) and an inequality similar to (4.8), we conclude that

$$\|z^n\| \le 2\varepsilon, \quad \text{for} \quad n \le \frac{1}{\varepsilon^{r-1}}$$

which yields to (4.2).
Now using (4.6) and the fact that $\|y^n\| \le 2\varepsilon$ we see that for $n \le \varepsilon^{1-r}$ we have

$$\forall\, a \in \mathcal{N}_K, \quad |I_a(y^{n+1}) - I_a(y^n)| \le 2^{r+1} C^\beta \varepsilon^{r+1/2}$$

whence

$$\forall\, a \in \mathcal{N}_K, \quad |I_a(y^n) - I_a(y^0)| \le 2^{r+1} C^\beta n \varepsilon^{r+1/2}$$

Now we have for all $a \in \mathcal{N}_K$

$$|I_a(y^n) - I_a(z^n)| = \big||\zeta_a^n|^2 - |\xi_a^n|^2\big| = \big||\zeta_a^n| - |\xi_a^n|\big| \times \big||\zeta_a^n| + |\xi_a^n|\big|,$$

whence

$$|I_a(y^n) - I_a(z^n)| \leq |\zeta_a^n - \xi_a^n|(\|y^n\| + \|z^n\|) \leq \|\tau_K(y^n) - y^n\| \, (\|y^n\| + \|z^n\|).$$

Using (4.4) we see that for all $n \leq \varepsilon^{1-r}$ and all $a \in \mathcal{N}_K$,

$$\|\tau_K(y^n) - y^n\| \leq 4C^\beta \varepsilon^{3/2}.$$

and hence, as $\|z^n\| \leq 2\varepsilon$,

$$|I_a(y^n) - I_a(z^n)| \leq 8C^\beta \varepsilon^{5/2}.$$

Using (4.8), we thus see that

$$\forall\, n \leq \varepsilon^{1-r} \quad \forall\, a \in \mathcal{N}_K, \quad |I_a(z^n) - I_a(z^0)| \leq 2^{r+4} C^\beta (\varepsilon^{5/2} + n\varepsilon^{r+1/2})$$

and this easily gives the result. ■

Remark 4.3 As usual in such procedure, the previous constructive proof yields a very small constant σ for large parameter r. The estimation of the optimal σ is a very difficult problem and may depend on the particular case considered. ■

4.2 Examples

In this section we present two examples, other examples like the Klein Gordon equation on the sphere (in the spirit of [3]) or the nonlinear Schrödinger operator with harmonic potential (in the spirit of [18]) could also be considered with these techniques.

4.2.1 Nonlinear Schrödinger equation

We first consider nonlinear Schrödinger equations of the form

$$i\partial_t \psi = -\Delta\psi + V \star \psi + \partial_2 g(\psi, \bar{\psi}), \quad x \in \mathbb{T}^d \tag{4.9}$$

where $V \in C^\infty(\mathbb{T}^d, \mathbb{R})$, $g \in C^\infty(\mathcal{U}, \mathbb{C})$ where $\mathcal{U}$ is a neighborhood of the origin in $\mathbb{C}^2$. We assume that $g(u, \bar{u}) \in \mathbb{R}$, and that $g(u, \bar{u}) = \mathcal{O}(|u|^3)$. The corresponding Hamiltonian functional is given by

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

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

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

the (abstract) Hamiltonian associated with the equation (4.9) can be formally written

$$H(\xi,\eta) = \sum_{a\in\mathbb{Z}^d} \omega_a \xi_a \eta_a + P(\xi,\eta). \tag{4.10}$$

Here $\omega_a = |a|^2 + \hat{V}_a$ are the eigenvalues of the operator

$$\psi \mapsto -\Delta\psi + V \star \psi,$$

and we see that ω_a satisfy (3.5) with $m = 2$. Moreover, the nonlinearity function $P(\xi,\eta)$ posesses a zero of order 3 at the origin. In this situation, it can be shown that the Hypothesis 3.4 is fulfilled for a large set of potential V (see for instance theorem 5.7 in [17]).

Following [14], a space discretization of this equation using spectral collocation methods yields a problem of the form (3.6) with

$$\mathcal{N}_K = [-K,\dots,K-1]^d$$

and, with

$$u_K = \Big(\frac{1}{2\pi}\Big)^{d/2} \sum_{a\in\mathcal{N}_K} \xi_a \phi_a(x) \quad \text{and} \quad v_K = \Big(\frac{1}{2\pi}\Big)^{d/2} \sum_{a\in\mathcal{N}_K} \eta_a \bar{\phi}_a(x) \tag{4.11}$$

the nonlinearity reads

$$P^{(K)}(\xi,\eta) = \int_{\mathbb{T}^d} \mathcal{Q}(g(u_K, v_K))\mathrm{d}x$$

where, for a function $\psi = (\frac{1}{2\pi})^{d/2} \sum_{a\in\mathbb{Z}^d} \psi_a \phi_a(x)$

$$\mathcal{Q}(\psi) = \sum_{a\in\mathcal{N}_K} \Big(\sum_{b\in\mathbb{Z}^d} \psi_{a+2Kb} \Big) \phi_a(x)$$

is the collocation operator associated with the points $x_a = a\frac{\pi}{K} \in \mathbb{T}^d$, $a \in \mathcal{N}_K$. It is easy to verify that $P^{(K)}$ satisfies (3.8) for some constants $C(\ell)$ depending on g and $\beta(\ell)$ depending on g and the dimension d.

Note that starting from a real initial value $u_K^0(x)$ (see (4.11)) this system reduces to solving the system of ordinary differential equation

$$\forall\, a \in \mathcal{N}_a \quad i\frac{\mathrm{d}}{\mathrm{d}t} u_K(x_a,t) = \mathcal{F}_{2K} \Omega \mathcal{F}_{2K}^{-1} u_K(x_a,t) + \partial_2 g(u_K(x_a,t), \overline{u_K(x_a,t)})$$

where Ω is the matrix $(\omega_a)_{a\in\mathcal{N}_K}$ and $\mathcal{F}_{2K}$ the Fourier transform associated with $\mathcal{N}_K$. In this case, the numerical solution (1.2) is easily implemented: The linear part is diagonal and can be solved explicitely in the Fourier space, while the nonlinear part is an ordinary differential equation with fixed parameter x_a at each step. If moreover $g(u, \bar{u}) = G(|u|^2)$ for some real function G then the solution of the nonlinear part is given explicitely by $\varphi^h_{P^{(K)}}(u) = \exp(-2ihG'(|u|^2))u$ using the fact that $|u|^2$ is constant for a fixed point x_a.

For high dimension d, the previous discretization is usually replaced by a discretization on sparse grid, i.e. with

$$\mathcal{N}_K = \{ a = (a_1, \ldots, a_d) \in \mathbb{Z}^d \mid (1 + |a_1|) \cdots (1 + |a_d|) \leq K \} \subset \mathbb{Z}^d.$$

As explained in [22, Chap III.1], methods exist to write the corresponding system under the symplectic form (3.6), upon a possible loss in the approximation properties of the exact solution of (4.9) by the solution of the discretized Hamiltonian $H^{(K)}$. Note that this does not influence the long time results proven here: In some sense we do not impose the nonlinearity $P^{(K)}(z)$ to approximate an exact nonlinearity $P(z)$.

We first give a numerical illustration of resonance effects. We consider the equation

$$i\partial_t \psi = -\Delta\psi + V \star \psi + \varepsilon^2 |\psi|^2 \psi$$

in the one dimensional torus $\mathbb{T}^1$, with initial value

$$\psi_0(x) = \frac{2}{2 - \cos(x)}.$$

Note that this problem is equivalent to solving (4.9) with a small initial value of order ε. We take $\varepsilon = 0.1$, V with Fourier coefficients $\hat{V}_a = 2/(10 + 2a^2)$ and $K = 200$ (i.e. 400 collocation points). In Figure 1, we plot the actions of the numerical solution given by the Lie splitting algorithm (1.2) in logarithmic scale. In the right we use the resonant stepsize $h = 2\pi/(\omega_7 - \omega_1) \simeq 0.17459\ldots$. In the left we plot the same result but with the non resonant stepsize $h = 0.174$.

In Figure 2, we show the long time almost conservation of the action in the case where $h = 0.1$ (non resonant), and $\varepsilon = 0.1$ and $\varepsilon = 0.01$ after 10^5 iterations.

4.2.2 Nonlinear wave equation

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

$$u_{tt} - u_{xx} + mu = g(u) , \quad x \in S^1 , \; t \in \mathbb{R} , \tag{4.12}$$

with Dirichlet boundary condition: $u(0, t) = u(\pi, t) = 0$ for any t. Here $m > 0$ is a constant and g is a C^∞ function in a neighbourhood of the origin in $\mathbb{R}$. We assume that g has a zero of order two at $u = 0$ in such a way that $g(u)$ appears, in the neighborhood of $u = 0$, as a perturbation term.

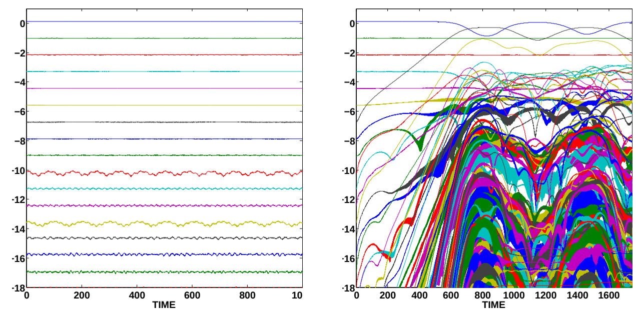

Figure 1: Plot of the actions for non-resonant and resonant step size.

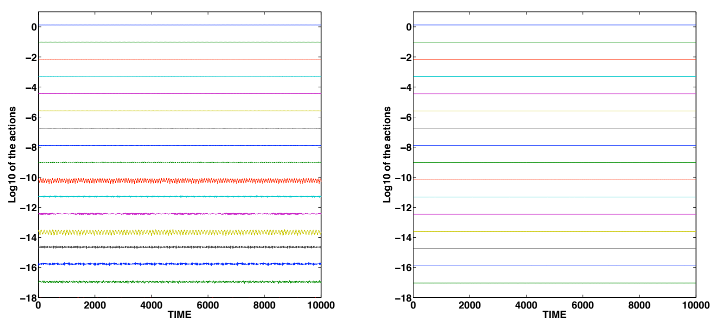

Figure 2: Conservation of the actions for $\varepsilon = 0.1$ (left) and $\varepsilon = 0.01$ (right).

Defining $v = u_t$, (4.12) reads

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

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

$$H(u,v) = \int_{S^1} \left(\frac{1}{2} v^2 + \frac{1}{2} u_x^2 + \frac{1}{2} mu^2 + G(x,u) \right) dx \tag{4.13}$$

where G is such that $\partial_u G = -g$, then (4.12) reads as an Hamiltonian system

$$\begin{aligned} \partial_t \begin{pmatrix} u \\ v \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -u_{xx} + mu + \partial_u G \\ v \end{pmatrix} \\ &= J \nabla_{u,v} H(u,v) \end{aligned} \tag{4.14}$$

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

Define the operator $A := (-\partial_{xx} + m)^{1/2}$, and introduce the variables (p, q) given by

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

Then, on $H^s(S^1) \times H^s(S^1)$ with $s \geq 1/2$, the Hamiltonian (4.13) takes the form $H_0 + P$ with

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

and

$$P(q,p) = \int_{S^1} G(x, A^{-1/2}q)dx$$

Now denote by $(\omega_a)_{a\in\mathbb{N}}$ the eigenvalues of A with Dirichlet boundary conditions and ϕ_a, $a \in \mathbb{N} =: \mathcal{N}$, the associated eigenfunctions. We have $\phi_a(x) = \sin ax$ and $\omega_a = \sqrt{a^2 + m}$.

Plugging the decompositions

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

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

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

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

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

the Hamiltonian function can be written under the form (4.10) with a nonlinearity depending on G. As in the previous case, it can be shown that the condition (3.11) is fulfilled for a set of constant m of full measure (see for instance Theorem 4.18 in [2]). A collocation discretization on equidistant points of $[0, 2\pi]$ yields the same kind of discretization as before (with $d = 1$).

In this situation, the symmetric Strang splitting scheme

$$\varphi^{h/2}_{P^{(K)}} \circ \varphi^{h}_{H_0^{(K)}} \circ \varphi^{h/2}_{P^{(K)}}$$

corresponds to the Deuflhard's method [10]. If moreover we consider the Hamiltonian

$$H^{(K)}(z) = H_0^{(K)}(z) + P^{(K)}(\Phi(h\Omega)z)$$

where Ω is the matrix with elements ω_a, $a \in \mathcal{N}_K$, and $\Phi(x)$ a smooth function that is real, bounded and such that $\Phi(0) = 1$, then the splitting schemes associated with this decomposition coincide with the symplectic mollified impulse methods (see [20, Chap. XIII] and [8]).

5 Proof of the normal form result

The rest of the paper consists in proving Theorem 4.2.

In the following, we denote by $\mathcal{T}_r$ the set of polynomial of order r on $\mathbb{C}^{\mathcal{Z}_K}$ (for sake of simplicity, we do note write the dependance in K in the notation $\mathcal{T}_r$). If

$$Q = \sum_{\ell=0}^{r} \sum_{\boldsymbol{j} \in \mathcal{Z}_K^\ell} Q_{\boldsymbol{j}} z_{\boldsymbol{j}}$$

is an element of $\mathcal{T}_r$, we set

$$|Q|_{\mathcal{T}_r} = \max_{\ell=0,\dots,r} \max_{\boldsymbol{j} \in \mathcal{Z}_K^\ell} |Q_{\boldsymbol{j}}|.$$

If moreover $Q \in \mathcal{C}([0,1], \mathcal{T}_r)$ we set

$$\|Q\|_{\mathcal{T}_r} = \max_{\lambda \in [0,1]} |Q(\lambda)|_{\mathcal{T}_r}.$$

Using the assumptions on $P^{(K)}$, we can write a Taylor expansion of P around 0,

$$P^{(K)}(z) = P_r + Q_r = \sum_{\ell=3}^{r} \sum_{\boldsymbol{j} \in \mathcal{Z}_K^\ell} P_{\boldsymbol{j}} z_{\boldsymbol{j}} + Q_r(z)$$

where

$$|P_{\boldsymbol{j}}| \leq C K^{\beta_0}$$

where C and β_0 depend on $\beta(\ell)$ and $C(\ell)$, $\ell = 0, \dots, r$ in (3.8).

Notice that $Q_r(z) \in \mathcal{C}^\infty(\mathbb{C}^{\mathcal{Z}_K}, \mathbb{C})$ admits a zero of order $r+1$ and satisfies

$$\|X_{Q_r}(z)\| \leq C K^{\beta_0} \|z\|^r$$

for $z \in \mathcal{U}_K$, provided $\beta_0 = \beta_0(r,d)$ is large enough.

Before giving the proof of Theorem 4.2, we give easy results on non autonomous polynomials Hamiltonian[1].

[1] In [13] we study the case $K = +\infty$ which requires much more elaborate tools about class of polynomials with infinite number of variables.

Lemma 5.1 *Let $k \geq 1$ and let $P(\lambda) \in \mathcal{C}([0,1], \mathcal{T}_{k+1})$ be a homogeneous polynomial of degree $k+1$ depending on $\lambda \in [0,1]$. Then*

(i) There exists a constant C depending on k such that for all $z \in \mathbb{C}^{\mathcal{Z}_K}$ and all $\lambda \in [0,1]$, we have

$$|P(\lambda, z)| \leq CK^{d(k+1)} \|P\|_{\mathcal{T}_{k+1}} \|z\|^{k+1}.$$

(ii) There exists a constant C depending on k such that for any $z \in \mathbb{C}^{\mathcal{Z}_K}$ and all $\lambda \in [0,1]$,

$$\|X_{P(\lambda)}(z)\| \leq CK^{d(k+1)} \|P\|_{\mathcal{T}_{k+1}} \|z\|^{k}.$$

Moreover, Let k_1 and k_2 two fixed integers. Let P and Q two homogeneous polynomials of degree k_1+1 and k_2+1 such that $P \in \mathcal{C}([0,1], \mathcal{T}_{k_1+1})$ and $Q \in \mathcal{C}([0,1], \mathcal{T}_{k_2+1})$. Then $\{P, Q\} \in \mathcal{C}([0,1], \mathcal{T}_{k_1+k_2})$ and we have

$$\|\{P, Q\}\|_{\mathcal{T}_{k_1+k_1}} \leq C \|P\|_{\mathcal{T}_{k_1+1}} \|Q\|_{\mathcal{T}_{k_2+1}}$$

for some constant C depending on k_1 and k_2.

Proof. We have

$$|P(\lambda, z)| \leq \|P\|_{\mathcal{T}_{k+1}} \sum_{\boldsymbol{j} \in \mathcal{Z}_K^{k+1}} |z_{\boldsymbol{j}}|$$

where we have set for $\boldsymbol{j} = (j_1, \ldots, j_\ell) \in \mathcal{Z}_K^\ell$,

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

Using $|z_j| \leq \|z\|$ we easily obtain *(i)* using $\sharp \mathcal{Z}_K \leq (2K+1)^d$. The second statement is proven similarly. The estimate on the Poisson brackets is trivial. ∎

Lemma 5.2 *Let $r \geq 3$,*

$$Q(\lambda, z) = \sum_{\ell=3}^{r} \sum_{\boldsymbol{j} \in \mathcal{Z}_K^\ell} Q_{\boldsymbol{j}}(\lambda) z_{\boldsymbol{j}}$$

be an element of $\mathcal{C}([0,1], \mathcal{T}_r)$. Let $\varphi^\lambda_{Q(\lambda)}$ be the flow associated with the non autonomous real Hamiltonian $Q(\lambda)$. Then there exists a constant C_r depending on r such that

$$\rho < \inf\big(1/2, C_r K^{-dr} \|Q\|_{\mathcal{T}_r}^{-1}\big) \quad \Longrightarrow \quad \forall \lambda \in [0,1], \quad \varphi^\lambda_{Q(\lambda)}(B_K(\rho)) \subset B_K(2\rho). \tag{5.1}$$

Moreover, if $F(\lambda) \in \mathcal{C}([0,1], \mathcal{C}^\infty(B_K(\rho), \mathbb{C}))$ has a zero of order r at the origin, then $F(\lambda) \circ \varphi^\lambda_{Q(\lambda)}$ has a zero of order r at the origin in $B_K(\rho)$.

Proof. Let $z^\lambda = \varphi^\lambda_{Q(\lambda)}(z^0)$. Using the estimates of the previous lemma, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\lambda}\|z^\lambda\|^2 &= 2\langle z^\lambda, X_{Q(\lambda)}(z^\lambda)\rangle \\ &\leq c_r K^{dr}\|Q\|_{\mathcal{T}_r}\|z^\lambda\|\left(\|z^\lambda\|^2 + \|z^\lambda\|^{r-1}\right)\end{aligned}$$

for some constant c_r depending on r. Hence, as long as $\|z^\lambda\| \leq 1$, we have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\|z^\lambda\|^2 \leq 2c_r K^{dr}\|Q\|_{\mathcal{T}_r}\|z^\lambda\|^3.$$

By a standard comparison argument, we easily get that for $z^0 \in B_K(\rho)$ we have

$$\forall\, \lambda \in [0,1], \quad \|z^\lambda\| \leq 2\|z^0\|.$$

This shows (5.1) and the rest follows. ∎

We now give the general strategy to prove the normal form Theorem 4.2, showing in particular the need of working with non autonomous Hamiltonians and of considering the non-resonance condition (3.10).

We consider a fixed step size h satisfying (3.10). As in this section K will be considered as fixed, we denote shortly $P^{(K)}$ by P and $H_0^{(K)}$ by H_0. We consider the propagator

$$\varphi^h_{H_0} \circ \varphi^h_P = \varphi^h_{H_0} \circ \varphi^1_{hP}.$$

We embed this application into the family of applications

$$\varphi^h_{H_0} \circ \varphi^\lambda_{hP}, \quad \lambda \in [0,1].$$

Formally, we would like to find a canonical change of variable, $\varphi^\lambda_{\chi(\lambda)}$, constructed as a time λ flow of a real Hamiltonian $\chi = \chi(\lambda)$ and a real Hamiltonian under normal form $Z = Z(\lambda)$ and such that

$$\forall\, \lambda \in [0,1] \quad \varphi^h_{H_0} \circ \varphi^\lambda_{hP} \circ \varphi^\lambda_{\chi(\lambda)} = \varphi^\lambda_{\chi(\lambda)} \circ \varphi^h_{H_0} \circ \varphi^\lambda_{hZ(\lambda)}. \tag{5.2}$$

Let $z^0 \in \mathbb{C}^{\mathcal{Z}_K}$ and $z^\lambda = \varphi^h_{H_0} \circ \varphi^\lambda_{hP} \circ \varphi^\lambda_{\chi(\lambda)}(z^0)$. Deriving the previous equation with respect to λ yields

$$\begin{aligned}\frac{\mathrm{d}z^\lambda}{\mathrm{d}\lambda} = (D_z\varphi^h_{H_0})_{\varphi^{-h}_{H_0}(z^\lambda)} X_{hP}(\varphi^{-h}_{H_0}(z^\lambda)) + \\ (D_z(\varphi^h_{H_0} \circ \varphi^\lambda_{hP}))_{\varphi^{-\lambda}_{hP}\circ\varphi^{-h}_{H_0}(z^\lambda)} X_{\chi(\lambda)}(\varphi^{-\lambda}_{hP} \circ \varphi^{-h}_{H_0}(z^\lambda)).\end{aligned}$$

Using Lemma 3.1 that remains obviously valid for non autonomous Hamiltonian, we thus have

$$\frac{\mathrm{d}z^\lambda}{\mathrm{d}\lambda} = X_{A(\lambda)}(z^\lambda)$$

where $A(\lambda)$ it the time dependent real Hamiltonian given by

$$A(\lambda) = hP \circ \varphi_{H_0}^{-h} + \chi(\lambda) \circ \varphi_{hP}^{-\lambda} \circ \varphi_{H_0}^{-h}.$$

Using the same calculations for the right-hand side, (5.2) is formally equivalent to the following equation (up to an integration constant)

$$\forall\, \lambda \in [0,1] \quad hP \circ \varphi_{H_0}^{-h} + \chi(\lambda) \circ \varphi_{hP}^{-\lambda} \circ \varphi_{H_0}^{-h} = \chi(\lambda) + hZ(\lambda) \circ \varphi_{\chi(\lambda)}^{-\lambda} \circ \varphi_{H_0}^{-h}. \quad (5.3)$$

which is equivalent to

$$\forall\, \lambda \in [0,1] \quad \chi(\lambda) \circ \varphi_{H_0}^{h} - \chi(\lambda) \circ \varphi_{hP}^{-\lambda} = hP - hZ(\lambda) \circ \varphi_{\chi(\lambda)}^{-\lambda}. \quad (5.4)$$

In the following, we will solve this equation in $\chi(\lambda)$ and $Z(\lambda)$ with a remainder term of order $r+1$ in z. So instead of (5.4), we will solve the equation

$$\forall\, \lambda \in [0,1] \quad \chi(\lambda) \circ \varphi_{H_0}^{h} - \chi(\lambda) \circ \varphi_{hP}^{-\lambda} = hP - (hZ(\lambda) + R(\lambda)) \circ \varphi_{\chi(\lambda)}^{-\lambda}. \quad (5.5)$$

where the unknown are $\chi(\lambda)$, and $Z(\lambda)$ are polynomials of order r, with Z under normal form, and where $R(\lambda)$ possesses a zero of order $r+1$ at the origin.

We formally write

$$\chi(\lambda) = \sum_{\ell=3}^{r} \chi_{[\ell]}(\lambda) := \sum_{\ell=3}^{r} \sum_{\boldsymbol{j} \in \mathcal{Z}_K^{\ell}} \chi_{\boldsymbol{j}}(\lambda) z_{\boldsymbol{j}}$$

and

$$Z(\lambda) = \sum_{\ell=3}^{r} Z_{[\ell]}(\lambda) := \sum_{\ell=3}^{r} \sum_{\boldsymbol{j} \in \mathcal{Z}_K^{\ell}} Z_{\boldsymbol{j}}(\lambda) z_{\boldsymbol{j}}$$

where here the coefficients $Z_{\boldsymbol{j}}(\lambda)$ are unknown and where we denote by $\chi_{[\ell]}(\lambda)$ and $Z_{[\ell]}(\lambda)$ the homogeneous part of degree ℓ in the polynomials $\chi(\lambda)$ and $Z(\lambda)$.

Identifying the coefficients of degree $\ell \leq r$ in equation (5.5), we obtain

$$\chi_{[\ell]}(\lambda) \circ \varphi_{H_0}^{h} - \chi_{[\ell]}(\lambda) = hP_{[\ell]} - hZ_{[\ell]}(\lambda) + hG_{[\ell]}(\lambda; \chi_*, P_*, Z_*).$$

where G is a real Hamiltonian homogeneous of degree ℓ depending on the polynomials $\chi_{[k]}$, $P_{[k]}$ and $Z_{[k]}$ for $k < \ell$. In particular, its coefficients are polynomials of order $\leq \ell$ of the coefficients χ_j, P_j and Z_j for $j \in \mathcal{Z}_K^k$, $k < \ell$.

Writing down the coefficients, this equation is equivalent to

$$\forall\, \boldsymbol{j} \in \mathcal{Z}_K^r \quad (e^{ih\Omega(\boldsymbol{j})} - 1)\chi_{\boldsymbol{j}} = hP_{\boldsymbol{j}} - hZ_{\boldsymbol{j}} + hG_{\boldsymbol{j}}$$

and hence we see that the key is to control the small divisors $e^{ih\Omega(\boldsymbol{j})} - 1$ in order to solve these equations recursively.

We first give two results on the change of variables generated by the flow of a non autonomous real Hamiltonian.

Lemma 5.3 *Let $\chi(\lambda)$ be an element of $\mathcal{C}([0,1],\mathcal{T}_r)$. Let $\tau(\lambda) := \varphi^{\lambda}_{\chi(\lambda)}$ be the flow associated with the non autonomous real Hamiltonian $\chi(\lambda)$. Let $g \in \mathcal{C}([0,1],\mathcal{T}_r)$, then we can write for all $\sigma_0 \in [0,1]$,*

$$g(\sigma_0)\circ\tau(\sigma_0) = g(\sigma_0) + \sum_{k=0}^{r-1}\int_0^{\sigma_0}\cdots\int_0^{\sigma_k}\Big(\mathrm{Ad}_{\chi(\sigma_k)}\circ\cdots\circ\mathrm{Ad}_{\chi(\sigma_1)}g(\sigma_0)\Big)\mathrm{d}\sigma_1\cdots\mathrm{d}\sigma_k + R(\sigma_0) \quad (5.6)$$

where by definition $\mathrm{Ad}_P(Q) = \{Q,P\}$

$$R(\sigma_0) = \int_0^{\sigma_0}\cdots\int_0^{\sigma_r}\Big(\mathrm{Ad}_{\chi(\sigma_r)}\circ\cdots\circ\mathrm{Ad}_{\chi(\sigma_1)}g(\sigma_0)\Big)\circ\tau(\sigma_r)\,\mathrm{d}\sigma_1\cdots\mathrm{d}\sigma_r. \quad (5.7)$$

Each term in the sum in Eqn. (5.6) belongs (at least) to the space $\mathcal{C}([0,1],\mathcal{T}_{kr})$. The term $R(\sigma_0)$ defines an element of $\mathcal{C}([0,1],\mathcal{C}^\infty(\mathbb{C}^{\mathcal{Z}_K},\mathbb{C}))$ and has a zero of order at least $r+1$ at the origin.

The classical proof of this lemma is for instance given in [13].

As mentioned previously, for a given polynomial $\chi \in \mathcal{C}([0,1],\mathcal{T}_r)$ with $r \geq 3$, we use the following notation

$$\chi(\lambda,z) = \sum_{\ell=3}^{r}\chi_{[\ell]}(\lambda) = \sum_{\ell=3}^{r}\sum_{\boldsymbol{j}\in\mathcal{Z}_K^\ell}\chi_{\boldsymbol{j}}(\lambda)z_{\boldsymbol{j}} \quad (5.8)$$

where $\chi_{[\ell]}(\lambda) \in \mathcal{C}([0,1],\mathcal{T}_r)$ is a homogeneous polynomial of degree ℓ. We now precise the result of Lemma 5.3:

Proposition 5.4 *Let $\chi(\lambda)$ be an element of $\mathcal{C}([0,1],\mathcal{T}_r)$ having a zero of order at least 3 at the origin. Let $\varphi^{\lambda}_{\chi(\lambda)}$ be the flow associated with the non autonomous real Hamiltonian $\chi(\lambda)$. Let $g \in \mathcal{C}([0,1],\mathcal{T}_r)$, then we can write for all $\lambda \in [0,1]$,*

$$g(\lambda)\circ\varphi^{\lambda}_{\chi(\lambda)} = S^{(r)}(\lambda) + T^{(r)}(\lambda)$$

where

- $S^{(r)}(\lambda) \in \mathcal{C}([0,1],\mathcal{T}_r)$. *Moreover, if we write*

$$S(z) = \sum_{\ell=3}^{r} S_{[\ell]}(\lambda)$$

where $S_{[\ell]}(\lambda)$ is a homogeneous polynomial of degree ℓ, then we have for all $\ell = 3,\dots,r$,

$$S_{[\ell]}(\lambda) = g_{[\ell]}(\lambda) + G_{[\ell]}(\lambda;\chi_*,g_*)$$

where $G_{[\ell]}(\lambda;\chi_*,g_*)$ is a homogeneous polynomial depending on λ and the coefficients S_j are polynomials of order $< \ell$ of the coefficients appearing in the decomposition of g and χ. Moreover, we have

$$\|G_{[\ell]}(\lambda;\chi_*,g_*)\| \le \Big(1+\sum_{m=3}^{\ell-1}\|g_{[m]}\|^{\ell}\Big)\Big(1+\sum_{m=3}^{\ell-1}\|\chi_{[m]}\|^{\ell}\Big). \tag{5.9}$$

- *$T^{(r)}(\lambda) \in \mathcal{C}([0,1],\mathcal{C}^\infty(\mathbb{C}^{\mathcal{Z}_K},\mathbb{C}))$ has a zero of order at least $r+1$ at the origin and satisfies for all $z \in B_K(1/2)$,*

$$\|X_{T^{(r)}(\lambda)}(z)\| \le C_r K^{2rd} C_r(\chi_*,g_*)\|z\|^r$$

where

$$C_r(\chi_*,g_*) \le C\Big(1+\sum_{m=3}^{r}\|g_{[m]}\|_{\mathcal{T}_r}^{r}\Big)\Big(1+\sum_{m=3}^{r}\|\chi_{[m]}\|_{\mathcal{T}_r}^{r}\Big) \tag{5.10}$$

with C depending on r.

Proof. Using the previous lemma, we define $S^{(r)}$ as the polynomial part of degree less or equal to r in the expression (5.6): this polynomial part may be computed iteratively, from the homogeneity degree 3 to r. Actually, every Poisson bracket appearing in (5.6) is taken with a polynomial $\chi(\sigma_k)$, which decomposes into homogeneous polynomials with degree 3 at least. The terms appearing in the sum in (5.6) hence have an increasing valuation, and this allows the iterative computation. The remainder terms, together with the term $R(\lambda)$ in (5.7), define the term $T^{(r)}$ (which is an element of $\mathcal{C}([0,1],\mathcal{T}_{2r})$). The properties of $S^{(r)}(\lambda)$ and $T^{(r)}(\lambda)$ are then easily shown using Lemma 5.1. ∎

The next result (Proposition 5.5 below) yields the construction of the *normal form* term ψ_K of Theorem 4.2.

Proposition 5.5 *Assume that $H := H^{(K)}$ satisfies (3.6) with $P := P^{(K)}$ fulfilling (3.8) and assume that $h \le h_0$ satisfies the hypothesis (3.10). Then there exist*

- *a polynomial $\chi \in \mathcal{C}([0,1],\mathcal{T}_r)$*

$$\chi(\lambda) = \sum_{\ell=3}^{r}\chi_{[\ell]}(\lambda) := \sum_{\ell=3}^{r}\sum_{\boldsymbol{j}\in\mathcal{Z}_K^\ell}\chi_{\boldsymbol{j}}(\lambda)z_{\boldsymbol{j}}$$

- *a polynomial $Z \in \mathcal{C}([0,1],\mathcal{T}_r)$*

$$Z(\lambda) = \sum_{\ell=3}^{r} Z_{[\ell]}(\lambda) := \sum_{\ell=3}^{r}\sum_{\boldsymbol{j}\in\mathcal{A}_K^\ell} Z_j(\lambda)z_{\boldsymbol{j}}$$

in normal form,

- *a function $R(\lambda) \in \mathcal{C}([0,1], \mathcal{C}^\infty(B_K(\rho), \mathbb{C}))$ with $\rho < c_0 K^{-\beta}$ for some constant $c_0 > 0$ and $\beta > 1$ depending on r and d, and having a zero of order at least $r+1$ at the origin*

such that the following equation holds:

$$\forall\, \lambda \in [0,1] \quad \chi(\lambda) \circ \varphi^h_{H_0} - \chi(\lambda) \circ \varphi^{-\lambda}_{hP} = hP - (hZ(\lambda) + R(\lambda)) \circ \varphi^{-\lambda}_{\chi(\lambda)}. \tag{5.11}$$

Furthermore there exists a constant C_0 depending on r and d such that

$$\|\chi\|_{\mathcal{I}_r} + \|Z\|_{\mathcal{I}_r} \leq C_0 K^\beta$$

and such that for all $\rho < c_0 K^{-\beta}$ and all $z \in B_K(\rho)$, we have

$$\forall\, \lambda \in [0,1], \quad \|X_{R(\lambda)}(z)\| \leq C_0 K^\beta \|z\|^r.$$

Proof. Identifying the coefficients of degree $\ell \leq r$ in the equation (5.11), we get

$$\chi_{[\ell]} \circ \varphi^h_{H_0} - \chi_{[\ell]} = hP_{[\ell]} - hZ_{[\ell]} + hG_{[\ell]}(\chi_*, P_*, Z_*).$$

where G is a real Hamiltonian homogeneous of degree ℓ depending on the polynomials $\chi_{[k]}$, $P_{[k]}$ and $Z_{[k]}$ for $k < \ell$. In particular, its coefficients are polynomials of order $\leq \ell$ of the coefficients $\chi_{\boldsymbol{j}}$, $P_{\boldsymbol{j}}$ and $Z_{\boldsymbol{j}}$ for $\boldsymbol{j} \in \mathcal{Z}^k_K$, $k < \ell$ and satisfy bounds like (5.9). Writing down the coefficients, this equation is equivalent to

$$\forall\, \boldsymbol{j} \in \mathcal{I}_r \quad (e^{ih\Omega(\boldsymbol{j})} - 1)\chi_{\boldsymbol{j}} = hP_{\boldsymbol{j}} - hZ_{\boldsymbol{j}} + hG_{\boldsymbol{j}}.$$

We solve this equation by setting

$$Z_{\boldsymbol{j}} = P_{\boldsymbol{j}} + G_{\boldsymbol{j}} \quad \text{and} \quad \chi_{\boldsymbol{j}} = 0 \quad \text{for} \quad \boldsymbol{j} \in \mathcal{A}^\ell_K$$

and

$$Z_{\boldsymbol{j}} = 0 \quad \text{and} \quad \chi_{\boldsymbol{j}} = \frac{h}{e^{ih\Omega(\boldsymbol{j})} - 1}(P_{\boldsymbol{j}} + G_{\boldsymbol{j}}) \quad \text{for} \quad \boldsymbol{j} \notin \mathcal{A}^\ell_K.$$

Using (3.10) and the result of Proposition 5.4 we get the claimed bound for some β depending on r.

To define R, we simply define it by the equation (5.11). By construction and the assumption on $P = P^{(K)}$, and using bounds of the form (5.10), it is easy to show that it satisfies the hypothesis. ■

Proof of Theorem 4.2. Integrating the equation (5.11) in λ, it is clear that the following equation holds:

$$\forall\, \lambda \in [0,1] \quad \varphi^h_{H_0} \circ \varphi^\lambda_{hP} \circ \varphi^\lambda_{\chi(\lambda)} = \varphi^\lambda_{\chi(\lambda)} \circ \varphi^h_{H_0} \circ \varphi^\lambda_{hZ(\lambda)+R(\lambda)}.$$

Note that using Proposition 5.4 and (5.1) we show that for $z \in B_K(\rho)$ with $\rho = cK^{-\beta}$ we have

$$\|\varphi^\lambda_{\chi(\lambda)}(z) - z\| \leq CK^\beta \|z\|^2.$$

This implies in particular that

$$\|z\| \leq \|\varphi^{\lambda}_{\chi(\lambda)}(z)\| + CK^{-\beta}\|z\|$$

For K sufficiently large, this shows that $\varphi^{\lambda}_{\chi(\lambda)}$ is invertible and maps $B_K(\rho)$ to $B_K(2\rho)$. Moreover, we have the estimate, for all $\lambda \in [0,1]$,

$$\|\big(\varphi^{\lambda}_{\chi(\lambda)}\big)^{-1}(z) - z\| \leq CK^{\beta}\|z\|^2 .$$

We then define $\tau_K = \varphi^1_{\chi(\lambda)}$ and $\psi_K = \varphi^1_{hZ(\lambda)+R(\lambda)}$ and verify that these applications satisfy the condition of the theorem for suitable constants C and β. ■

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