Birkhoff normal form for splitting methods applied to semi linear Hamiltonian PDEs. Part II: Abstract splitting

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May 16, 2009

Abstract

We consider Hamiltonian PDEs that can be split into a linear unbounded operator and a regular non linear part. We consider abstract splitting methods associated with this decomposition where no discretization in space is made. We prove a normal form result for the corresponding discrete flow under generic non resonance conditions on the frequencies of the linear operator and on the step size, and under a condition of zero momentum on the nonlinearity. This result implies the conservation of the regularity of the numerical solution associated with the splitting method over arbitrary long time, provided the initial data is small enough. This result holds for *rounded* numerical schemes avoiding at each step possible high frequency energy drift. We apply these results to nonlinear Schrödinger equations as well as the nonlinear wave equation.

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1 Introduction

This work is the second part of a series of two (see [11]). We consider a class of Hamiltonian partial differential equations whose Hamiltonian functions $H = H_0 + P$ can be divided into a linear unbounded operator H_0 with discrete spectrum and a non linear function P having a zero of order at least 3 at the origin of the phase space. Typical examples are given by the non linear wave equation on a segment with Dirichlet boundary conditions or the non linear Schrödinger equation on the torus. In this second part, we assume moreover that P satisfies a zero momentum property (see below for a definition and a discussion of this property).

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 schemes is based on the approximation

$$\varphi_H^h \simeq \varphi_{H_0}^h \circ \varphi_P^h \tag{1.1}$$

for small time h, and where φ_Q^t denotes the exact flow of the Hamiltonian PDE associated with the Hamiltonian Q. In this second paper, we consider splitting methods (1.1) without space discretization (abstract splitting), while the first part [11] deals with space discretizations of this scheme.

The understanding of the long-time behavior of numerical methods applied to Hamiltonian PDEs is a fundamental ongoing challenge in the field of geometric integration, as the classical arguments of backward error analysis (see for instance [18]) do not applied in this situation where the frequencies of the system are arbitrary large, and where resonances phenomenon are known to occur for some values of the step size. We refer to [10, 8, 17, 6, 13, 14] and the the introduction of [11] for a review.

As in the first part, we use normal form techniques to address the question of the long time preservation of the regularity of the numerical solutions associated with (1.1). Normal form techniques have proven to be one of the most important tool for the understanding of the long time behaviour of Hamiltonian PDE (see [1, 4, 15, 2, 3, 16]). 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 one dimension [4], Klein Gordon equation on spheres or Zoll manifolds [3] or nonlinear quantum harmonic oscillator on \mathbb{R}^d [16]).

In this paper, we mainly show that the same kind of results hold true for nu-merical solutions associated with the abstract splitting method (1.1) under some further restrictions specifically induced by the time discretization, but without any restriction on the space discretization parameter.

In the first part [11], we consider full discretizations of the Hamiltonian PDE, with a spectral discretization parameter K. We show that under the hypothesis $K \leq \varepsilon^{-\sigma}$ for some constant σ depending on the precision degree r, the same conclusions as in the continuous case can be drawn.

In some sense, the present paper 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, 15, 2]. However, instead of being valid for the (exact) abstract splitting (1.1), we have to consider rounded splitting methods of the form

$$\Pi_{\eta,s} \circ \varphi_{H_0}^h \circ \varphi_P^h \tag{1.2}$$

where $\Pi_{\eta,s}$ puts to zero all the modes ξ_j whose weighted energy $|j|^{2s}|\xi_j|^{2s}$ in the Sobolev space H^s is smaller than a given threshold η^2 . Hence, for small η , (1.2) is very close to the exact splitting method (1.1). The good news is that this threshold can be taken of the order ε^r , making this projection $\Pi_{\eta,s}$ very close to the identity.

The reasons for these restrictions in comparison with the continuous case are explained in the Section 2 of the first part [11]. They can be summarized as follows: In contrast with [4], the search for a normal form for the discrete flow (1.1) requires the control of small divisors of the form

$$e^{ih\Omega(\boldsymbol{j},\boldsymbol{k})} - 1 \tag{1.3}$$

where $\mathbf{j} = (j_1, \dots, j_p) \in \mathbb{N}^p$ and $\mathbf{k} = (k_1, \dots, k_q) \in \mathbb{N}^q$ are multi-indices, and where

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

are precisely the small divisors to be controlled in the continuous case (here the ω_j are the frequencies of the linear operator H_0). The non resonance condition used in [4] is of the form

$$\forall j \neq k, \quad |\Omega(j,k)| \ge \gamma \mu(j,k)^{-\alpha}$$
 (1.4)

where $\mu(j, k)$ denotes the third largest integer amongst $|j_1|, \ldots, |k_q|$. In this latter work, the authors show that such a condition is actually guaranteed in a large number of situations (see [4], [15] or [2] for precise results). In contrast, such a condition involving the third largest integer for the small divisors (1.3) turns out to be non generic with respect to h. Indeed in this case we cannot control the small divisors $|e^{ih\Omega(j,k)}-1|$ associated with the splitting scheme by the third largest integer in the multi index, but by the largest (see Hypothesis 3.4 and Lemma 3.6 in [11]).

In the continuous case (see for instance [4] and the Section 2 of [11]), in order to transform the original Hamiltonian $H_0 + P$ to the form $H_0 + Z + R$ where Z is the normal form term and R a polynomial having a zero of order r + 1, the following argument is used: a monomial containing at least three large indices among (j, k) has a vector field that is already small (in Sobolev norms). Hence the control of the small divisors with respect to the third largest index (cf. (1.4)) allows to construct the normal form: if (j, k) contains at least three large indices it is not necessary to solve the homological equation (the corresponding term is already small) and on the other hand if the third largest index among (j, k) is not large, then the small divisor is not so small and the homological equation can be solved.

In our case, with a control of the small divisors with respect to the largest index, the only solution is to put in the normal form Z the monomials containing at least *one* large index.

To control these terms, we assume a zero momentum property: all the monomials appearing in the procedure contain terms with indices (j, k) where $j = (j_1, \ldots, j_p) \in \mathbb{N}^p$ and $k = (k_1, \ldots, k_q) \in \mathbb{N}^q$ such that

$$\mathcal{M}(j, k) := j_1 + j_2 + \dots + j_p - k_1 - \dots - k_q = 0.$$
 (1.5)

This implies that if one index among (j, k) is large then necessarily an other index is also large (see Lemma 4.2). That is why, using a generic condition on $h \leq h_0$, we can prove a normal form result and show that the flow is conjugated to the flow of a Hamiltonian vector field of the form $H_0 + Z + R$ where R has a zero of order r + 1, but where Z now contains terms depending only on the actions, and supplementary terms containing at least two large indices. Here, large means greater than $\varepsilon^{-\sigma}$ where σ depends on r.

The normal form result that we obtain can be interpreted as follows: the non conservation of the actions can only come from two high modes (of order greater

than $\varepsilon^{-\sigma}$) interacting together and contaminating the whole spectrum. The role of the projection operator $\Pi_{\eta,s}$ is to destroy these high modes at each step but only when these high modes have an energy smaller than η (cf. (2.13)). Then, in our main result (Theorem 3.2), we assume that the initial data z^0 has all its high modes equal to zero (see Remark 3.4) and we verify that this property is preserved by the flow (1.2). That is, the projection $\Pi_{\eta,s}$ avoids possible high frequency energy drift. As we can take $\eta = \varepsilon^r$, the error induced in comparison with the exact splitting is very small¹.

We end this introduction with two comments on the possible extensions of our result. As explained before, the zero momentum property is crucial to the normal form reduction. In the examples described in section 3.2, this property is easily obtained because the basis of eigenfunctions of the linear part of the PDE is the Fourier basis and because a nonlinearity of the form

$$\int_{\mathbb{T}} g(\sum \xi_j e^{ijx}, \sum \eta_k e^{-ikx}) dx$$

has the zero momentum property. Clearly this situation is not generic. Therefore in order to extend our result to other examples, we would have to relax the zero momentum property. Actually we guess that a condition of the type

$$|G_{ik}| < be^{-a\mathcal{M}(j,k)}$$

for some constants a, b > 0 could be sufficient and of course much more generic.

We also notice that, in this present form, our results apply only to non resonant Hamiltonian PDEs (see section 3.2). 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 in the spirit of [16].

The structure of the present paper follows the lines of the first part. However, the use of infinite dimensional objects requires the introduction of specific tools developed in the next section (see also [1, 15]). To avoid any confusion and for ease of presentation we have sometimes written down results that look very close to the ones given in the first part [11], but are in nature very different. In [11] we actually take the advantage of the restriction $K \leq \varepsilon^{-\sigma}$ to work only in L^2 norm while here the natural spaces are Sobolev space H^s with large s.

¹and may in particular be beyond the round-off error in numerical simulations.

2 Setting of the problem

2.1 Abstract Hamiltonian formalism

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

$$|a|^2 = \max(1, a_1^2 + \dots + a_d^2).$$

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

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

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

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

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

For a given real number $s \geq 0$, we consider the Hilbert space $\mathcal{P}_s = \ell_s(\mathcal{Z}, \mathbb{C})$ made of elements $z \in \mathbb{C}^{\mathcal{Z}}$ such that

$$||z||_s^2 := \sum_{j \in \mathcal{Z}} |j|^{2s} |z_j|^2 < \infty,$$

and equipped with the symplectic form (2.1).

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

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

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

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

Let H(z) be a function defined on \mathcal{U} . 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 \mathcal{P}_s induced by the symplectic form (2.1). For two functions F and G, the Poisson Bracket is defined as

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

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

Definition 2.1 Let $s \geq 0$, and let \mathcal{U} be a neighborhood of the origin in \mathcal{P}_s . We denote by $\mathcal{H}^s(\mathcal{U})$ the space of real Hamiltonians P satisfying

$$P \in \mathcal{C}^{\infty}(\mathcal{U}, \mathbb{C}), \quad and \quad X_P \in \mathcal{C}^{\infty}(\mathcal{U}, \mathcal{P}_s).$$

Notice that $H_0 \notin \mathcal{H}^s$ but we will consider nonlinearities that belongs to \mathcal{H}^s . With a given Hamiltonian function H, we associate the Hamiltonian system

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

which can be written

$$\begin{cases}
\dot{\xi}_{a} = -i\frac{\partial H}{\partial \eta_{a}}(\xi, \eta) & a \in \mathcal{N} \\
\dot{\eta}_{a} = i\frac{\partial H}{\partial \xi_{a}}(\xi, \eta) & a \in \mathcal{N}.
\end{cases}$$
(2.2)

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

$$\dot{\xi}_a = -i\frac{\partial H}{\partial \eta_a}(\xi, \bar{\xi}), \quad a \in \mathcal{N}.$$
 (2.3)

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

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

the system (2.3) is 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 $H(q, p) = H(\xi, \bar{\xi})$.

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

$$(D_z \tau^t)_z^T J (D_z \tau^t)_z = J \tag{2.4}$$

where D_z denotes the derivative with respect to the initial conditions. The following result is classic:

Lemma 2.2 Let \mathcal{U} and \mathcal{W} be two domains of \mathcal{P}_s , and let $\tau = \varphi_{\chi}^1 \in \mathcal{C}^{\infty}(\mathcal{U}, \mathcal{W})$ be the flow of the real hamiltonian χ . Then for $K \in \mathcal{H}^s(\mathcal{W})$, we have

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

Moreover, if K is a real hamiltonian, $K \circ \tau$ is a real hamiltonian.

2.2 Function spaces

We describe now the hypothesis needed on the Hamiltonian H.

Let $\ell \geq 3$. We consider $\mathbf{j} = (j_1, \dots, j_\ell) \in \mathcal{Z}^\ell$, and we set for all $i = 1, \dots l$ $j_i = (a_i, \delta_i)$ where $a_i \in \mathcal{N}$ and $\delta_i \in \{\pm 1\}$. We define

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

We also use the notation

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

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

$$\mathcal{M}(j) = a_1 \delta_1 + \dots + a_{\ell} \delta_{\ell}. \tag{2.5}$$

We then define the set of indices with zero momentum

$$\mathcal{I}_{\ell} = \{ \boldsymbol{j} = (j_1, \dots, j_{\ell}) \in \mathcal{Z}^{\ell}, \text{ with } \mathcal{M}(\boldsymbol{j}) = 0 \}.$$
 (2.6)

We can now define precisely the zero momentum property:

Definition 2.3 We say that a Hamiltonian P has the zero momentum property if its Taylor's polynomials exhibit only monomials $a_{\mathbf{j}}z_{\mathbf{j}}$ having zero momentum, i.e. such that $\mathcal{M}(\mathbf{j}) = 0$ when $a_{\mathbf{j}} \neq 0$ and thus P formally reads

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

Let $\ell \geq 3$ be a given integer. For $\mathbf{j} = (j_1, \dots, j_r) \in \mathbb{Z}^r$, we define $\mu(\mathbf{j})$ as the third largest integer between $|j_1|, \dots, |j_r|$. Then we set $S(\mathbf{j}) = |j_{i_r}| - |j_{i_{r-1}}| + \mu(\mathbf{j})$ where $|j_{i_r}|$ and $|j_{i_{r-1}}|$ denote the largest and the second largest integer between $|j_1|, \dots, |j_r|$.

We recall the following definition from [15].

Definition 2.4 Let $k \geq 3$, M > 0 and $\nu \in [0, +\infty)$, and let

$$Q(z) = \sum_{\ell=3}^{k} \sum_{j \in \mathcal{I}_{\ell}} Q_{j} z_{j}.$$

We say that $Q \in \mathcal{T}_k^{M,\nu}$ if there exists a constant C depending on M such that

$$\forall \ell = 3, \dots, k, \quad \forall j \in \mathcal{I}_{\ell}, \quad |Q_{j}| \le C \frac{\mu(j)^{M+\nu}}{S(j)^{M}}.$$
 (2.7)

Note that Q is a real Hamiltonian if and only if

$$\forall \ell = 3, \dots, k, \quad \forall j \in \mathcal{I}_{\ell}, \quad Q_j = \overline{Q}_{\overline{j}}.$$
 (2.8)

We have that $\mathcal{T}_k^{M,\nu} \in \mathcal{H}^s$ for $s \ge \nu + 1/2$ (see [15]). The best constant in the inequality (2.7) defines a norm $|Q|_{\mathcal{T}_k^{M,\nu}}$ for which $\mathcal{T}_k^{M,\nu}$ is a Banach space. We set

$$T_k^{\infty,\nu} = \bigcap_{M \in \mathbb{N}} \mathcal{T}_k^{M,\nu}.$$

Definition 2.5 A function P is in the class T if

- P is a real hamiltonian and exhibits a zero of order at least 3 at the origin.
- P satisfies the zero momentum property.
- There exists $s_0 \ge 0$ such that for any $s \ge s_0$, $P \in \mathcal{H}^s(\mathcal{U})$ for some neighborhood \mathcal{U} of the origin in \mathcal{P}_s .
- For all $k \geq 1$, there exists $\nu \geq 0$ such that the Taylor expansion of degree k of P around the origin belongs to $\mathcal{T}_k^{\infty,\nu}$.

With previous notations, we consider in the following Hamiltonian functions of the form

$$H(z) = H_0(z) + P(z) = \sum_{a \in \mathcal{N}} \omega_a I_a(z) + P(z),$$
 (2.9)

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

$$I_a(z) = \xi_a \eta_a$$

are the *actions* associated with $a \in \mathcal{N}$ and where $\omega_a \in \mathbb{R}$ are frequencies satisfying

$$\forall a \in \mathcal{N}, \quad |\omega_a| \le C|a|^m \tag{2.10}$$

for some constants C > 0 and m > 0. The Hamiltonian system (2.2) can hence be written

$$\begin{cases}
\dot{\xi}_{a} = -i\omega_{a}\xi_{a} - i\frac{\partial P}{\partial \eta_{a}}(\xi, \eta) & a \in \mathcal{N} \\
\dot{\eta}_{a} = i\omega_{a}\eta_{a} + i\frac{\partial P}{\partial \xi_{a}}(\xi, \eta) & a \in \mathcal{N}.
\end{cases} (2.11)$$

2.3 Rounded splitting methods

When considering the numerical simulation of such Hamiltonian system, many methods can be interpreted as splitting methods associated with the decomposition (2.9). This means that for small step size h, we approximate the flow φ_H^h by the composed flow

$$\varphi_H^h \simeq \varphi_{H_0}^h \circ \varphi_P^h$$
.

For a given time t, and a small step size h with t = nh, the approximation of φ_H^t is then written

$$\varphi_H^t \simeq \left(\varphi_{H_0}^h \circ \varphi_P^h\right)^n.$$
(2.12)

We give examples of such schemes in the next section.

In order to control the possible numerical instabilities due to the interaction of high frequencies, we introduce the following projection operator: Let $\eta>0$ and s be given, we define

$$\Pi_{n,s}:\mathcal{P}_s\to\mathcal{P}_s$$

by the formula

$$\forall j \in \mathcal{Z}, \quad \left(\Pi_{\eta, s} z\right)_{j} = \begin{cases} z_{j} & \text{if } |j|^{s} |z_{j}| \geq \eta \\ 0 & \text{if } |j|^{s} |z_{j}| < \eta. \end{cases}$$
 (2.13)

The goal of this paper is the studying of the long-time behavior of *rounded* splitting schemes associated with the operator

$$\Pi_{\eta,s} \circ \varphi_{H_0}^h \circ \varphi_P^h$$

to which we associate the numerical solution

$$z^{n} = \left(\Pi_{\eta,s} \circ \varphi_{H_0}^{h} \circ \varphi_{P}^{h}\right)^{n} (z^{0}). \tag{2.14}$$

Obviously, for $\eta = 0$, $\Pi_{\eta,s}$ is the identity operator.

In the following, we show a normal form result on the abstract splitting method

$$\varphi_{H_0}^h \circ \varphi_P^h$$

and then draw some dynamical consequences for the discrete solution (2.14).

3 Statement of the result and applications

3.1 Main result

Let $\mathbf{j} = (j_1, \dots, j_r) \in \mathbb{Z}^r$, and denote by $j_i = (a_i, \delta_i) \in \mathcal{N} \times \{\pm 1\}$ for $i = 1, \dots, r$. We set

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

We say that $j = (j_1, ..., j_r) \in \mathcal{I}_r$ is resonant and we write $j \in \mathcal{A}_r$ if r is even and if we can write up to a permutation of indices

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

for some $a_i \in \mathcal{N}$. Note that in this situation,

$$z_{j} = z_{j_{1}} \cdots z_{j_{r}} = \xi_{a_{1}} \eta_{a_{1}} \cdots \xi_{a_{r/2}} \eta_{a_{r/2}}$$

= $I_{a_{1}} \cdots I_{a_{r/2}}$

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

$$I_a(z) = \xi_a \eta_a$$

denotes the action associated with the index a. Note that if z satisfies the condition $z_{\overline{j}} = \overline{z_j}$ for all $j \in \mathcal{Z}$, then we have $I_a(z) = |\xi_a|^2$. For odd r, \mathcal{A}_r is the empty set.

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

Hypothesis 3.1 For all $r \in \mathbb{N}$, there exist constants γ^* and α^* such that $\forall N \in \mathbb{N}^*$ and $\forall \mathbf{j} = (j_1, \dots, j_r) \notin \mathcal{A}_r$,

$$|j_1|, \dots, |j_r| \le N \implies |1 - e^{ih\Omega(\mathbf{j})}| \ge \frac{h\gamma^*}{N^{\alpha^*}}.$$
 (3.1)

Theorem 3.2 Assume that $P \in \mathcal{T}$ and that the frequencies and the step size $h < h_0$ satisfy the condition (3.1). Let $r \in \mathbb{N}^*$ be fixed. Then there exists a constant s_0 depending on r such that for all $s > s_0$, there exist constants C and ε_0 depending on r and s such that the following holds: For all $\varepsilon < \varepsilon_0$ and for all $z^0 \in \mathcal{P}_{2s}$ real such that $\Pi_{\eta,s}z^0 = z^0$ with $\eta = \varepsilon^{r+1/4}$ and

$$\left\|z^{0}\right\|_{s} \leq \varepsilon \quad and \quad \left\|z^{0}\right\|_{2s} \leq 1,$$

if we define

$$z^{n} = \left(\Pi_{\eta,s} \circ \varphi_{H_0}^{h} \circ \varphi_{P}^{h}\right)^{n} (z^{0}) \quad \text{with} \quad \eta = \varepsilon^{r+1/4}$$
(3.2)

then z^n is still real, and moreover

$$\|z^n\|_s \le 2\varepsilon \quad \text{for} \quad n \le \frac{1}{\varepsilon^{r-2}},$$
 (3.3)

and

$$\sum_{a \in \mathcal{N}} |a|^{2s} |I_a(z^n) - I_a(z^0)| \le \varepsilon^{5/2} \quad \text{for} \quad n \le \frac{1}{\varepsilon^{r-2}}$$
 (3.4)

The proof is postponed to section 4.3.

Remark 3.3 As r is arbitrary, the condition $\eta = \varepsilon^{r+1/4}$ implies that $\Pi_{\eta,s}$ is $\varepsilon^{r+1/4}$ close to the identity in \mathcal{P}_s (cf. (2.13)). From the practical point of view, we may assume that ε^r is beyond the round-off error, so that we can consider that (3.2) coincides with the numerical solution associated with the splitting method at each time step up to some round-off error. However, the full understanding of the real numerical phenomenon taking into account the round-off error is clearly out of the scope of this paper. We refer to [12] for works in this direction.

Remark 3.4 The condition $||z_0||_{2s} \le 1$ together with $\Pi_{\eta,s}z^0 = z^0$ implies that $z_j^0 = 0$ for j large enough which is actually the assumption we need.

In [11, Lemma 3.6], it is shown that the non resonance condition (3.1) is generic under the following hypothesis on the frequencies ω_a , $a \in \mathcal{N}$ (in the next section we will verify this condition in different concrete cases):

Hypothesis 3.5 For all $r \in \mathbb{N}$, there exist constants $\gamma(r)$ and $\alpha(r)$ such that $\forall N \in \mathbb{N}^*$ and $\forall j = (j_1, \ldots, j_r) \notin \mathcal{A}_r$,

$$|j_1|, \dots, |j_r| \le N \implies |\Omega(\mathbf{j})| \ge \frac{\gamma}{N^{\alpha}}.$$
 (3.5)

Under this assumption the set of $h \leq h_0$ satisfying (3.1) is indeed a dense open subset of $(0, h_0)$ (see [11, Lemma 3.6] for a precise statement).

3.2 Examples

3.2.1 Nonlinear Schrödinger equation

We first consider non linear Schrödinger equations of the form

$$i\partial_t \psi = -\Delta \psi + V \star \psi + \partial_2 g(\psi, \bar{\psi}), \quad x \in \mathbb{T}^d$$
 (3.6)

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 $g(z, \bar{z}) \in \mathbb{R}$, and that $g(z, \bar{z}) = \mathcal{O}(|z|^3)$. The corresponding hamiltonian functional is given by

$$H(\psi, \bar{\psi}) = \int_{\mathbb{T}^d} \left(|\nabla \psi|^2 + \bar{\psi}(V \star \psi) + g(\psi, \bar{\psi}) \right) dx$$

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

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

the Hamiltonian associated with the equation (3.6) can be (formally) written

$$H(\xi,\eta) = \sum_{a \in \mathbb{Z}^d} \omega_a \xi_a \eta_a + \sum_{r \ge 3} \sum_{\boldsymbol{a},\boldsymbol{b}} P_{\boldsymbol{a}\boldsymbol{b}} \, \xi_{a_1} \cdots \xi_{a_p} \eta_{b_1} \cdots \eta_{b_q}. \tag{3.7}$$

Here $\omega_a = |a|^2 + \hat{V}_a$ satisfying (2.10) with m = 2 and are the eigenvalues of the operator

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

Note that in (3.7) the sum is made over the set of multi-indices

$$\{(\boldsymbol{a},\boldsymbol{b}) = (a_1,\dots,a_p,b_1,\dots,b_q) \in (\mathbb{Z}^d)^p \times (\mathbb{Z}^d)^q \quad \text{with} \quad p+q=r$$
and $a_1+\dots+a_p-b_1-\dots-b_q=0\},$

which corresponds to the set (2.6) in variables $(z_j)_{j\in\mathcal{Z}}$ (here we set $\mathcal{N}=\mathbb{Z}^d$).

The relation $H(\xi,\bar{\xi}) \in \mathbb{R}$ is equivalent to the fact that the coefficients P_{ab} satisfy $P_{ab} = \overline{P}_{ba}$ which corresponds to the hypothesis (2.8) in variables $(z_j)_{j \in \mathbb{Z}}$. The fact that the nonlinearity P belongs to T can be verified using the regularity of g and the properties of the basis functions ϕ_a , see [15, 4]. Furthermore the fact that the eigenfunctions basis is the Fourier basis, and the fact that the nonlinearity g does not depend on g insure that the zero momentum condition is satisfied. In this situation, it can be shown that the Hypothesis 3.1 is fulfilled for a large set of potential V (see for instance Theorem 5.7 in [15]).

The numerical implementation of the splitting method is very easy in the case of Eqn. (3.6): The part corresponding to the equation

$$i\partial_t \psi = -\Delta \psi + V \star \psi$$

is easily solved in terms of Fourier coefficients, while the non linear part

$$i\partial_t \psi = \partial_2 g(\psi, \bar{\psi})$$

is a simple differential equation with fixed $x \in \mathbb{T}^d$. The use of a fast Fourier transform allows to compute alternatively the solution of the linear part and the solution of the non-linear part.

3.2.2 Nonlinear wave equation

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

$$u_{tt} - u_{xx} + mu = g(u) , \quad x \in (0, \pi) , \ t \in \mathbb{R} ,$$
 (3.8)

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.

Defining $v = u_t$, (3.8) reads

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

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

$$H(u,v) = \int_{S^1} \left(\frac{1}{2}v^2 + \frac{1}{2}u_x^2 + \frac{1}{2}mu^2 + G(x,u) \right) dx$$
 (3.9)

where G is such that $\partial_u G = -g$, then (3.8) reads as an Hamiltonian system

$$\partial_t \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -u_{xx} + mu + \partial_u G \\ v \end{pmatrix}$$
$$= J\nabla_{u,v}H(u,v)$$
(3.10)

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

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

Then, on $H^s(0,\pi) \times H^s(0,\pi)$ with $s \ge 1/2$, the Hamiltonian (3.9) 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 , $a\in\mathbb{N}\setminus\{0\}=:\mathcal{N}$, the associated eigenfunctions. We have $\phi_a(x)=\sin ax$

and $\omega_a = \sqrt{a^2 + m}$.

Plugging the decompositions

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

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

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

the Hamiltonian function can be written under the form (3.7) with a nonlinearity depending on G. As in the previous case, it can be shown that the condition (3.5) is fulfilled for a set of constant m of full measure (see for instance Theorem 4.18 in [2]).

In this situation, the symmetric Strang splitting scheme

$$\varphi_P^{h/2} \circ \varphi_{H_0}^h \circ \varphi_P^{h/2}$$

corresponds to the Deuflhard's method [9]. If moreover we consider the Hamiltonian

$$H(z) = H_0(z) + P(\Phi(hH_0)z)$$

where $\Phi(x)$ is 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 [18, Chap. XIII] and [6]). The fact that Φ is bounded makes that the functional $z \mapsto P(\Phi(H_0)z)$ obviously belongs to \mathcal{T} . Notice that the nonlinearity satisfies the zero momentum property because in complex variables the eigenfunctions basis is again the Fourier basis.

4 A normal form result

4.1 Normal form

Definition 4.1 Let N > 0 be a real number. For a given multi-index $j \in \mathbb{Z}^r$, let i_p be the permutation such that

$$|j_{i_1}| \leq \cdots \leq |j_{i_r}|$$

We define the set

$$\mathcal{J}_r(N) = \{ \boldsymbol{j} \in \mathcal{I}_r \mid j_{i_r} | \leq (r-1)N \quad and \quad |j_{i_{r-1}}| \leq N \}.$$

Lemma 4.2 Let $r \geq 3$, and assume that $j \notin \mathcal{J}_r(N)$. Then j contains at least two indices with modulus greater than N.

Proof. Let $\mathbf{j} = (j_1, \dots, j_r) \in \mathcal{I}_r \backslash \mathcal{J}_r(N)$. We have $\mathcal{M}(\mathbf{j}) = 0$ where $\mathcal{M}(\mathbf{j})$ is defined in (2.5). Assume that there exists only one index of modulus greater than N. We can assume that $|j_1| > N$ and hence all the other indices are of modulus $\leq N$ (in particular, with the previous notation, we have $j_1 = j_{i_r}$). Hence we have

$$|j_1| \le |j_2| + \dots + |j_r| \le (r-1)N$$

and this implies that $j \in \mathcal{J}_r(N)$ which is a contradiction.

We motivate now the definition of normal form terms we introduce in the sequel. For a given number N and $z \in \mathcal{P}_s$ we define

$$\mathsf{N}_s^N(z) = \sum_{|a| \le N} |a|^{2s} \xi_a \eta_a$$

and

$$\mathsf{R}^N_s(z) = \sum_{|a| > N} |a|^{2s} \xi_a \eta_a$$

so that

$$||z||_s^2 = \mathsf{N}_s^N(z) + \mathsf{R}_s^N(z).$$

Proposition 4.3 Let $N \in \mathbb{N}$ and $r \geq 3$. Assume that the homogeneous polynomial

$$Z = \sum_{\boldsymbol{j} \in \mathcal{I}_r \setminus \mathcal{J}_r(N)} Z_{\boldsymbol{j}} z_{\boldsymbol{j}}$$

defines an element of $\mathcal{T}_r^{M,\nu}$ for some constants M and ν . Then we have for all $s > 2\nu + 4$, M > s + 2 and for all $z \in \mathcal{P}_s(\mathbb{C})$,

$$|\{\mathsf{N}_{s}^{N}, Z\}(z)| \le C_{0}|Z|_{\mathcal{T}_{s}^{M,\nu}} N^{\nu+2+d/2-s} ||z||_{s}^{r-2} \mathsf{R}_{s}^{N}(z). \tag{4.1}$$

and

$$\forall a \in \mathcal{N}, \quad |a| \le N, \quad |\{I_a, Z\}| \le C_0 |Z|_{\mathcal{T}_r^{M,\nu}} N^{\nu + 2 - s} ||z||_s^{r-2} \mathsf{R}_s^N(z). \tag{4.2}$$

Moreover

$$|\{\mathsf{R}_{s}^{N},Z\}(z)| \le C_{0}|Z|_{\mathcal{T}_{r}^{M,\nu}} \|z\|_{s}^{r-2} \,\mathsf{R}_{s}^{N}(z) \tag{4.3}$$

where C_0 is a constant depending on s, r and the dimension d of $\mathcal{N} = \mathbb{N}^d$ of \mathbb{Z}^d .

Roughly speaking, (4.1) and (4.2) say that, if s and N are large, the flow generated by Z does not move a lot the first actions, I_a , $|a| \leq N$. On the other hand, (4.3) implies, by using Gronwall lemma, that, if in the principle $\mathsf{R}^N_s(z)$ is small, the flow generated by Z will preserve this smallness during finite time. These two facts will be used in the proof of Theorem 3.2. The proof of Proposition 4.3 is technical and is given in the Appendix.

Definition 4.4 An element $Z \in \mathcal{T}_r^{M,\nu}$ is said to be in normal form if we can write it

$$Z = \sum_{\ell=3}^{r} \sum_{\{j \in \mathcal{A}_{\ell} \cup \mathcal{I}_{\ell} \setminus \mathcal{J}_{\ell}(N)\}} Z_{j} z_{j}.$$

In other words, a normal form term either depends only on the actions or contains at least two terms with index greater than N (cf. Lemma 4.2).

4.2 Statement of the normal form result

In the following, we set

$$B_s(\rho) = \{ z \in \mathcal{P}_s \, | \, ||z||_s \le \rho \}.$$

Theorem 4.5 Assume that $P \in \mathcal{T}$ and that the frequencies and the step size $h < h_0$ satisfy the Hypothesis 3.1. Let $r_0 \geq 3$ be fixed. Then there exist constants s_0 , β and N_0 such that for all $s \geq s_0$, there exists a constant C and for all $N \geq N_0$ there exists a canonical transformation τ from $B_s(\rho)$ into $B_s(2\rho)$ with $\rho = (CN)^{-\beta}$ satisfying for all $z \in B_s(\rho)$,

$$\|\tau(z) - z\|_{s} \le (CN)^{\beta} \|z\|_{s}^{2} \quad and \quad \|\tau^{-1}(z) - z\|_{s} \le (CN)^{\beta} \|z\|_{s}^{2}$$
 (4.4)

and such that the restriction of τ to the high modes is the identity, i.e.

$$(\tau(z))_j = z_j \quad \text{for} \quad |j| > (r_0 - 1)N.$$
 (4.5)

Moreover, τ puts φ_H^h in normal form up to order r_0 in the sense that

$$\varphi_{H_0}^h \circ \varphi_P^h \circ \tau = \tau \circ \varphi_{H_0}^h \circ \psi \tag{4.6}$$

where ψ is the solution at time $\lambda = 1$ of a non-autonomous hamiltonian $hZ(\lambda) + R(\lambda)$ with

• $Z(\lambda) \in \mathcal{C}([0,1], \mathcal{T}_{r_0}^{M_1,\nu_1})$ for some M_1 and ν_1 depending on P, r_0 , s and h_0 , and for all $\lambda \in [0,1]$, $Z(\lambda)$ is a real polynomial of degree r under normal form such that

$$|Z(\lambda)|_{T_{r_0}^{M_1,\nu_1}} \le (CN)^{\beta}.$$
 (4.7)

• $R(\lambda) \in \mathcal{C}([0,1], \mathcal{H}^s(B_s(\rho)))$ with $\rho \leq (CN)^{-\beta}$ has a zero of order $r_0 + 1$ at the origin and satisfies and for all $z \in B_s(\rho)$,

$$\forall \lambda \in [0,1], \quad \|X_{R(\lambda)}(z)\|_{s} \le (CN)^{\beta} \|z\|_{s}^{r}.$$
 (4.8)

The proof is postponed to section 4.4 and 4.6. We first verify that this normal form theorem has the dynamical consequences announced in Theorem 3.2.

4.3 Proof of the main Theorem 3.2

We now give the proof of Theorem 3.2.

First, let us note that as the Hamiltonian functions H_0 , P, Z and R are real Hamiltonians, and by definition of $\Pi_{\eta,s}$ (which is symmetric in ξ and η), it is clear that there exist $\xi^n \in \mathbb{C}^{\mathcal{N}}$ such that for all n, we have $z^n = (\xi^n, \bar{\xi}^n)$.

Let $r_0 = r$, and let C = C(r, s), $s_0 = s_0(r)$ and $\beta = \beta(r)$ be the constants appearing in Theorem 4.5. We can always assume that

$$s_0(r) \ge 2(r+1)\beta(r).$$
 (4.9)

Let $s \geq s_0(r)$. Let ε_0 be such that

$$\varepsilon_0^{1/2} \le \frac{(r-1)^s}{2C^s}. (4.10)$$

Let $\varepsilon < \varepsilon_0$. We define N such that

$$(CN)^{\beta} = \varepsilon^{-1/2}. (4.11)$$

Notice that the assumption $\|z^0\|_s \leq \varepsilon$ implies $z^0 \in B_s(\rho)$ with $\rho = (CN)^{-\beta}$. Furthermore we have $\|z^0\|_{2s} \leq 1$ and together with $\Pi_{\eta,s}z^0 = z^0$, this hypothesis implies that $z_j^0 = 0$ for j large enough. Actually let $j \in \mathcal{Z}$ be such that |j| > (r-1)N, we have

$$|j^s||z_j^0| \le |j|^{-s} \le ((r-1)N)^{-s}$$
.

using (4.11) we have $N = C^{-1} \varepsilon^{-\frac{1}{2\beta}}$ and hence

$$|j^s||z_j^0| \le (r-1)^{-s} C^s \varepsilon^{\frac{s}{2\beta}}.$$

Now condition (4.9) implies that $\frac{s}{2\beta} \ge r+1$ and hence (as we can always assume that $\varepsilon < 1$),

$$\varepsilon^{\frac{s}{2\beta}} \le \varepsilon^{r+1}$$
.

Therefore we get using (4.10)

$$|j^{s}||z_{j}^{0}| \le \varepsilon^{r+1/2} \Big((r-1)^{-s} C^{s} \varepsilon^{1/2} \Big) \le \varepsilon^{r+1/2}.$$

As $\Pi_{\eta,s}z^0=z^0$ and $\eta=\varepsilon^{r+1/4}$, this implies that

$$\forall |j| > (r-1)N, \quad z_j^0 = 0.$$

Let τ defined by Theorem 4.5, and let $y^n = \tau^{-1}(z^n)$. As τ is the flow of a real Hamiltonian, there exists $\zeta^n \in \mathbb{C}^{\mathcal{N}}$ such that $y^n = (\zeta^n, \bar{\zeta}^n)$ for all n. By definition, we have

$$\forall n \ge 0, \quad y^{n+1} = (\tau^{-1} \circ \Pi_{\eta,s} \circ \tau) \circ (\varphi_{H_0}^h \circ \psi)(y^n). \tag{4.12}$$

and as τ is the identify for high modes (see (4.5)), we have $y_j^0 = 0$ for |j| > (r-1)N.

Using the definition of N, the transformation τ in the previous Theorem satisfies (taking $\rho := 2\varepsilon < \sqrt{\varepsilon}$): for all z such that $||z||_{\varepsilon} \leq 2\varepsilon$,

$$\|\tau^{-1}(z) - z\|_{s} \leq \varepsilon^{-1/2} \|z\|_{s}^{2}$$

$$\leq 4\varepsilon^{3/2}$$

$$\leq \frac{1}{4}\varepsilon$$
(4.13)

provided ε_0 is sufficiently small. Hence, we have $\|y^0\|_s = \|\tau^{-1}(z^0)\|_s \leq \frac{5}{4}\varepsilon$. We will show by induction that the following holds for all $n \in \mathbb{N}$:

- (i) $\|y^n\|_a^2 \le \|y^0\|_a^2 + 2n\varepsilon^{r+1/8}$
- (ii) $y_j^n = 0 \text{ for } j \ge (r-1)N$.

These assumptions are satisfied for n=0. Assume that they hold for $n \geq 0$. Let ψ be the application defined by Theorem 4.5 and $\psi^{\lambda}(z)$ be the flow associated with the Hamiltonian $hZ(\lambda) + R(\lambda)$ defining the application ψ for $\lambda = 1$.

Using the results of Lemmas 4.6 and 4.7 below, we easily see that there exists a constant c depending on r such that for all $\lambda \in [0,1]$, $\|\psi^{\lambda}(y^n)\|_{c} \leq c\varepsilon$.

Let $N_1 = (r-1)N$. We have by hypothesis that $\mathsf{R}^{N_1}_s(y^n) = 0$. Furthermore

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathsf{R}_s^{N_1}(\psi^\lambda(y^n)) = \{\mathsf{R}_s^{N_1}, hZ + R\}.$$

Thus using the equation (4.3), (4.7) and (4.8) we get

$$\left| \frac{\mathrm{d}}{\mathrm{d}\lambda} \mathsf{R}_s^{N_1}(\psi^{\lambda}(y^n)) \right|$$

$$\leq C_1 N^{\beta} \mathsf{R}_s^{N_1} (\psi^{\lambda}(y^n)) (\|\psi^{\lambda}(y^n)\|_s + \|\psi^{\lambda}(y^n)\|_s^{r-2}) + C_1 N^{\beta} \|\psi^{\lambda}(z)\|_s^{r+1}$$

for some constant C_1 depending on r and s. Hence we have

$$\left| \frac{\mathrm{d}}{\mathrm{d}\lambda} \mathsf{R}_s^{N_1}(\psi^{\lambda}(y^n)) \right| \le C_1 \left(\varepsilon^{1/2} \mathsf{R}_s^{N_1}(\psi^{\lambda}(y^n)) + \varepsilon^{r+1/2} \right).$$

where C_1 depends on r and s. Using the Gronwall Lemma, we obtain for all $\lambda \in [0,1]$

$$\mathsf{R}_s^{N_1}(\psi^{\lambda}(y^n)) \le \varepsilon^{r+1/2} C_1 e^{\varepsilon^{1/2} \lambda C_1}.$$

We can always assume that $\varepsilon_0^{1/4} C_1 e^{\varepsilon_0^{1/2} C_1} < 1$. Hence we get

$$\forall \lambda \in [0,1], \quad \mathsf{R}_s^{N_1}(\psi^{\lambda}(y^n)) \le \varepsilon^{r+1/4}.$$

On the other hand, using (4.1) we have

$$\left| \frac{\mathrm{d}}{\mathrm{d}\lambda} \mathsf{N}_s^{N_1}(\psi^{\lambda}(y^n)) \right| \le$$

$$C_1 N^{\beta+\nu+2+d/2-s} \mathsf{R}_s^{N_1}(\psi^\lambda(y^n)) \big(\left\|\psi^\lambda(z)\right\|_s + \left\|\psi^\lambda(z)\right\|_s^{r-2} \big) + C_1 N^\beta \left\|\psi^\lambda(z)\right\|_s^{r+1}$$

for some constant C_1 depending on r and s. We can always assume that $s > \beta + \nu + d/2 + 2$. Using the previous estimates, we get

$$\left| \frac{\mathrm{d}}{\mathrm{d}\lambda} \mathsf{N}_s^{N_1}(\psi^{\lambda}(y^n)) \right| \le C_1 \varepsilon^{r+1/2}$$

and then

$$\mathsf{N}_s^{N_1}(\psi^{\lambda}(y^n)) \le \|y^n\|_s^2 + C_1 \varepsilon^{r+1/2}.$$

Let $\tilde{y}^n = \varphi_{H_0}^h \circ \psi(y^n)$. As for all z we have $\|z\|_s^2 = \mathsf{N}_s^{N_1}(z) + \mathsf{R}_s^{N_1}(z)$ and as $\varphi_{H_0}^h$ preserves all the actions, therefore

$$\|\tilde{y}^n\|_s^2 \le \|y^n\|_s^2 + C_1 \varepsilon^{r+1/2}$$
 and $\mathsf{R}_s^{N_1}(\tilde{y}^n) \le \varepsilon^{r+1/4}$. (4.14)

Now by construction (cf. (4.12))

$$y^{n+1} = \tau^{-1} \circ \Pi_{n,s} \circ \tau(\tilde{y}^n).$$

As τ is the identity for modes $|j| > N_1$, we have

$$\mathsf{R}^{N_1}_s(\tau(\tilde{\boldsymbol{y}}^n)) = \mathsf{R}^{N_1}_s(\tilde{\boldsymbol{y}}^n) \le \varepsilon^{r+1/4} = \eta.$$

Hence by definition of the projection $\Pi_{\eta,s}$ we get that

$$\left(\Pi_{\eta,s} \circ \tau(\tilde{y}^n)\right)_j = 0, \text{ for } |j| > (r-1)N = N_1.$$

As τ^{-1} is the identity for modes greater than (r-1)N, this shows (ii) for n+1, i.e.

$$y_j^{n+1} = 0$$
 for $|j| > (r-1)N$.

Let z be such that $z_j = 0$ for |j| > (r-1)N. We have

$$\left\|\Pi_{\eta,s}z - z\right\|_{s} \leq \sum_{|j| \leq N} \eta \leq \eta N^{d} \leq \varepsilon^{r+1/4 - d/2\beta} \leq \varepsilon^{r+1/8}$$

since we can always assume $\beta > 4d$.

Writing

$$\tau^{-1} \circ \Pi_{\eta,s} \circ \tau = I + \tau^{-1} \circ (\Pi_{\eta,s} - I) \circ \tau$$

and as τ leaves the set $(z_j)_{|j| \ge N_1}$ invariant, we get using (4.4),

$$\begin{split} \left\| y^{n+1} \right\|_s^2 &= \mathsf{N}_s^{N_1}(y^{n+1}) \leq \mathsf{N}_s^{N_1}(\tilde{y}^n) + (1 + (CN)^{\beta} \varepsilon^2) \eta N^d \\ &\leq \mathsf{N}_s^{N_1}(\tilde{y}^n) + \frac{3}{2} \varepsilon^{(r+1/8)} \end{split}$$

Thus we get

$$\|y^{n+1}\|_{s}^{2} \le \|y^{n}\|_{s}^{2} + c\varepsilon^{r+1/4} + \frac{3}{2}\varepsilon^{r+1/8} \le \|y^{n}\|_{s}^{2} + 2\varepsilon^{r+1/8}.$$

This shows (i) for n + 1.

In particular, for all $n \leq \varepsilon^{-r+2}$ we have (recall $||y^0||_{\alpha} \leq \frac{5}{4}\varepsilon$)

$$\|y^n\|_s^2 \le \left(\frac{5}{4}\varepsilon\right)^2 + 2\varepsilon^{2+1/8}$$

and hence (provided ε_0 is small enough)

$$||y^n||_{\varepsilon} \leq \frac{7}{4}\varepsilon.$$

Now using (4.13) for the application τ , we easily see that $||z^n|| \leq 2\varepsilon$ as long as $n \leq \varepsilon^{r-2}$. This proves (3.3).

The proof of (3.4) is obtained similarly using (4.2) and we do not give the details here.

4.4 Formal equations

We consider a fixed step size h satisfying (3.1) and the associated propagator

$$\varphi_{H_0}^h \circ \varphi_P^h = \varphi_{H_0}^h \circ \varphi_{hP}^1.$$

As in [11], we embed this application into the family of applications

$$\varphi_{H_0}^h \circ \varphi_{hP}^{\lambda}, \quad \lambda \in [0, 1].$$

Formally, we would like to find a real hamiltonian $\chi = \chi(\lambda)$ and a real hamiltonian under normal form $Z = Z(\lambda)$ and such that

$$\forall \lambda \in [0,1] \quad \varphi_{H_0}^h \circ \varphi_{hP}^\lambda \circ \varphi_{\chi(\lambda)}^\lambda = \varphi_{\chi(\lambda)}^\lambda \circ \varphi_{H_0}^h \circ \varphi_{hZ(\lambda)}^\lambda. \tag{4.15}$$

Following the formal calculations made in [11] by taking the derivative of this expression with respect to λ , see equations (5.3)–(5.5), this amounts to solve the equation

$$\forall \lambda \in [0,1] \quad \chi(\lambda) \circ \varphi_{H_0}^h - \chi(\lambda) \circ \varphi_{hP}^{-\lambda} = hP - (hZ(\lambda) + R(\lambda)) \circ \varphi_{\chi(\lambda)}^{-\lambda} \quad (4.16)$$

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.

In the following, we formally write

$$\chi(\lambda) = \sum_{\ell=3}^{r} \chi_{[\ell]}(\lambda) := \sum_{\ell=3}^{r} \sum_{\mathbf{j} \in \mathcal{I}_{\ell}} \chi_{\mathbf{j}}(\lambda) z_{\mathbf{j}}$$

and

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

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

Using the assumptions on P, we can write

$$P = A + B = \sum_{\ell=3}^{r} P_{[\ell]} + B$$

where $A \in \mathcal{T}_r^{\infty,\nu}$ and $B \in \mathcal{H}^s(B_s(\rho_0))$ for $s > s_0$ and ρ_0 sufficiently small. Moreover, B has a zero of order r+1 at the origin.

Identifying the coefficients of degree $\ell \leq r$ in equation (4.16), 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 polynomial of order $\leq \ell$ of the coefficients χ_j , P_j and Z_j for $j \in \mathcal{I}_k$, $k < \ell$.

Writing down the coefficients, this equation is equivalent to

$$\forall j \in \mathcal{I}_r \quad (e^{ih\Omega(j)} - 1)\chi_j = hP_j - hZ_j + hG_j$$

and hence we see that the key is to control the small divisors $e^{ih\Omega(j)} - 1$.

4.5 Non autonomous Hamiltonians

Before giving the proof of Theorem 3.2, we give easy results on the flow of non autonomous Hamiltonian. Let $Q(\lambda) \in \mathcal{C}([0,1],\mathcal{T}_r^{M,\nu})$ for some $r \geq 3, M > 0$ and $\nu > 0$. We set

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

The following results extend the properties already proved in [15] or [2] and needed in the proofs below.

Lemma 4.6 Let $k \in \bar{\mathbb{N}}$, $M \in \mathbb{N}$, $\nu \in [0, \infty)$, $s \in \mathbb{R}$ with $s > \nu + 3/2$, and let $P(\lambda) \in \mathcal{C}([0, 1], \mathcal{T}_{k+1}^{M, \nu})$ be a homogeneous polynomial of order k+1 depending on $\lambda \in [0, 1]$. Then

(i) P extends as a continuous polynomial on $\mathcal{P}_s(\mathbb{C})$ depending continuously on $\lambda \in [0,1]$, and there exists a constant C such that for all $z \in \mathcal{P}_s(\mathbb{C})$ and all $\lambda \in [0,1]$,

$$|P(\lambda, z)| \le C ||P||_{\mathcal{T}_{k+1}^{M, \nu}} ||z||_s^{k+1}.$$

(ii) Assume moreover that M > s+1, then the Hamiltonian vector field $X_{P(\lambda)}$ extends as a bounded function from $\mathcal{P}_s(\mathbb{C})$ to $\mathcal{P}_s(\mathbb{C})$ depending continuously on $\lambda \in [0,1]$. Furthermore, for any $s > \nu + 1$, there exists a constant C such that for any $z \in \mathcal{P}_s(\mathbb{C})$ and $\lambda \in [0,1]$,

$$||X_{P(\lambda)}(z)||_{s} \le C||P||_{\mathcal{T}_{k+1}^{M,\nu}} ||z||_{s}^{k}.$$

Lemma 4.7 Let $r \geq 3$, M > 0 and let

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

be an element of $C([0,1], \mathcal{T}_r^{M,\nu})$. Let $\varphi_{Q(\lambda)}^{\lambda}$ be the flow associated with the non autonomous real Hamiltonian $Q(\lambda)$. Then for $s > \nu + 3/2$ there exists a constant C_r depending on r such that

$$\rho < \inf(1/2, C_r \|Q\|_{\mathcal{I}_r^{M,\nu}}^{-1}) \quad \Longrightarrow \quad \forall \lambda \in [0,1], \quad \varphi_{Q(\lambda)}^{\lambda}(B_s(\rho)) \subset B_s(2\rho). \tag{4.17}$$

Moreover, if $F(\lambda) \in \mathcal{C}([0,1], \mathcal{H}^s(B_s(2\rho)))$ has a zero of order r at the origin, then $F(\lambda) \circ \varphi_{Q(\lambda)}^{\lambda}$ has a zero of order r at the origin in $B_s(\rho)$.

Proof. The proof is very similar to the one of Lemma 5.2 in [11] and is omitted.

The next result is a consequence of Prop 6.3 in [15]. The only specificity is the control of the sum of the indices, and the evolution of the norm

Proposition 4.8 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 $P \in \mathcal{C}([0,1], \mathcal{T}_{k_1+1}^{M,\nu_1})$ and $Q \in \mathcal{C}([0,1], \mathcal{T}_{k_2+1}^{M,\nu_2})$ for some $\nu_1 > 0$, $\nu_2 > 0$ and M > 0.

Then $\{P,Q\}$ defines a homogeneous polynomial of degree $k_1 + k_2$, and for all M' and ν' such that

$$M' < M - \max(\nu_1, \nu_2) - 1$$
 and $\nu' > \nu_1 + \nu_2 + 1$,

we have $\{P,Q\} \in \mathcal{C}([0,1],\mathcal{T}_{k_1+k_1}^{M',\nu'})$ and

$$\left\|\{P,Q\}\right\|_{\mathcal{T}_{k_1+k_1}^{M',\nu'}} \leq C \|P\|_{\mathcal{T}_{k_1+1}^{M,\nu_1}} \left\|Q\right\|_{\mathcal{T}_{k_2+1}^{M,\nu_2}}$$

for some constant C depending on M, ν , M', ν' , k_1 and k_2 .

Proof. The proof is clear using Proposition 6.3 in [15]. We only need to verify the fact that the summations are always made over sets of indices with zero moment $\mathcal{M}(j)$, which is trivial.

Lemma 4.9 Let $\chi(\lambda)$ be an element of $\mathcal{C}([0,1], \mathcal{T}_r^{M,\nu})$ for some M > 0 and $\nu > 0$. Let $\tau(\lambda) := \varphi_{\chi(\lambda)}^{\lambda}$ be the flow associated with the non autonomous real Hamiltonian $\chi(\lambda)$. Let $g \in \mathcal{C}([0,1], \mathcal{T}_r^{M,\nu})$, then we can write for all $\sigma_0 \in [0,1]$,

$$g(\sigma_0) \circ \tau(\sigma_0) = g(\sigma_0)$$

$$+\sum_{k=0}^{r-1} \int_0^{\sigma_0} \cdots \int_0^{\sigma_k-1} \left(\operatorname{Ad}_{\chi(\sigma_k)} \circ \cdots \circ \operatorname{Ad}_{\chi(\sigma_1)} g(\sigma_0) \right) d\sigma_1 \cdots d\sigma_k + R(\sigma_0) \quad (4.18)$$

where by definition $Ad_P(Q) = \{Q, P\}$

$$R(\sigma_0) = \int_0^{\sigma_0} \cdots \int_0^{\sigma_{r-1}} \left(\operatorname{Ad}_{\chi(\sigma_r)} \circ \cdots \circ \operatorname{Ad}_{\chi(\sigma_1)} g(\sigma_0) \right) \circ \tau(\sigma_r) \, d\sigma_1 \cdots d\sigma_r. \tag{4.19}$$

Each term in the sum in (4.18) belongs (at least) to the space $C([0,1], \mathcal{T}_{kr}^{M',\nu'})$ where

$$\nu' = (r+1)(\nu+2)$$
 and $M' = M - \nu'$.

The term $R(\sigma_0)$ defines an element of $\mathcal{H}^s(B_s(\rho))$ for $s > \nu' + 3/2$ and $\rho \leq \inf(1/2, C_r \|\chi\|_{\mathcal{T}_r^{M,\nu}}^{-1})$ and has a zero of order at least r+1 at the origin.

Proof. For a fixed $\sigma_0 \in [0,1]$, we have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}g(\sigma_0)\circ\tau(\lambda)=\{g(\sigma_0),\chi(\lambda)\}\circ\tau(\lambda).$$

Hence, we have that

$$g(\sigma_0) \circ \tau(\sigma_0) = g(\sigma_0) + \int_0^{\sigma_0} \left(\operatorname{Ad}_{\chi(\sigma_1)} g(\sigma_0) \right) \circ \tau(\sigma_1) \, d\sigma_1.$$

Repeating again the same argument, we have

$$g(\sigma_0) \circ \tau(\sigma_0) = g(\sigma_0) + \int_0^{\sigma_0} (\operatorname{Ad}_{\chi(\sigma_1)} g(\sigma_0)) d\sigma_1 + \int_0^{\sigma_0} \int_0^{\sigma_1} \left(\operatorname{Ad}_{\chi(\sigma_2)} \circ \operatorname{Ad}_{\chi(\sigma_1)} g(\sigma_0) \right) \circ \tau(\sigma_2) d\sigma_1 d\sigma_2.$$

The equation (4.18) is then easily shown by induction. The result then follows from the previous propositions.

For a given polynomial $\chi \in \mathcal{C}([0,1], \mathcal{T}_r^{M,\nu})$ with $r \geq 3$, we use the following notation

$$\chi(\lambda, z) = \sum_{\ell=3}^{r} \chi_{[\ell]}(\lambda) = \sum_{\ell=3}^{r} \sum_{\mathbf{j} \in \mathcal{I}_{\ell}} \chi_{\mathbf{j}}(\lambda) z_{\mathbf{j}}$$

$$(4.20)$$

where $\chi_{[\ell]}(\lambda) \in \mathcal{C}([0,1], \mathcal{T}_r^{M,\nu})$ is a homogeneous polynomial of degree ℓ .

Proposition 4.10 Let $\chi(\lambda)$ be an element of $C([0,1], T_r^{M,\nu})$ for some M > 0 and $\nu > 0$. Let $\varphi_{\chi(\lambda)}^{\lambda}$ be the flow associated with the non autonomous real hamiltonian $\chi(\lambda)$. Let $g \in C([0,1], T_r^{M,\nu})$, then we can write for all $\lambda \in [0,1]$,

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

where

• $S^{(r)}(\lambda) \in C^{\infty}([0,1], \mathcal{T}_r^{M_1,\nu_1})$ with $\nu_1 = (r+1)(\nu+2)$ and $M_1 = M - \nu_1$. 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 $\ell = 3, \ldots, r$,

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

where $G_{[\ell]}(\chi_*, g_*)$ 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

$$\|G_{[\ell]}(\chi_*, g_*)\|_{\mathcal{T}_r^{M_1, \nu_1}} \le C \left(1 + \sum_{m=3}^{\ell-1} \|g_{[m]}\|_{\mathcal{T}_r^{M, \nu}}^{\ell}\right) \left(1 + \sum_{m=3}^{\ell-1} \|\chi_{[m]}\|_{\mathcal{T}_r^{M, \nu}}^{\ell}\right)$$

$$(4.21)$$

where C depends on ℓ , M and ν .

• $T^{(r)}(\lambda) \in \mathcal{H}^s(B_s(\rho))$ for $s > \nu' + 3/2$ and $\rho \leq \inf(1/2, C_r \|\chi\|_{\mathcal{T}_r^{M,\nu}}^{-1})$ and has a zero of order at least r+1 in the origin. Moreover, we have for all $z \in B_s(\rho)$,

$$\forall \lambda \in [0,1], \quad \|X_{T^{(r)}(\lambda)}(z)\|_{s} \leq C_{r}(\chi_{*}, g_{*})\|z\|_{s}^{r}$$

where

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

with C depending on r, M and ν .

Proof. Using the previous lemma, we define $S^{(r)}$ as the polynomial part of degree less than r in the expression (4.18). The remainder terms, together with the term $R(\lambda)$ in (4.19), define the term $T^{(r)}(\lambda)$. The properties of $S^{(r)}(\lambda)$ and $T^{(r)}(\lambda)$ are then easily shown.

4.6 Proof of the normal form result

Proposition 4.11 Let $P \in \mathcal{T}$ and N be a fixed integer. Let $M > \nu' := (r + 1)(\nu + 2)$ and $M' = M - \nu'$. Then there exist

• a polynomial $\chi \in \mathcal{C}([0,1], \mathcal{T}_r^{M',\nu'})$

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

• a polynomial $Z \in \mathcal{C}([0,1], \mathcal{T}_r^{M',\nu'})$

$$Z(\lambda) = \sum_{\ell=3}^{r} Z_{[\ell]}(\lambda) := \sum_{\ell=3}^{r} \sum_{\{j \in \mathcal{A}_{\ell} \cup \mathcal{I}_{\ell} \setminus \mathcal{J}_{\ell}(N)\}} Z_{j}(\lambda) z_{j}$$

under normal form,

• a function $R(\lambda) \in \mathcal{C}([0,1], \mathcal{H}_s(B_s(\rho)))$ with $\rho < c_0 N^{-\beta}$ for some constant $c_0 > 0$ and $\beta > 1$ depending on r, M, P, and having a zero of order r + 1 at the origin

such that the following equation holds:

$$\forall \lambda \in [0,1] \quad \chi(\lambda) \circ \varphi_{H_0}^h - \chi(\lambda) \circ \varphi_{hP}^{-\lambda} = hP - (hZ(\lambda) + R(\lambda)) \circ \varphi_{\chi(\lambda)}^{-\lambda}. \quad (4.22)$$

Furthermore there exists $C_0 > 0$ depending on P, ν , r, M such that

$$|\chi|_{\mathcal{T}_{-}^{M',\nu'}} + |Z|_{\mathcal{T}_{-}^{M',\nu'}} \le C_0 N^{\beta}$$

and

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

for $z \in B_s(\rho)$ with $\rho < c_0 N^{-\beta}$.

Proof. Identifying the coefficients of degree $\ell \leq r$ in the equation (4.22), we get

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

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 polynomial of order $\leq \ell$ of the coefficients $\chi_{\boldsymbol{j}}$, $P_{\boldsymbol{j}}$ and $Z_{\boldsymbol{j}}$ for $\boldsymbol{j} \in \mathcal{I}_k$, $k < \ell$ and satisfy estimates of the form (4.21). 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

$$Z_{\boldsymbol{i}} = P_{\boldsymbol{i}} + G_{\boldsymbol{i}}$$
 and $\chi_{\boldsymbol{i}} = 0$ for $\boldsymbol{j} \in \mathcal{A}_{\ell} \cup \mathcal{I}_{\ell} \setminus \mathcal{J}_{\ell}(N)$

and

$$Z_{j} = 0$$
 and $\chi_{j} = \frac{h}{e^{ih\Omega(j)} - 1} (P_{j} + G_{j})$ for $j \in \mathcal{J}_{\ell}(N) \setminus \mathcal{A}_{\ell}$.

Using (3.1) and the result of Proposition 4.10 we get the claimed bound for some β depending on r.

To define R, we simply define it by the equation (4.22). By construction, it will satisfies the announced properties.

Proof of Theorem 4.5. Integrating the equation (4.22) in λ , it is clear that the following equation holds:

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

Note that using Proposition 4.10 and (4.17) we show that for $s > \nu' + 1$ and $z \in B_s(\rho)$ with $\rho = cN^{-\beta}$ we have

$$\left\|\varphi_{\chi(\lambda)}^{\lambda}(z)-z\right\|_{s}\leq CN^{\beta}\left\|z\right\|_{s}^{2}.$$

This implies in particular that

$$\|z\|_{s} \leq \|\varphi_{\chi(\lambda)}^{\lambda}(z)\|_{s} + CN^{-\beta}\|z\|_{s}$$

For N sufficiently large, this shows that $\varphi_{\chi(\lambda)}^{\lambda}$ is invertible and send $B_s(\rho)$ to $B_s(2\rho)$. Moreover, we have the estimate, for all $\lambda \in [0,1]$,

$$\|\left(\varphi_{\gamma(\lambda)}^{\lambda}\right)^{-1}(z)-z\|_{s} \leq CN^{\beta}\|z\|_{s}^{2}$$
.

We then define $\tau = \varphi^1_{\chi(\lambda)}$ and $\psi = \varphi^1_{hZ(\lambda)+R(\lambda)}$ and verify that these application satisfy the condition of the theorem.

5 Appendix: Proof of Proposition 4.3

Let $j \in \mathcal{I}_r \setminus \mathcal{J}_r(N)$. It is clear that for $a \in \mathcal{N}$, we have, with the notation $I_a = \xi_a \eta_a$,

$$\{I_a, z_j\} = 0$$

unless (a,1) or (a,-1) appears in j. Moreover, if this is the case, we have

$$|\{I_a, z_j\}| \le 2|z_j|.$$

where we set

$$|z_{\boldsymbol{i}}| = |z_{i_1}| \cdots |z_{i_r}|$$

for $\boldsymbol{j}=(j_1,\ldots,j_r)\in\mathcal{Z}^r$. Hence we can write

$$|\{\mathbf{N}_s^N,Z\}(z)| \leq 2\sum_{|k| \leq N} |k|^{2s} \sum_{\{\boldsymbol{j} \in \mathcal{I}_r \backslash \mathcal{J}_r(N) | \boldsymbol{j} \supset k\}} |Z_{\boldsymbol{j}}| |z_{\boldsymbol{j}}|$$

where $k = (a, \pm 1) \in \mathcal{Z}$ in the first sum and the notation $j \supset k$ means that the index k belongs the set $\{j_1, \dots, j_r\}$. We thus get using (2.7)

$$|\{\mathsf{N}_s^N,Z\}(z)| \leq 2|Z|_{\mathcal{I}_r^{M,\nu}} \sum_{|k| \leq N} \sum_{\{\boldsymbol{j} \in \mathcal{I}_r \setminus \mathcal{J}_r(N) | \boldsymbol{j} \supset k\}} |k|^{2s} \frac{\mu(\boldsymbol{j})^{M+\nu}}{S(\boldsymbol{j})^M} |z_{\boldsymbol{j}}|.$$

Using Lemma 4.2, the indices in the previous sum are such that at least two of them are greater than N. As $|k| \leq N$, these indices cannot be equal to k. Hence we can rewrite each index j containing k as (\tilde{j}, k) where $\tilde{j} \in \mathbb{Z}^{r-1}$ contains at least two indices greater than N. Using the symmetries in the sum, we can moreover assume that the indices are ordered in such a way that $|j_1| > |j_2| > \dots$ Hence, we can rewrite the previous sum as

$$|\{\mathsf{N}_{s}^{N},Z\}(z)| \leq C|Z|_{\mathcal{I}_{r}^{M,\nu}} \sum_{\boldsymbol{j} \in \mathcal{Z}_{r-1}, |j_{1}|, |j_{2}| > N, |k| \leq N} |k|^{2s} \frac{\mu(\boldsymbol{j},k)^{M+\nu}}{S(\boldsymbol{j},k)^{M}} |z_{\boldsymbol{j}}| |z_{k}| \quad (5.1)$$

where $\mu(\boldsymbol{j},k)$ and $S(\boldsymbol{j},k)$ denote the values of μ and S associated with the r-tuple $(j_1,j_2,\ldots,j_{r-1},k)$. Here, C denotes a constant depending on r. Since $\mu(\boldsymbol{j},k) \leq S(\boldsymbol{j},k)$ and $\mu(\boldsymbol{j},k) \leq |j_2|$ we have for $M \geq 2$

$$|\{\mathsf{N}^N_s,Z\}(z)| \leq C|Z|_{\mathcal{T}^{M,\nu}_r} \sum_{\boldsymbol{j} \in \mathcal{Z}_{r-1}, \, |j_1|, |j_2| > N, \, |k| \leq N} |k|^{2s} \left(\frac{1}{1+|j_1|-|j_2|}\right)^2 |j_2|^{\nu+2} |z_{\boldsymbol{j}}| |z_k|.$$

Then use $|k| \leq |j_1|$ to obtain

$$|\{\mathsf{N}_{s}^{N},Z\}(z)| \leq C|Z|_{\mathcal{T}_{r}^{M,\nu}} \sum_{\boldsymbol{j}\in\mathcal{Z}_{r-1},\,|j_{1}|,|j_{2}|>N,\,|k|\leq N} \left(\frac{1}{1+|j_{1}|-|j_{2}|}\right)^{2} |j_{2}|^{\nu+2}|j_{1}|^{s}|z_{\boldsymbol{j}}||k|^{s}|z_{k}|.$$

$$(5.2)$$

By Cauchy-Schwarz, one has for s > 1/2

$$\sum_{l \in \mathcal{Z}} |z_l| \le ||z||_s \left(\sum_{l \in \mathcal{Z}} |l|^{-2s}\right)^{1/2} \tag{5.3}$$

and thus we get from (5.2)

$$|\{\mathsf{N}^N_s,Z\}(z)| \leq C|Z|_{\mathcal{T}^{M,\nu}_r} \, ||z||_s^{r-3} \sum_{|j_1|,|j_2|>N,\, |k|\leq N} \left(\frac{1}{1+|j_1|-|j_2|}\right)^2 |j_2|^{\nu+2} |j_1|^s |z_{\boldsymbol{j}}| |k|^s |z_k|.$$

Hence, introducing the sequence $(b_j)_{j\in\mathcal{Z}}=(|j|^s|z_j|)_{j\in\mathcal{Z}}\in\ell^2(\mathcal{Z})$ we can write

$$|\{\mathsf{N}_{s}^{N},Z\}(z)| \leq C|Z|_{\mathcal{T}_{r}^{M,\nu}} ||z||_{s}^{r-3} \sum_{|j_{1}|,|j_{2}|>N,\,|k|\leq N} \left(\frac{1}{1+|j_{1}|-|j_{2}|}\right)^{2} |j_{2}|^{\nu+2-s} b_{j_{2}} b_{j_{1}} b_{k}.$$

$$(5.4)$$

Moreover, the sum in $|k| \leq N$ in (5.4) yields by Cauchy-Schwarz inequality

$$\sum_{|k| \le N} b_k \le C N^{d/2} \sqrt{\mathsf{N}_s^N(z)} \le C N^{d/2} \|z\|_s \,.$$

where d is the dimension of $\mathcal{N}=\mathbb{N}^d$ or \mathbb{Z}^d . Hence, we get from (5.4) using $|j_2|>N$

$$|\{\mathsf{N}_s^N,Z\}(z)| \le CN^{-s+2+\nu+d/2}|Z|_{\mathcal{T}_r^{M,\nu}} ||z||^{r-2} \sum_{|j_1| > |j_2| > N} \left(\frac{1}{1+|j_1|-|j_2|}\right)^2 b_{j_2} b_{j_1}$$

and this concludes the proof of (4.1) since, if a and c are two sequences in $\ell^2(\mathcal{Z})$ we have by a convolution argument

$$\sum_{i,l} \left(\frac{1}{1+|j|-|l|} \right)^2 |a_l| \ |c_j| \le C||a||_{\ell^2(\mathcal{Z})} \ ||c||_{\ell^2(\mathcal{Z})}$$
 (5.5)

for some universal constant C.

Note that (4.2) is easily shown by similar calculations (the only difference lies in the fact that there is no summation in $|k| \leq N$).

We now show (4.3).

As R^N_s contains only indices greater than N, we can write (see (5.1))

$$|\{\mathsf{R}_{s}^{N}, Z\}(z)| \le C|Z|_{\mathcal{I}_{r}^{M,\nu}} \sum_{\mathbf{j} \in \mathcal{I}_{r-1}, |j_{1}| > N, |k| > N} |k|^{2s} \frac{\mu(\mathbf{j}, k)^{M+\nu}}{S(\mathbf{j}, k)^{M}} |z_{\mathbf{j}}| |z_{k}|$$
 (5.6)

where the sum is made over ordered indices $|j_1| > |j_2| > \cdots$. Note that in opposition with the previous situation, we cannot ensure that $|j_2| > N$ in this sum. We first notice that, for all k and j,

$$|k|\frac{\mu(\boldsymbol{j},k)}{S(\boldsymbol{j},k)} \le 2|j_1|,\tag{5.7}$$

Actually, if $|k| \leq 2j_1$ then (5.7) holds true since $\frac{\mu(j,k)}{S(j,k)} \leq 1$. Now if $k \geq 2j_1$ then $S(l,j) \geq ||k| - |j_1|| \geq 1/2|k|$ and thus

$$|k|\frac{\mu(\boldsymbol{j},k)}{S(\boldsymbol{j},k)} \le 2\mu(\boldsymbol{j},k) \le 2|j_1|.$$

Then we distinguish two cases in this sum (5.6):

$$|\{\mathsf{R}_{s}^{N},Z\}(z)| \leq C|Z|_{\mathcal{T}_{s}^{M,\nu}}(I_{1}+I_{2})$$

corresponding to the two cases $|j_2| \leq |k|$, (I_1) and $|k| < |j_2|$, (I_2) .

Case 1: $|j_2| \le |k|$

In this situation, we use (5.7), $\mu(\boldsymbol{j},k) = |j_2|, \ \mu(\boldsymbol{j},k) \leq S(\boldsymbol{j},k)$ to conclude for $M \geq s+2$

$$I_1 \leq 2^s \sum_{\boldsymbol{j} \in \mathcal{I}_{r-1}, \, |j_1| > N, \, |k| > N} |k|^s |j_1|^s \left(\frac{1}{1 + ||j_1| - |k||} \right)^2 |j_2|^{2 + \nu} |z_{\boldsymbol{j}}| |z_k|.$$

Then use (5.3) and the notation $(b_j)_{j\in\mathcal{Z}} = (|j|^s|z_j|)_{j\in\mathcal{Z}} \in \ell^2(\mathcal{Z})$ to get

$$\begin{split} I_1 &\leq 2^s ||z||_s^{r-3} \sum_{j_2,|j_1|>N,\,|k|>N} \left(\frac{1}{1+||j_1|-|k||}\right)^2 |j_2|^{2+\nu-s} b_{j_2} b_k b_{j_1} \\ &\leq C ||z||_s^{r-2} \mathsf{R}_s^N(z) \end{split}$$

where we have used again (5.5) for $\sum_{j_1,k}$ and (5.3) for \sum_{j_2} .

Case 2: $|j_2| \ge |k|$

In this situation, we still have $\mu(j,k) \leq |j_2|$ and using that both $|j_1|$ and $|j_2|$ are greater than |k| we get for $M \geq 2$

$$I_{2} \leq C \|z\|_{s}^{r-3} \sum_{|j_{1}| > N, |j_{2}| \geq |k| > N} |j_{1}|^{s} |j_{2}|^{s/2} |k|^{s/2} \left(\frac{1}{1 + |j_{1}| - |j_{2}|}\right)^{2} |j_{2}|^{2+\nu} |z_{j_{1}}| z_{k} ||z_{j_{2}}|$$

$$\leq C \|z\|_{s}^{r-3} \sum_{|j_{1}| > N, |j_{2}| \geq |k| > N} \left(\frac{1}{1 + |j_{1}| - |j_{2}|}\right)^{2} b_{j_{1}} \frac{b_{k}}{|k|^{s/2}} \frac{b_{j_{2}}}{|j_{2}|^{s/2 - 2 - \nu}}$$

$$\leq C \|z\|_{s}^{r-3} R_{s}^{N}(z)^{3/2}$$

where in the last inequality, we used that b_{j_1} , $\frac{b_k}{|k|^{s/2}}$ and $\frac{b_{j_2}}{|j_2|^{s/2-2-\nu}}$ are respectively in $\ell^2(\mathcal{Z})$, $\ell^1(\mathcal{Z})$ (for s > 1) and $\ell^2(\mathcal{Z})$ (for $s \ge 4 + 2\nu$) and we used again (5.5) and (5.3).

References

- [1] D. Bambusi, Birkhoff normal form for some nonlinear PDEs, Comm. Math. Physics 234 (2003), 253–283.
- [2] D. Bambusi, A birkhoff normal form theorem for some semilinear PDEs, Hamiltonian Dynamical Systems and Applications, Springer, 2007, pp. 213–247.
- [3] D. Bambusi, J.-M. Delort, B. Grébert, and J. Szeftel, Almost global existence for Hamiltonian semilinear Klein-Gordon equations with small Cauchy data on Zoll manifolds, Comm. Pure Appl. Math. 60 (2007), no. 11, 1665–1690.
- [4] D. Bambusi and B. Grébert, Birkhoff normal form for PDE's with tame modulus. Duke Math. J. 135 no. 3 (2006), 507-567.
- [5] D. Cohen, E. Hairer and C. Lubich, Long-time analysis of nonlinearly perturbed wave equations via modulated Fourier expansions, Arch. Ration. Mech. Anal. 187 (2008) 341-368.
- [6] D. Cohen, E. Hairer and C. Lubich, Conservation of energy, momentum and actions in numerical discretizations of nonlinear wave equations, Numerische Mathematik 110 (2008) 113–143.
- [7] J. M. Delort and J. Szeftel, Long-time existence for semi-linear Klein-Gordon equations with small cauchy data on Zoll manifolds, Amer. J. Math 128 (2006), 1187–1218.
- [8] A. Debussche and E. Faou, Modified energy for split-step methods applied to the linear Schrödinger equation, preprint (2009) http://hal.archives-ouvertes.fr/hal-00348221/fr/
- [9] P. Deuflhard A study of extrapolation methods based on multistep schemes without parasitic solutions. Z. angew. Math. Phys. 30 (1979) 177-189.
- [10] G. Dujardin and E. Faou, Normal form and long time analysis of splitting schemes for the linear Schrödinger equation with small potential. Numerische Mathematik 106, 2 (2007) 223–262
- [11] E. Faou, B. Grébert and E. Paturel, Birkhoff normal form for splitting methods applied to semi linear Hamiltonian PDEs. Part I: Finite dimensional discretization.
- [12] E. Hairer, R. I. McLachlan and A. Razakarivony, Achieving Brouwer's law with implicit Runge-Kutta methods, BIT 48 (2008) 231–243.
- [13] L. Gauckler and C. Lubich, Nonlinear Schrödinger equations and their spectral discretizations over long times, to appear in Found. Comput. Math. (2009).

- [14] L. Gauckler and C. Lubich, Splitting integrators for nonlinear Schrödinger equations over long times, to appear in Found. Comput. Math. (2009).
- [15] B. Grébert, Birkhoff normal form and Hamiltonian PDEs. Séminaires et Congrès 15 (2007), 1–46
- [16] B. Grébert, E. Paturel and R. Imekraz, Long time behavior for solutions of semilinear Schrödinger equation with harmonic potential and small Cauchy data on \mathbb{R}^d , to appear in Comm. Math. Phys. (2008)
- [17] E. Hairer and C. Lubich, Spectral semi-discretisations of weakly nonlinear wave equations over long times, Found. Comput. Math. 8 (2008) 319-334.
- [18] E. Hairer, C. Lubich and G. Wanner Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations. Second Edition. Springer 2006.
- [19] Z. Shang Resonant and Diophantine step sizes in computing invariant tori of Hamiltonian systems Nonlinearity 13 (2000), 299–308.