# Boundary effects on the dynamics of chains of coupled oscillators 

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#### Abstract

We study the dynamics of a chain of coupled particles subjected to a restoring force (Klein-Gordon lattice) in the cases of either periodic or Dirichlet boundary conditions. Precisely, we prove that, when the initial data are of small amplitude and have long wavelength, the main part of the solution is interpolated by a solution of the nonlinear Schrödinger equation, which in turn has the property that its Fourier coefficients decay exponentially. The first order correction to the solution has Fourier coefficients that decay exponentially in the periodic case, but only as a power in the Dirichlet case. In particular our result allows one to explain the numerical computations of the paper [BMP07].


## 1 Introduction.

The dynamics of chains of coupled particles has been the object of a huge number of studies, but only recently some numerical works (see [BG08, BMP07]) have shown that the boundary conditions have some relevance on FPU type investigations. The goal of the present paper is to study analytically the effects of the boundary conditions ( BC ) on the dynamics of a simple 1-dimensional model, namely the so called Klein Gordon lattice (coupled particles subjected to an on site restoring force). Precisely, we concentrate on the cases of periodic and of Dirichlet boundary conditions, and use the methods of normal form to study the dynamics. This leads to a quite clear understanding of the role of the boundary conditions and to an explanation of the numerical results of [BMP07]. On the contrary, our theory does not allow one to explain the results of [BG08].

More precisely, we study the dynamics of a large lattice corresponding to small amplitude initial data with long wavelength; we show that if the size $N$ is large enough and the amplitude of the initial excitation is of order $\mu:=\frac{1}{N}$, then the solution $z$ has the form

$$
\begin{equation*}
z=\mu z^{a}(t)+\mu^{2} z_{1}(t), \tag{1.1}
\end{equation*}
$$

up to times $|t| \leq \mathcal{O}\left(\mu^{-2}\right)$. In (1.1) $z^{a}$ is interpolated by a solution of the nonlinear Schrödinger equation (NLS) and has a behaviour which is independent of the BC. On the contrary $z_{1}$ depends on the BC. Precisely, its Fourier coefficients decrease exponentially in the periodic case, but only as $|k|^{-3}$ in the Dirichlet case.

The theory we develop in order to give the representation (1.1) provides a clear interpretation of the phenomenon. Indeed, it turns out that the normal form of the system is independent of the BC (and coincides with the NLS), but the coordinate transformation introducing the normal form has properties which are different in the periodic and in the Dirichlet case. In particular, in the Dirichlet case it maps sequences which decay fast into sequences which decay as $|k|^{-3}$. This introduces the slow decay in the Dirichlet case.

It should be pointed out that our result still depends on the size $N$ of the lattice. ${ }^{1}$ Nevertheless, we think that (within the range of validity of our result) we clearly show the role of the boundary conditions and provide a good interpretation of the numerical results.

The present situation has many similarities with the one occurring in the theory of the Navier Stokes equation (see e.g. [Tem91]), where it is well known that the spectrum of the solution depends on the boundary conditions. Moreover, we recall that a power law decay of localized object has been previously observed in nonlinear lattice dynamics in [DP03, Pey04, Fla98, GF05] and that the connection between the nonlinear Schrödinger equation and the dynamics of long chains of particles was studied in many papers (see e.g. [Kal89, KSM92, Sch98, GM06]).

The paper is organized as follows: in sect. 2 we present the model, state our main result and discuss its relation with numerical computations. In sect. 3 we give the proof of the normal form construction. In sect. 4 we use the normal form (in a way similar to that introduced in [BCP02, BP06, Bam05]) and deduce the proof of the decomposition (1.1). Some technical details are deferred to the appendix. Each section is split into several subsections.

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## 2 Main result

In this chapter we present the model, we recall some numerical simulations (see [BMP07]) which clearly show the dependence of the metastable Fourier decay

[^0]on the boundary conditions and we finally state the main theoretical result and use it to explain the numerics.

### 2.1 The model.

We consider a chain of particles described by the Hamiltonian function

$$
\begin{equation*}
H(p, q)=\sum_{j} \frac{p_{j}^{2}}{2}+\sum_{j} V\left(q_{j}\right)+\sum_{j} W\left(q_{j}-q_{j-1}\right) \tag{2.1}
\end{equation*}
$$

where $j$ runs from 0 to $N$ in the case of Dirichlet boundary conditions (DBC), namely $q_{0}=q_{N+1}=0$, while it runs from $-(N+1)$ to $N$ in the case of periodic boundary conditions (PBC), i.e. $q_{-N-1}=q_{N+1}$. The corresponding Hamilton equations are

$$
\begin{equation*}
\ddot{q}_{j}=-V^{\prime}\left(q_{j}\right)-W^{\prime}\left(q_{j}-q_{j-1}\right)+W^{\prime}\left(q_{j+1}-q_{j}\right) . \tag{2.2}
\end{equation*}
$$

We recall that the standard Fermi Pasta Ulam model is obtained by taking $V \equiv 0$ and $W(x)=\frac{x^{2}}{2}+\alpha \frac{x^{3}}{3}+\beta \frac{x^{4}}{4}$. Here instead we will take

$$
\begin{equation*}
V(x)=\frac{1}{2} x^{2}+\frac{1}{3} \alpha x^{3}+\frac{1}{4} \beta x^{4}, \quad W(x)=\frac{1}{2} a x^{2}, \alpha, \beta, a \geq 0 . \tag{2.3}
\end{equation*}
$$

Explicitly our Hamiltonian has the form

$$
\begin{align*}
H & =H_{0}+H_{1}+H_{2},  \tag{2.4}\\
H_{0}(p, q) & :=\sum_{j} \frac{p_{j}^{2}+q_{j}^{2}}{2}+a \frac{\left(q_{j}-q_{j-1}\right)^{2}}{2},  \tag{2.5}\\
H_{1}(p, q) & :=\alpha \sum_{j} \frac{q_{j}^{3}}{3}, \quad H_{2}(p, q):=\beta \sum_{j} \frac{q_{j}^{4}}{4} . \tag{2.6}
\end{align*}
$$

Remark 2.1. In the case where

$$
\begin{equation*}
V(x)=V(-x) \tag{2.7}
\end{equation*}
$$

the equations (2.2) with PBC are invariant under the involution $q_{j} \mapsto-q_{-j}$, $p_{j} \mapsto-p_{-j}$. As a consequence the submanifold of the periodic sequences which are also skew-symmetric, is invariant under the dynamics. For this reason when (2.7) is fulfilled the case of DBC is just a subcase of the case of PBC. This happens in the standard FPU model and also in the case of the Hamiltonian (2.1) with the potential (2.3) and $\alpha=0$. The case $\alpha \neq 0$ is the simplest one where a difference between DBC and PBC is possible.

Consider the vectors

$$
\hat{e}_{k}(j)= \begin{cases}\frac{\delta_{P D}}{\sqrt{N+1}} \sin \left(\frac{j k \pi}{N+1}\right), & k=1, \ldots, N,  \tag{2.8}\\ \frac{1}{\sqrt{N+1}} \cos \left(\frac{j k \pi}{N+1}\right), & k=-1, \ldots,-N, \\ \frac{1}{\sqrt{2 N+2}}, & k=0, \\ \frac{(-1)^{j}}{\sqrt{2 N+2}}, & k=-N-1,\end{cases}
$$



Figure 1: Averaged harmonic energies distribution. DBC (dots) and PBC (crosses) with $N=511, a=0.5, \mathcal{E}=0.001, T=10^{5}$. Panel (a): $\alpha$ model with $\alpha=0.25$. Panel (b): $\beta$ model with $\beta=0.25$.
then the Fourier basis is formed by $\hat{e}_{k}, k=1, \ldots, N$ and $\delta_{P D}=\sqrt{2}$ in the case of DBC, and by $\hat{e}_{k}, k=-N-1, \ldots, N$ and $\delta_{P D}=1$ in the case of PBC. Here we will treat in a unified way both the cases of DBC and PBC, thus we will not specify the set where the indexes $j$ and $k$ vary. Introducing the rescaled Fourier variables $\left(\hat{p}_{k}, \hat{q}_{k}\right)$ defined by

$$
\begin{equation*}
p_{j}=\sum_{k} \sqrt{\omega_{k}} \hat{p}_{k} \hat{e}_{k}(j), \quad q_{j}=\sum_{k} \frac{\hat{q}_{k}}{\sqrt{\omega_{k}}} \hat{e}_{k}(j) \tag{2.9}
\end{equation*}
$$

where the frequencies are defined by

$$
\begin{equation*}
\omega_{k}=\sqrt{1+4 a \sin ^{2}\left(\frac{k \pi}{2 N+2}\right)} \tag{2.10}
\end{equation*}
$$

the Hamiltonian $H_{0}$ is changed to

$$
\begin{equation*}
H_{0}=\sum_{k} \omega_{k} \frac{\hat{p}_{k}^{2}+\hat{q}_{k}^{2}}{2} . \tag{2.11}
\end{equation*}
$$

### 2.2 The phenomenon and its numerical evidence.

Let us define the energy of a normal mode and its time average by

$$
E_{k}:=\omega_{k} \frac{\hat{p}_{k}^{2}+\hat{q}_{k}^{2}}{2}, \quad\left\langle E_{k}\right\rangle(t):=\frac{1}{t} \int_{0}^{t} E_{k}(s) d s
$$

In the case of PBC the oscillators of index $k$ and $-k$ are in resonance, so the relevant quantity to be observed is the average $\overline{\left\langle E_{k}\right\rangle}=\frac{1}{2}\left(\left\langle E_{k}\right\rangle+\left\langle E_{-k}\right\rangle\right)$.



Figure 2: DBC with parameters $N=511, a=0.5, \alpha=0.1, T=10^{5}$. Panel (a): distribution of $\left\langle E_{k}\right\rangle$ in semi-log scale. Energy densities: $\mathcal{E}=0.05,0.025,0.01,0.005,0.001$. Panel (b): distribution of $\left\langle E_{k}\right\rangle$ in log-log scale. Energy densities: $\mathcal{E}=0.01,0.001,0.0001,0.00001$.

Take an initial datum with all the energy concentrated on the first Fourier mode with energy density $\mathcal{E} \equiv H_{0} / N=0.001$. Integrating the system numerically one can see that after a short transient time, the averages of the harmonic energies relax to well defined steady values, which persist for very long times. In figures 1 we plot in a semi-log scale the time-average energies $\left\langle E_{k}\right\rangle(T)$ (or $\left.\overline{\left\langle E_{k}\right\rangle}(T)\right)$ at time $T=10^{5}$ (subsequent to the relaxation time) as a function of the index $k$. The parameters in the two panels are $\alpha=0.25, \beta=0$ and $\alpha=0, \beta=0.25$ respectively. In both cases $a=0.5$. In each distribution the dots refer to the DBC case while the crosses pertain to the PBC one ${ }^{2}$.

While in panel (b) one clearly observes a perfect overlapping of the exponential part of the decays, in panel (a) a sharp difference arises. Indeed, while the PBC solution is once more characterized by an exponential distribution, in the case of DBC one sees a richer behavior: at an energy approximately equal to $10^{-8}$ there is crossover and a new regime appears. Nevertheless, a striking similarity among the exponential part of the two dynamics is evident.

To describe more carefully the situation in the case of DBC we plot in figures 2 four different distributions of the quantities $\left\langle E_{k}\right\rangle$, in a semi-log and in a loglog scale respectively. They correspond to different values of the energy density (see the caption). In the first panel we plot the first part of the distribution: we notice that by decreasing the energy density, the slope of the exponential decay of the low frequencies increases. In the second figure, instead, we focus our attention on the second part of the distribution: we see that the corresponding curves are parallel. So a change of energy only induces a translation. Except for the last part, that we will interpret as due to discreteness effects, the curves are very well interpolated by a straight line giving a power decay with an exponent close to -6 . A similar behavior is also obtained if one excites a few modes of large wave length.

[^1]
### 2.3 Explanation of the phenomenon.

In order to state our main result we need a topology in the phase space.
Definition 2.1. Let us define the spaces $\ell_{s, \sigma}^{2}$ of the sequences $p=\left\{\hat{p}_{k}\right\}$ s.t.

$$
\begin{equation*}
\|p\|_{s, \sigma}^{2}:=\mu \sum_{k}[k]^{2 s} \mathrm{e}^{2 \sigma|k|}\left|\hat{p}_{k}\right|^{2}<\infty, \quad[k]:=\max \{1,|k|\} \tag{2.12}
\end{equation*}
$$

and the phase spaces $\mathcal{P}_{s, \sigma}:=\ell_{s, \sigma}^{2} \times \ell_{s, \sigma}^{2} \ni(p, q)$.
The main part of the solution will be described by the NLS (its Hamiltonian will appear as the first term of the normal form, see Corollary 3.5), so we consider a smooth solution $\varphi(x, \tau)$ of the nonlinear Schrödinger equation

$$
\begin{equation*}
-\mathrm{i} \partial_{\tau} \varphi=-\partial_{x x} \varphi+\gamma \varphi|\varphi|^{2}, \quad \gamma:=\frac{3}{8 a}\left(\beta-\frac{10}{9} \alpha^{2}\right), \quad x \in \mathbb{T}:=\mathbb{R} / 2 \pi \mathbb{Z} \tag{2.13}
\end{equation*}
$$

For fixed $\tau$ we will measure the size of a function $\varphi$ by the norm

$$
\begin{equation*}
\|\varphi\|_{s, \sigma}^{2}:=\sum_{k}[k]^{2 s} \mathrm{e}^{2 \sigma|k|}\left|\hat{\varphi}_{k}\right|^{2} \tag{2.14}
\end{equation*}
$$

where $\hat{\varphi}_{k}$ are the Fourier coefficients of $\varphi$, which are defined by

$$
\begin{equation*}
\varphi(x):=\sum_{k} \hat{\varphi}_{k} \hat{e}_{k}^{c}(x) ; \tag{2.15}
\end{equation*}
$$

here $\hat{e}_{k}^{c}(x)$ is the continuous Fourier basis,

$$
\hat{e}_{k}^{c}:=\left\{\begin{array}{cc}
\frac{1}{\sqrt{\pi}} \cos k x & k>0  \tag{2.16}\\
\frac{1}{\sqrt{2 \pi}} & k=0 \\
\frac{\delta_{P D}}{\sqrt{\pi}} \sin (-k x) & k<0
\end{array} .\right.
$$

Remark that the definition of the norm (2.14) for interpolating functions differs from the definition (2.12) of the norm of sequences, because of the factor $\mu$ contained in the latter one.
Remark 2.2. The dynamics of (2.13) is well known [FT87, GK03]. Precisely, if $\gamma<\gamma^{*}$ with a suitable positive constant $\gamma^{*}$, then $\forall \sigma \geq 0$ there exists $0 \leq \sigma^{\prime}<\sigma$ such that from $\|\varphi(x, 0)\|_{s, \sigma}=1$ it follows $\|\varphi(x, t)\|_{s, \sigma^{\prime}} \leq C_{s} \sim 1$ for all times.

Corresponding to $\varphi(x, \tau)$ we define an approximate solution of the original model by

$$
\begin{equation*}
z_{j}^{a}(t) \equiv\left(p_{j}^{a}(t), q_{j}^{a}(t)\right):=\left(\operatorname{Re}\left(e^{i t} \varphi\left(\mu j, a \mu^{2} t\right)\right), \operatorname{Im}\left(e^{i t} \varphi\left(\mu j, a \mu^{2} t\right)\right)\right) \tag{2.17}
\end{equation*}
$$

Our main result concerns the comparison between $z^{a}(t)$ and the solution $z(t)$ of the original system with initial datum

$$
z(0):=\mu z^{a}(0)
$$

Theorem 2.1. Assume $\left\|\varphi^{0}(x)\right\|_{s, \sigma} \leq 1$, then $\forall T>0$ there exists $\mu^{*}>0$ with the following properties: if $\mu<\mu_{*}$ then there exists $z_{1}(t)$ defined for $|t| \leq T \mu^{-2}$ such that

$$
\begin{equation*}
z(t)=\mu z^{a}(t)+\mu^{2} z_{1}(t) \tag{2.18}
\end{equation*}
$$

where $z^{a}$ is the approximate solution just defined and,

$$
\begin{equation*}
\left\|z_{1}(t)\right\|_{s, \sigma^{\prime}} \leq C \tag{2.19}
\end{equation*}
$$

with

$$
\begin{array}{lll}
\frac{1}{2}<s, & \sigma^{\prime}>0 & \text { if } P B C \\
\frac{1}{2}<s<\frac{5}{2}, & \sigma^{\prime}=0 & \text { if } D B C \tag{2.20}
\end{array}
$$

The above result gives an upper estimate of the error $z_{1}(t)$. We want now to compute it at first order and for short times, i.e to construct the first correction to $z^{a}$. To this end we anticipate from the theory of next sections that the transformation putting the system in normal form is similar to the map $\varphi(x) \mapsto \varphi(x)+c \mu \varphi(x)^{2}$, with a suitable complex constant $c$. Now, the wanted correction will be constructed as follows: first introduce the normalizing coordinates, then evolve linearly the so obtained data, finally transform back to the original coordinates. To state in a precise way the result we assume, for simplicity, that $\varphi^{0}$ is purely imaginary, i.e. that the initial datum has zero velocity, and consider the complex function $\psi_{10}$ with Fourier coefficients given by

$$
\begin{equation*}
\left(\widehat{\psi_{10}}\right)_{k}:=\frac{\alpha}{6 \sqrt{2}}\left[4 e^{\mathrm{i} \omega_{k} t}-3 e^{2 \mathrm{i} t}-e^{-2 \mathrm{i} t}-6 \mathrm{i} e^{\mathrm{i} \omega_{k} t}+6 \mathrm{i}\right] \hat{\Phi}_{k} \tag{2.21}
\end{equation*}
$$

where $\Phi(x):=-\mathrm{i} \varphi^{0}(x)^{2}$, and let $z_{10} \equiv\left(p_{10}, q_{10}\right)$ be the sequence with

$$
\frac{p_{10, j}+\mathrm{i} q_{10, j}}{\sqrt{2}}=\psi_{10}(\mu j) .
$$

We have the following
Theorem 2.2. For any $0<b<1$, one has

$$
\begin{equation*}
\left\|z_{1}(t)-z_{10}(t)\right\|_{s, \sigma^{\prime}} \leq C \mu^{1-b}, \quad|t| \leq \frac{T}{\mu^{b}} \tag{2.22}
\end{equation*}
$$

The above theorems provide the interpretation for the numerical results of the previous paragraph. Referring to fig. 1, we identify the exponential part of the distribution as due to the main part of the solution, namely $z^{a}$, which is the same for both the boundary conditions. In the case of PBC , the inequality (2.19) implies that also the error $z_{1}$ is exponentially decreasing; thus the whole solution is in particular exponentially localized in Fourier space.

In the case of DBC the situation is different. Indeed the correction, namely $z_{1}$, is ensured to have coefficients such that the series with general term $|k|^{2 s}\left|\hat{z}_{1, k}(t)\right|^{2}$ is convergent; this is very close to say that

$$
\left|\hat{z}_{1, k}(t)\right|^{2}<\frac{C}{|k|^{2 s+1}}
$$

which, taking $s$ very close to $5 / 2$ essentially gives a power law decay like $|k|^{-6}$.
Then Theorem 2.2 shows that this is actually optimal, as seen by taking

$$
\begin{equation*}
\varphi^{0}(x)=\mathrm{i} \sin x \tag{2.23}
\end{equation*}
$$

(as in the numerical computations). Indeed in such a case one has

$$
\begin{equation*}
\hat{\Phi}_{k}=\left(\sin ^{2} x\right)_{k}^{\wedge} \sim \frac{1}{k^{3}} \tag{2.24}
\end{equation*}
$$

so that (2.22) shows that after a time of order 1 the energy of the $k$-th mode is of order $\mu^{2} / k^{6}$ as shown by the numerics.

## 3 The normal form construction.

In this part we introduce and use the methods of the normal form theory for the proof of our main result. Accordingly one looks for a canonical transformation putting the system in a simpler form.

### 3.1 Preliminaries and main claim.

We first need to introduce some notations:

- $z$ will denote a phase point. In particular a phase point can be represented using the coordinates $\left(p_{j}, q_{j}\right)$ of the lattice's particles or the Fourier coordinates $\left(\hat{p}_{k}, \hat{q}_{k}\right)$.
- In the phase space we will also use coordinates $\psi$ defined by

$$
\hat{\psi}_{k}:=\frac{\hat{p}_{k}+\mathrm{i} \hat{\mathrm{q}}_{k}}{\sqrt{2}}
$$

and, in real space

$$
\psi_{j}:=\sum_{k} \hat{\psi}_{k} \hat{e}_{k}(j)
$$

- Given a Hamiltonian function $H$, we will denote by $X_{H}$ the corresponding Hamiltonian vector field. Thus if one uses for example the variables ( $p_{j}, q_{j}$ ), one has

$$
X_{H}(p, q)=\left(-\frac{\partial H}{\partial q_{j}}, \frac{\partial H}{\partial p_{j}}\right) \quad \text { or } \quad X_{H}(\psi):=\left(\mathrm{i} \frac{\partial H}{\partial \bar{\psi}_{j}}\right)
$$

Correspondingly we will write the Hamilton equations of a Hamiltonian function $H$ by

$$
\dot{z}=X_{H}(z)
$$

- The Lie transform $\Phi_{\chi}^{1}$ generated by a Hamiltonian function $\chi$ is the time one flow of the corresponding Hamilton equations, namely

$$
\Phi_{\chi}^{1}:=\left.\Phi_{\chi}^{t}\right|_{t=1}, \quad \frac{d}{d t} \Phi_{\chi}^{t}(z)=X_{\chi}\left(\Phi_{\chi}^{t}(z)\right),\left.\quad \Phi_{\chi}^{t}\right|_{t=0}=\mathbb{I}
$$

- The Poisson bracket $\{f, g\}$ of two functions $f, g$ is defined by

$$
\{f, g\}:=d f X_{g} \equiv \sum_{j}\left(\frac{\partial f}{\partial q_{j}} \frac{\partial g}{\partial p_{j}}-\frac{\partial f}{\partial p_{j}} \frac{\partial g}{\partial q_{j}}\right)
$$

The normalizing transformation will be constructed by composing two Lie transforms $\mathcal{T}_{1}=\Phi_{\chi_{1}}^{1}$ and $\mathcal{T}_{2}=\Phi_{\chi_{2}}^{1}$ generated by two functions $\chi_{1}$ and $\chi_{2}$. Taking $\chi_{1}$ and $\chi_{2}$ to be homogeneous polynomials of degree 3 and 4 respectively, an elementary computation shows that

$$
\begin{align*}
H \circ \mathcal{T}_{1} \circ \mathcal{T}_{2} & =H_{0}  \tag{3.1}\\
& +\left\{\chi_{1}, H_{0}\right\}+H_{1}  \tag{3.2}\\
& +\left\{\chi_{2}, H_{0}\right\}+\frac{1}{2}\left\{\chi_{1},\left\{\chi_{1}, H_{0}\right\}\right\}+\left\{\chi_{1}, H_{1}\right\}+H_{2}  \tag{3.3}\\
& + \text { h.o.t. } \tag{3.4}
\end{align*}
$$

where the term (3.2) is a homogeneous polynomial of degree 3 , the term (3.3) has degree 4 and h.o.t denotes higher order terms. We will construct a function $\chi_{1}$ such that (3.2) vanishes and we will show that there exists a $\chi_{2}$ such that (3.3) is reduced to a form which as simple as possible, namely the normal form (see below for a precise definition).

To make precise the construction we need to split $H_{0}$ as follows

$$
\begin{align*}
H_{0} & =H_{00}+H_{01}, \quad H_{00}(z):=\sum_{k} \frac{\hat{p}_{k}^{2}+\hat{q}_{k}^{2}}{2},  \tag{3.5}\\
H_{01}(z) & :=\sum_{k} \nu_{k} \frac{\hat{p}_{k}^{2}+\hat{q}_{k}^{2}}{2}, \quad \nu_{k}:=\omega_{k}-1=a \frac{4 \sin ^{2}\left(\frac{k \pi}{2 N+2}\right)}{\omega_{k}+1} \leq 2 a
\end{align*}
$$

Definition 3.1. A polynomial $Z$ will be said to be in normal form if it Poisson commutes with $H_{00}$, i.e. if

$$
\begin{equation*}
\left\{H_{00}, Z\right\} \equiv 0 \tag{3.6}
\end{equation*}
$$

Remark 3.1. In order to study the system with DBC we will always extend the system to a system defined for $j=-(N+1), \ldots, N$ with PBC, which is invariant under the involution $q_{j} \mapsto-q_{-j}, p_{j} \mapsto-p_{-j}$. When $\alpha=0$ the extension is obtained without modifying the equations, while, when $\alpha \neq 0$, the extension is given by the system

$$
\begin{equation*}
\dot{q}_{j}=p_{j}, \quad \dot{p}_{j}=-q_{j}-a\left(\Delta_{1} q\right)_{j}-\alpha s_{j} q_{j}^{2}-\beta q_{j}^{3}, \tag{3.7}
\end{equation*}
$$

where $s_{j}$ is a discretization of the step function given by

$$
s_{j}:=\left\{\begin{array}{cl}
1 & \text { if } j \geq 1  \tag{3.8}\\
0 & \text { if } j=0 \\
-1 & \text { if } j \leq 1
\end{array}\right.
$$

and

$$
\begin{equation*}
\left(\Delta_{1} q\right)_{j}=2 q_{j}-q_{j+1}-q_{j-1} \tag{3.9}
\end{equation*}
$$

is the discrete Laplacian. The need of the introduction of the sequence $s_{j}$ is at the origin of the finite smoothness of the solution in the DBC case.

We are going to prove the following
Theorem 3.1. Assume $a<1 / 3$. Then, there exists an analytic canonical transformation $z=\mathcal{T}(\psi)$, defined in a neighborhood of the origin

$$
\begin{equation*}
H \circ \mathcal{T}=H_{0}(\psi)+Z(\psi)+\mathcal{R}(\psi), \tag{3.10}
\end{equation*}
$$

where $Z$ is in normal form and the following holds true

1) The remainder, the normal form and the canonical transformation are estimated by

$$
\begin{align*}
\left\|X_{\mathcal{R}}(\psi)\right\|_{s, \sigma} & \leq C_{\mathcal{R}}\|\psi\|_{s, \sigma}^{4}  \tag{3.11}\\
\left\|X_{Z}(\psi)\right\|_{s, \sigma} & \leq C_{Z}\|\psi\|_{s, \sigma}^{3}  \tag{3.12}\\
\|\psi-\mathcal{T}(\psi)\|_{s, \sigma} & \leq C_{\mathcal{T}}\|\psi\|_{s, \sigma}^{2} \tag{3.13}
\end{align*}
$$

where

$$
\begin{array}{lll}
\frac{1}{2}<s, & \sigma \geq 0 & \text { if } P B C  \tag{3.14}\\
\frac{1}{2}<s<\frac{5}{2}, & \sigma=0 & \text { if } D B C
\end{array}
$$

and $C_{\mathcal{R}, Z, \mathcal{T}}$ are constants independent of $N$.
2) One has $\mathcal{T}=\mathbb{I}+X_{\chi_{10}}+\mathcal{R}_{\mathcal{T}}$ with $\chi_{10}$ given by

$$
\begin{equation*}
\chi_{10}(\psi)=-\frac{\alpha}{6 \sqrt{2}} \sum_{j}\left(\frac{1}{3} \psi_{j}^{3}-\frac{\mathrm{i}}{3} \bar{\psi}_{j}^{3}+3 \psi_{j} \bar{\psi}_{j}^{2}-3 \mathrm{i} \psi_{j}^{2} \bar{\psi}_{j}\right) . \tag{3.15}
\end{equation*}
$$

and

$$
\begin{equation*}
\left\|\mathcal{R}_{\mathcal{T}}(\psi)\right\|_{s-s_{1}, \sigma} \leq C_{\mathcal{R}_{\mathcal{T}}} \mu^{s_{1}}\|\psi\|_{s, \sigma}^{2} \tag{3.16}
\end{equation*}
$$

where the parameters vary in the range

$$
\begin{gather*}
0 \leq s_{1}<s-\frac{1}{2}<2, \sigma=0 \text { for } D B C  \tag{3.17}\\
0 \leq s_{1}<s-\frac{1}{2}, s_{1} \leq 2, \sigma \geq 0 \text { for } P B C
\end{gather*}
$$

3) The normal form has the following structure

$$
Z(\psi, \bar{\psi})=Z_{0}+Z_{r}
$$

where

$$
\begin{equation*}
Z_{0}:=\tilde{\gamma} \sum_{j}\left|\psi_{j}\right|^{4}, \quad \tilde{\gamma}:=\frac{3}{8}\left(\beta-\frac{10}{9} \alpha^{2}\right) \tag{3.18}
\end{equation*}
$$

and

$$
\begin{equation*}
\left\|X_{Z_{r}}(\psi)\right\|_{s-s_{1}, \sigma} \leq \mu^{s_{1}} C_{r}\|\psi\|_{s, \sigma}^{3} \tag{3.19}
\end{equation*}
$$

with the parameters varying in the range (3.17).

The proof of this theorem is divided into three parts. In the first one we will prove an abstract normal form theorem under the assumption that the non-linearity corresponding to the system (2.4) is smooth. In the second part we will prove that this smoothness assumption is satisfied by the system under consideration. In the third part we will compute the first order term of the normal form and of the transformation and we will estimate the corresponding errors.

We point out that there are 3 delicate points in the proof: the first one is to solve the homological equation (see Lemma 3.3); the second one is to prove smoothness of the perturbation in the optimal space, and the third one is the actual computation of the main part of the normal form and of the canonical transformation.

### 3.2 An abstract normal form theorem.

First we recall that a homogeneous polynomial map $F: \mathcal{P}_{s, \sigma} \rightarrow \mathcal{P}_{s, \sigma}$ of degree $r$ is continuous and also analytic if and only if it is bounded, i.e. if there exists a constant $C$ such that

$$
\begin{equation*}
\|F(z)\|_{s, \sigma} \leq C\|z\|_{s, \sigma}^{r} \quad \forall z \in \mathcal{P}_{s, \sigma} \tag{3.20}
\end{equation*}
$$

Definition 3.2. The best constant such that (3.20) holds is called the norm of $F$, and will be denoted by $|F|_{s, \sigma}$. One has

$$
\begin{equation*}
\mid F \mathbf{|}_{s, \sigma}:=\sup _{\|z\|_{s, \sigma}=1}\|F(z)\|_{s, \sigma} \tag{3.21}
\end{equation*}
$$

Definition 3.3. A polynomial function $f$, homogeneous of degree $r+2$, will be said to be of class $\mathcal{H}_{s, \sigma}^{r}$ if its Hamiltonian vector field $X_{f}$ is bounded as a map from $\mathcal{P}_{s, \sigma}$ to itself.

Theorem 3.2. Let $H_{0}$ be as above (see (2.11)) with $a<1 / 3$. Assume that $H_{j} \in \mathcal{H}_{s, \sigma}^{j}$ for some fixed $s, \sigma$ and for $j=1,2$; then there exists an analytic
canonical transformation $\mathcal{T}=\mathcal{T}_{1} \circ \mathcal{T}_{2}$, defined in a neighborhood of the origin in $\mathcal{P}_{s, \sigma}$ such that

$$
\begin{equation*}
H \circ \mathcal{T}=H_{0}+Z+\mathcal{R} \tag{3.22}
\end{equation*}
$$

where $Z$ is in normal form and the remainder, the normal form and the canonical transformation are bounded by

$$
\begin{align*}
\left\|X_{\mathcal{R}}(z)\right\|_{s, \sigma} & \leq C_{\mathcal{R}}\|z\|_{s, \sigma}^{4}  \tag{3.23}\\
\left\|X_{Z}(z)\right\|_{s, \sigma} & \leq C_{Z}\|z\|_{s, \sigma}^{3}  \tag{3.24}\\
\|z-\mathcal{T}(z)\|_{s, \sigma} & \leq C_{\mathcal{T}}\|z\|_{s, \sigma}^{2} \tag{3.25}
\end{align*}
$$

with constants $C_{\mathcal{R}, Z, \mathcal{T}}$ depending only on a, $\left|X_{H_{1}}\right|_{s, \sigma},\left|X_{H_{2}}\right|_{s, \sigma}$.
The rest of this subsection will be occupied by the proof of Theorem 3.2. First we need some simple estimates.

Lemma 3.1. Let $f \in \mathcal{H}_{s, \sigma}^{r}$ and $g \in \mathcal{H}_{s, \sigma}^{r_{1}}$, then $\{f, g\} \in \mathcal{H}_{s, \sigma}^{r+r_{1}}$, and

$$
\begin{equation*}
\left|X_{\{f ; g\}}\right|_{s, \sigma} \leq\left(r+r_{1}+2\right)\left|X_{f}\right|_{s, \sigma}\left|X_{g}\right|_{s, \sigma} \tag{3.26}
\end{equation*}
$$

Proof. First remember that

$$
\begin{equation*}
X_{\{f, g\}}=\left[X_{f} ; X_{g}\right]=d X_{f} X_{g}-d X_{g} X_{f} \tag{3.27}
\end{equation*}
$$

We recall now that, given a polynomial $X$ of degree $r+1$, there exists a unique $(r+1)$-linear symmetric form $\widetilde{X}$ such that

$$
X(z)=\widetilde{X}(z, \ldots, z)
$$

then, (3.27) is explicitly given by

$$
\begin{equation*}
X_{\{f ; g\}}=(r+1) \widetilde{X}_{f}\left(X_{g}(z), z, z, \ldots, z\right)-\left(r_{1}+1\right) \widetilde{X}_{g}\left(X_{f}(z), z, z, \ldots, z\right) \tag{3.28}
\end{equation*}
$$

moreover from (3.21) one has

$$
\begin{equation*}
\left\|\widetilde{X}\left(z_{1}, \ldots, z_{r+1}\right)\right\|_{s, \sigma} \leq|X|_{s, \sigma}\left\|z_{1}\right\|_{s, \sigma} \cdots\left\|z_{r+1}\right\|_{s, \sigma} \tag{3.29}
\end{equation*}
$$

from which the thesis immediately follows.
Remark 3.2. Let $f \in \mathcal{H}_{s, \sigma}^{r}$, then the corresponding vector field generates a flow in a neighborhood of the origin in $\mathcal{P}_{s, \sigma}$.
Lemma 3.2. Let $\chi$ be of class $\mathcal{H}_{s, \sigma}^{r}$, and let $f \in \mathcal{H}_{s, \sigma}^{r_{1}}$. Let $\Phi_{\chi}^{1}$ be the Lie transform generated by $\chi$, then each term of the Taylor expansion of $f \circ \Phi_{\chi}^{1}$ is a polynomial with bounded vector field.

Proof. Iterating the relation

$$
\frac{d}{d t}\left(f \circ \Phi_{\chi}^{t}\right)=\{\chi, f\} \circ \Phi_{\chi}^{t}
$$

one gets that the Taylor expansion of $f \circ \Phi_{\chi}^{1}$ is given by

$$
\begin{aligned}
f \circ \Phi_{\chi}^{1} & =\sum_{l \geq 0} f_{l} \\
f_{0} & =f, \quad f_{l}=\frac{1}{l}\left\{\chi, f_{l-1}\right\}, \quad l \geq 1
\end{aligned}
$$

Then, the thesis follows from Lemma 3.1
A key role in the proof of Theorem 3.2 is played by the so called homological equation, namely

$$
\begin{equation*}
\left\{\chi_{j} ; H_{0}\right\}+f_{j}=Z_{j} \tag{3.30}
\end{equation*}
$$

where $f_{j} \in \mathcal{H}_{s, \sigma}^{j}$ is a given polynomial, and $\chi_{j} \in \mathcal{H}_{s, \sigma}^{j}, Z_{j} \in \mathcal{H}_{s, \sigma}^{j}$ are to be determined with the property that $Z_{j}$ is in normal form.
Lemma 3.3. Consider the homological equation (3.30) with $f_{j}$ of class $\mathcal{H}_{s, \sigma}^{j}$, with $j=1,2$. Assume that $a<\frac{1}{3}$, then (3.30) admits a solution $\chi_{j}, Z_{j} \in \mathcal{H}_{s, \sigma}^{j}$ with

$$
\begin{equation*}
\left|X_{\chi_{j}}\right|_{s, \sigma} \leq \frac{1}{2(1-3 a)}\left|X_{f_{j}}\right|_{s, \sigma} . \tag{3.31}
\end{equation*}
$$

Proof. First we rewrite the homological equation as

$$
\begin{equation*}
\left(L_{0}+L_{1}\right) \chi_{j}=f_{j}-Z_{j} \tag{3.32}
\end{equation*}
$$

where the operators $L_{0}$ and $L_{1}$ are defined by

$$
L_{0} \chi_{j}:=\left\{H_{00}, \chi_{j}\right\}, \quad L_{1} \chi_{j}:=\left\{H_{01}, \chi_{j}\right\}
$$

and $H_{00}$ and $H_{01}$ are defined by (3.5). We will invert $L_{0}$ and solve (3.32) by Neumann series (see [BDGS07]).

We begin by showing that the space $\mathcal{H}_{s, \sigma}^{j}, j \leq 2$ decompose into the sum of the kernel $\operatorname{Ker}\left(L_{0}\right)$ of $L_{0}$ and of its range $\operatorname{Im}\left(L_{0}\right)$. Moreover, we show that $L_{0}$ is invertible on its range.

Given $f \in \mathcal{H}_{s, \sigma}^{j}$ with $j=1,2$ define

$$
\begin{align*}
Z & :=\frac{1}{T} \int_{0}^{T} f\left(\Psi^{t}(z)\right) d t  \tag{3.33}\\
\chi & :=\frac{1}{T} \int_{0}^{T} t\left[f\left(\Psi^{t}(z)\right)-Z\left(\Psi^{t}(z)\right)\right] d t \tag{3.34}
\end{align*}
$$

where $\Psi^{t}$ is the flow of $X_{H_{00}}$ and $T=1$ is its period. Then an explicit computation shows that $Z \in \operatorname{Ker}\left(L_{0}\right)$, and that (see [BG93])

$$
\begin{equation*}
L_{0} \chi=f-Z \tag{3.35}
\end{equation*}
$$

Thus denoting by $Q$ the projector on the kernel of $L_{0}$, and $P=\mathbb{I}-Q$ the projector on the range, one sees that (3.33) is a concrete definition of $Q$, while (3.34) is the definition of $L_{0}^{-1}$ restricted to $\operatorname{Im}\left(L_{0}\right)$. It remains to show that $Z, \chi \in \mathcal{H}_{s, \sigma}^{j}$. Remark that, since $\Psi^{t}$ is a canonical transformation one has

$$
\begin{align*}
X_{Z}(z) & \equiv X_{Q f}(z)=\frac{1}{T} \int_{0}^{T}\left(\Psi^{-t} \circ X_{f} \circ \Psi^{t}\right)(z) d t  \tag{3.36}\\
X_{\chi}(z) & \equiv X_{L_{0}^{-1} P f}(z)=\frac{1}{T} \int_{0}^{T}\left(\Psi^{-t} \circ X_{P f} \circ \Psi^{t}\right)(z) t d t \tag{3.37}
\end{align*}
$$

From which it follows that

$$
\begin{align*}
\left|X_{Q f}\right|_{s, \sigma} & \leq\left|X_{f}\right|_{s, \sigma}  \tag{3.38}\\
\left|X_{L_{0}^{-1} P f}\right|_{s, \sigma} & \leq \frac{1}{2}\left|X_{P f}\right|_{s, \sigma} \leq \frac{1}{2}\left|X_{f}\right|_{s, \sigma} \Longrightarrow\left\|L_{0}^{-1}\right\| \leq \frac{1}{2} \tag{3.39}
\end{align*}
$$

where the last norm is the norm of $L_{0}^{-1}$ as a linear operator acting on the space $\mathcal{H}_{s, \sigma}^{j}$, and thus $Q f \in \mathcal{H}_{s, \sigma}^{j}, L_{0}^{-1} P f \in \mathcal{H}_{s, \sigma}^{j}$.

We come now to the true homological equation (3.32). We look for a solution $\chi_{j}=P \chi_{j}$ and $Z_{j}=Q Z_{j}$. Applying $P$ or $Q$ to (3.32), remarking that since $\left[L_{0}, L_{1}\right]=0$ one has $\left[P, L_{1}\right]=\left[Q, L_{1}\right]=0$, we get

$$
\begin{equation*}
\left(L_{0}+L_{1}\right) \chi_{j}=P f_{j}, \quad Q f_{j}=Z_{j} \tag{3.40}
\end{equation*}
$$

The first equation of (3.40) is formally solved by Neumann series, i.e. defining

$$
\begin{equation*}
\left(L_{0}+L_{1}\right)^{-1}:=\sum_{k \geq 0}(-1)^{k}\left(L_{0}^{-1} L_{1}\right)^{k} L_{0}^{-1}, \quad \chi_{j}:=\left(L_{0}+L_{1}\right)^{-1} P f_{j} \tag{3.41}
\end{equation*}
$$

To show the convergence of the series in operator norm we need an estimate of $\left\|L_{1}\right\|$. To this end remark that, for any $s, \sigma$ one has

$$
\left|X_{H_{01}}\right|_{s \sigma} \leq 2 a
$$

which using Lemma 3.1 implies $\left\|L_{1}\right\| \leq 2 a(j+1) \leq 6 a$. It follows that the series (3.41) converges provided $a<1 / 3$, which is our assumption, and that

$$
\begin{equation*}
\left\|\left(L_{0}+L_{1}\right)^{-1}\right\| \leq \frac{1}{2(1-3 a)}, \tag{3.42}
\end{equation*}
$$

which concludes the proof.
End of the proof of Theorem 3.2. From Lemma 3.3 one has that the solution $\chi_{1}$ of the homological equation with $f_{1} \equiv H_{1}$ is well defined provided $H_{1} \in \mathcal{H}_{s, \sigma}^{1}$ for some $s, \sigma$. Then $\chi_{1}$ generates a Lie transform $\mathcal{T}_{1}$ which puts the system in normal form up to order 4 . Then the part of degree four of $H \circ \mathcal{T}_{1}$ takes the form

$$
\begin{equation*}
f_{2}:=\frac{1}{2}\left\{\chi_{1},\left\{\chi_{1}, H_{0}\right\}\right\}+\left\{\chi_{1}, H_{1}\right\}+H_{2} \equiv \frac{1}{2}\left\{\chi_{1}, H_{1}\right\}+H_{2} \tag{3.43}
\end{equation*}
$$

which is of class $\mathcal{H}_{s, \sigma}^{2}$. It follows that one can use the homological equation with such a known term and determine a $\chi_{2}$ which generates the Lie transformation putting the system in normal form up to order 4. This concludes the proof of Theorem 3.2.

### 3.3 Proof of the smoothness properties of the nonlinearity

In this subsection we prove the following lemma
Lemma 3.4. Let $H_{j}, j=1,2$ be given by (2.4). Consider the vector fields $X_{H_{j}}$ of the cubic and of the quartic terms of the Hamiltonian: they fulfill the estimates

$$
\left\|X_{H_{1}}(z)\right\|_{s, \sigma} \leq G_{1}\|z\|_{s, \sigma}^{2}, \quad\left\{\begin{array}{cll}
\frac{1}{2}<s, & \sigma \geq 0 & \text { if PBC }  \tag{3.44}\\
\frac{1}{2}<s<\frac{5}{2}, & \sigma=0 & \text { if DBC }
\end{array}\right.
$$

and

$$
\begin{equation*}
\left\|X_{H_{2}}(z)\right\|_{s, \sigma} \leq G_{2}\|z\|_{s, \sigma}^{3}, \quad \frac{1}{2}<s, \sigma \geq 0 \text { both cases } \tag{3.45}
\end{equation*}
$$

where we set $G_{j}:=\left|X_{H_{j}}\right|_{s, \sigma}$.
The proof will be split into two parts. First we show that it is possible to prove the result working on interpolating functions, and then we show that the "interpolating nonlinearities" have a smooth vector field when the parameters $s, \sigma$ vary in the considered range.
Remark 3.3. Define $T_{l}$ as the $\operatorname{map} q_{j} \mapsto q_{j}^{l+1}$ in the case of PBC, and $\left[T_{1}(q)\right]_{j}=$ $q_{j}^{2} s_{j}$ and $\left[T_{2}(q)\right]_{j}:=q_{j}^{3}$ in the case of DBC. Then the vector field $X_{H_{l}}$ has only $p$ components, moreover the norms are defined in terms of the Fourier variables, so we have to estimate the map constructed as follows

$$
\begin{aligned}
& \hat{q}_{k} \stackrel{1}{\mapsto} \hat{q}_{k}^{S}:=\frac{\hat{q}_{k}}{\sqrt{\omega_{k}}} \stackrel{\mathcal{F}}{\mapsto} q_{j}:=\sum_{k} \hat{q}_{k}^{S} \hat{e}_{k}(j) \mapsto T_{l}\left(q_{j}\right) \stackrel{\mathcal{F}^{-1}}{\mapsto} \\
& \stackrel{\mathcal{F}^{-1}}{\mapsto} p_{k}^{S}:=\sum_{j} q_{j}^{l+1} \hat{e}_{k}(j) \stackrel{2}{\mapsto} \hat{p}_{k}:=\sqrt{\omega_{k}} p_{k}^{S}
\end{aligned}
$$

It is immediate to realize that the maps 1 and 2 are smooth (the frequencies are between 1 and 3 ) so it is enough to estimate the remaining maps. The remaining maps essentially coincide with the map $T_{l}(q)$ read in terms of standard Fourier variables (without the factors $\sqrt{\omega_{k}}$ ). These are the maps we will estimate.

All along this section we will use a definition of the Fourier coefficients of a sequence not including the factors $\sqrt{\omega_{k}}$, namely we define $\hat{q}_{k}$ by

$$
q_{j}=\sum_{k} \hat{q}_{k} \hat{e}_{k}(j)
$$

We start by showing how to use the interpolation in order to make estimates. To this end we define an interpolation operator $I$ by

$$
\begin{equation*}
[I(q)](x):=\sum_{k} \sqrt{\mu} \hat{q}_{k} \hat{e}_{k}^{c}(x) \tag{3.46}
\end{equation*}
$$

We also define a restriction operator $R$ that associates to a function the corresponding sequence, by

$$
\begin{equation*}
[R(u)]_{j}:=u(\mu j) \tag{3.47}
\end{equation*}
$$

We remark that the operator $R$ is defined on functions which do not necessarily have finitely many non-vanishing Fourier coefficients.
Remark 3.4. With the definition (2.14) one has

$$
\begin{equation*}
\|I q\|_{s, \sigma}=\|q\|_{s, \sigma} \tag{3.48}
\end{equation*}
$$

Lemma 3.5. For any $s>1 / 2$ there exists a constant $C_{6}(s)$ such that one has

$$
\begin{equation*}
\|R u\|_{s, \sigma} \leq C_{6}\|u\|_{s, \sigma} \tag{3.49}
\end{equation*}
$$

Proof. Denote $q_{j}=(R u)_{j}$; using the formula

$$
\begin{equation*}
\hat{e}_{k}^{c}(\mu j)=\hat{e}_{k+2(N+1) m}^{c}(\mu j)=\frac{1}{\sqrt{\mu}} \hat{e}_{k}(j) \tag{3.50}
\end{equation*}
$$

one gets
$q_{j}=\sum_{k \in \mathbb{Z}} \hat{u}_{k} \hat{e}_{k}^{c}(\mu j)=\sum_{k=-(N+1)}^{N} \sqrt{\mu} \hat{e}_{k}^{c}(\mu j) \sum_{m \in \mathbb{Z}} \frac{\hat{u}_{k+2(N+1) m}}{\sqrt{\mu}}=\sum_{k=-(N+1)}^{N} \hat{e}_{k}(j) \hat{q}_{k}$,
from which

$$
\begin{equation*}
\hat{q}_{k}=\sum_{m \in \mathbb{Z}} \frac{\hat{u}_{k+2(N+1) m}}{\sqrt{\mu}} . \tag{3.51}
\end{equation*}
$$

Let's define
$\gamma_{m, k}(s, \sigma):=\frac{[k]^{s} e^{\sigma|k|}}{[k+2(N+1) m]^{s} e^{\sigma|k+2(N+1) m|}}=\left(\frac{[k]}{[k+2(N+1) m]}\right)^{s} \frac{e^{\sigma|k|}}{e^{\sigma|k+2(N+1) m|}}$ and replace (3.51) in the norm $\|q\|_{s, \sigma}^{2}$, then we get

$$
\begin{aligned}
\|q\|_{s, \sigma}^{2} & =\mu \sum_{k=-(N+1)}^{N}[k]^{2 s} e^{2 \sigma|k|}\left|\hat{q}_{k}\right|^{2}= \\
& =\sum_{k=-(N+1)}^{N}[k]^{2 s} e^{2 \sigma|k|}\left|\sum_{m \in \mathbb{Z}} \hat{u}_{k+2(N+1) m}\right|^{2}= \\
& =\sum_{k=-(N+1)}^{N}[k]^{2 s} e^{2 \sigma|k|}\left|\sum_{m \in \mathbb{Z}} \frac{\gamma_{m, k}(s, \sigma)}{\gamma_{m, k}(s, \sigma)} \hat{u}_{k+2(N+1) m}\right|^{2} \leq \\
& \leq \sum_{k=-(N+1)}^{N}\left(\sum_{m \in \mathbb{Z}} \gamma_{m, k}^{2}(s, \sigma)\right) \sum_{m \in \mathbb{Z}} \frac{[k]^{2 s} e^{2 \sigma|k|}}{\gamma_{m, k}^{2}(s, \sigma)}\left|\hat{u}_{k+2(N+1) m}\right|^{2} \leq \\
& \leq C_{6}(s)\|u\|_{s, \sigma}^{2} .
\end{aligned}
$$

Indeed, since $k=-(N+1), \ldots, N$, we can estimate the two factors of $\gamma_{m, k}$ as follows:

$$
|2(N+1) m+k| \geq|2(N+1)| m|-|k|| \geq\left\{\begin{array}{l}
|k|, \quad m=0, \\
N+1 \geq|k|, \quad m \neq 0
\end{array}\right.
$$

which gives

$$
\frac{e^{\sigma|k|}}{e^{\sigma|k+2(N+1) m|}} \leq 1
$$

$$
\frac{[k]}{[k+2(N+1) m]}=\left\{\begin{array}{l}
\frac{1}{[2(N+1) m \mid}<\frac{1}{\mid 2 m]}, \quad m=0, \\
\frac{|k|}{|k+2(N+1) m|} \leq \frac{1}{1+2 m}<\frac{1}{\mid 2 m]}, \quad m \neq 0
\end{array}\right.
$$

which gives

$$
\left(\frac{[k]}{[k+2(N+1) m]}\right)^{2 s} \leq \frac{1}{[2 m]^{2 s}}
$$

Corollary 3.3. Let $T: \mathbb{R}^{2(N+1)} \rightarrow \mathbb{R}^{2(N+1)}$ be a polynomial map, assume that there exists an "interpolating polynomial map $T^{c}$ " such that $T=R T^{c} I$. If the map $T^{c}$ is bounded in some space $H^{s, \sigma}$, with $s>1 / 2$, then $T$ is bounded in $\ell_{s, \sigma}^{2}$. Moreover one has

$$
\begin{equation*}
|T|_{s, \sigma} \leq C_{6}\left|T^{c}\right|_{s, \sigma} \tag{3.52}
\end{equation*}
$$

Now we define the interpolating maps we have to study. They are $T_{l}^{c}(u):=$ $u^{l+1}$ in the case of PBC and $T_{1}^{c}(u)=\operatorname{sgn}(x) u^{2}(x)$ and $T_{2}^{c}(u):=u^{3}$ in the case of DBC. Here we introduced the function

$$
\operatorname{sgn}(x):=\left\{\begin{array}{cl}
1 & \text { if } x>0 \\
0 & \text { if } x=0 \\
-1 & \text { if } x<1
\end{array}\right.
$$

The estimates (3.44) in the case of PBC and (3.45) for both boundary conditions are proved in Lemma A. 1 by a standard argument on the Sobolev norm of the product of two functions. We come to the estimate of $T_{1}^{c}$ in the case of DBC.

We will denote by $H_{o}^{s}$ the subspace of $H^{s, 0}$ composed by the odd functions $u(x)$ on $[-\pi, \pi]$.
Lemma 3.6. For any $1 / 2<s<5 / 2$, The operator

$$
T_{1}^{c}(u):=u^{2} \operatorname{sgn}(x)
$$

is smooth from $H_{o}^{s}$ in itself and there exists $C_{7}(s)$ such that

$$
\left\|T_{1}^{c} u\right\|_{s} \leq C_{7}\|u\|_{s}^{2}
$$

Proof. We begin with the case $2 \leq s<\frac{5}{2}$. First, observe that the function $T_{1}^{c}(u)$ is odd when $u$ is odd. We will prove the thesis by showing that the second weak derivative $d^{2} T_{1}^{c}(u)$ of $T_{1}^{c}(u)$ is in $H_{o}^{s-2}$. First remark that, by an explicit computation which exploits the fact that $u(0)=0$ one has

$$
d^{2} T_{1}^{c}(u)=2\left[\operatorname{sgn}(x)\left(u^{\prime 2}\right)+\operatorname{sgn}(x) u d^{2} u\right]
$$

We show now that both terms are in $H_{o}^{s-2}$. The second term can be considered as the product of the function $d^{2} u \in H_{o}^{s-2}$ and of $\operatorname{sgn}(x) u$. This last function is of class $H^{1}$, as it is seen by computing its derivative, namely

$$
d(\operatorname{sgn}(x) u)=\operatorname{sgn}(x) d u(x)+\delta(x) u(x)=\operatorname{sgn}(x) d u(x)
$$

which clearly belongs to $L^{2}$. From Lemma A. 1 it follows that the product $\operatorname{sgn}(x) u\left[d^{2} u\right] \in H^{s-2}$.

Concerning the term $\operatorname{sgn}(x)\left(u^{2}\right)$, it can be considered as the product of $u^{\prime 2} \in H^{s-1}$ and of $\operatorname{sgn}(x)$, which is of class $H_{o}^{r}$ for all $r<1 / 2$, as it can be seen by explicitly computing its Fourier coefficients. Thus Lemma A. 1 gives the result.

The case $1 \leq s<2$ is easier and works in a very similar way. Indeed, since $u(x) \operatorname{sgn}(x) \in H^{1}$ and $d u(x) \in H^{s}$ with $0 \leq s<1$, the derivative $d\left(u^{2}(x) \operatorname{sgn}(x)\right)=2 u(x)(d u(x)) \operatorname{sgn}(x)$ belongs to $H^{s}$ with $0 \leq s<1$, which gives the thesis.

Quite different is the case $\frac{1}{2}<s<1$, since by hypothesis no weak derivative exists for the function $u(x)$. We exploit the following equivalent definition of the norm of the Sobolev space $H_{o}^{s}([-\pi, \pi])$ with real exponent $s$

$$
\begin{equation*}
\|u\|_{s}^{2}:=\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{|u(x)-u(y)|^{2}}{|x-y|^{1+2 s}} d x d y \tag{3.53}
\end{equation*}
$$

and the skew-symmetry of the periodic function $u(x) \in H_{o}^{s}$. We want to prove that $g(x):=u(x) \operatorname{sgn}(x) \in H^{s}$ with $\frac{1}{2}<s<1$; more precisely

$$
\begin{equation*}
\|u(x) \operatorname{sgn}(x)\|_{s}^{2}<4\|u(x)\|_{s}^{2}, \quad \frac{1}{2}<s<1 \tag{3.54}
\end{equation*}
$$

The symmetries of $g(x)$ on the given domain allow to simplify the integral in (3.53)

$$
\begin{aligned}
\|g\|_{s}^{2} & =2 \int_{0}^{\pi} \int_{-\pi}^{\pi} \frac{|g(x)-g(y)|^{2}}{|x-y|^{1+2 s}} d x d y= \\
& =2 \int_{0}^{\pi} \int_{0}^{\pi}\left[\frac{|g(x)-g(y)|^{2}}{|x-y|^{1+2 s}}+\frac{|g(x)-g(y)|^{2}}{|x+y|^{1+2 s}}\right] d x d y= \\
& =2 \int_{0}^{\pi} \int_{0}^{\pi}\left[\frac{|u(x)-u(y)|^{2}}{|x-y|^{1+2 s}}+\frac{|u(x)-u(y)|^{2}}{|x+y|^{1+2 s}}\right] d x d y \leq \\
& \leq 4 \int_{0}^{\pi} \int_{0}^{\pi} \frac{|u(x)-u(y)|^{2}}{|x-y|^{1+2 s}} d x d y<4\|u\|_{s}^{2} .
\end{aligned}
$$

### 3.4 Computation of the normal form and of the transformation.

In this section we will concentrate on the case of DBC which is the most difficult one. Indeed in the case of PBC the formal computations are identical, but the estimates are less delicate.

Consider again the Hamiltonian (2.4), introduce complex variables $\xi_{j}, \eta_{j}$ defined by

$$
\begin{equation*}
\xi_{j}=\frac{p_{j}+\mathrm{i} q_{j}}{\sqrt{2}}, \quad \eta_{j}=\frac{p_{j}-\mathrm{i} q_{j}}{\mathrm{i} \sqrt{2}} \tag{3.55}
\end{equation*}
$$

and split $H_{0}=\mathcal{H}_{00}+\mathcal{H}_{01}$ with

$$
\begin{align*}
\mathcal{H}_{00} & :=\sum_{j} \frac{p_{j}^{2}+q_{j}^{2}}{2} \equiv \mathrm{i}\langle\xi ; \eta\rangle_{\ell^{2}}  \tag{3.56}\\
\mathcal{H}_{01} & :=\sum_{j} \frac{a}{2}\left(q_{j}-q_{j-1}\right)^{2} \equiv \frac{a}{2}\left\langle\frac{\xi-\mathrm{i} \eta}{\mathrm{i} \sqrt{2}} ;-\Delta_{1} \frac{\xi-\mathrm{i} \eta}{\mathrm{i} \sqrt{2}}\right\rangle_{\ell^{2}} \tag{3.57}
\end{align*}
$$

where $\langle\xi ; \eta\rangle_{\ell^{2}}:=\sum_{j} \xi_{j} \eta_{j}$.
Remark 3.5. The above splitting is different from the one introduced in (3.5) which had been used in the proof of Lemma 3.3, and which was based on the Fourier variables. In particular one has $\left\{H_{00} ; H_{01}\right\} \equiv 0$, but $\left\{\mathcal{H}_{00} ; \mathcal{H}_{01}\right\} \not \equiv 0$.

In the variables $(\xi, \eta)$ the flow $\Phi^{t}$ of $\mathcal{H}_{00}$ acts as follows

$$
\Phi^{t}(\xi, \eta):=\left\{\begin{array}{l}
\xi_{j} \mapsto e^{\mathrm{i} t} \xi_{j},  \tag{3.58}\\
\eta_{j} \mapsto e^{-\mathrm{it} t} \eta_{j} .
\end{array}\right.
$$

The third order part of the Hamiltonian takes the form

$$
\begin{equation*}
H_{1}=\frac{\alpha}{3} \sum_{j}\left(\frac{\xi_{j}-\mathrm{i} \eta_{j}}{\mathrm{i} \sqrt{2}}\right)^{3} s_{j} \tag{3.59}
\end{equation*}
$$

where $s_{j}$ is the discrete step function defined in (3.8). The form of $H_{2}$ will be given below.

Denoting

$$
\begin{equation*}
\mathcal{L}_{0}:=\left\{\mathcal{H}_{00}, .\right\}, \quad \mathcal{L}_{1}:=\left\{\mathcal{H}_{01} ; .\right\} \tag{3.60}
\end{equation*}
$$

we rewrite the homological equation for $\chi_{1}$ as follows

$$
\begin{equation*}
\left(\mathcal{L}_{0}+\mathcal{L}_{1}\right) \chi_{1}=H_{1} \tag{3.61}
\end{equation*}
$$

which is solvable since the kernel of $\mathcal{L}_{0}+\mathcal{L}_{1}=L_{0}+L_{1}$ on polynomials of third order is empty. The solution $\chi_{1}$ of (3.61) is unique and, as shown in Lemma 3.3, exists.

By a direct computation one has

$$
\begin{equation*}
\chi_{1}=\mathcal{L}_{0}^{-1} H_{1}-\left(\mathcal{L}_{0}+\mathcal{L}_{1}\right)^{-1} \mathcal{L}_{1} \mathcal{L}_{0}^{-1} H_{1} ; \tag{3.62}
\end{equation*}
$$

we are going to show that the second term is much smaller than the first one. Before starting, a couple of remarks are in order.

Remark 3.6. The discrete Laplacian is $\ell^{2}$-symmetric on periodic sequences

$$
\begin{equation*}
<\Delta_{1} \xi, \eta>_{\ell^{2}}=<\xi, \Delta_{1} \eta>_{\ell^{2}} \tag{3.63}
\end{equation*}
$$

This is an immediate consequence of the fact that in Fourier variables it acts as a multiplier by a real factor.
Remark 3.7. In Fourier coordinates the discrete Laplacian $\Delta_{1}$ defined in (3.9) acts as a multiplier by $\sin ^{2} k \mu$. It follows that it has norm 1 when acting on anyone of the spaces $\ell_{s, \sigma}^{2}$. Moreover, since

$$
\left|\sin ^{2}(k \mu)\right| \leq k^{s_{1}} \mu^{s_{1}}, \quad s_{1} \in[0,2], \quad k \mu \in[0, \pi]
$$

one also has

$$
\begin{equation*}
\left\|\Delta_{1} \xi\right\|_{s-s_{1}, \sigma} \leq \mu^{s_{1}}\|\xi\|_{s, \sigma}, \quad s_{1} \in[0,2] . \tag{3.64}
\end{equation*}
$$

From (3.64) and (3.57) it follows

$$
\begin{equation*}
\left\|X_{\mathcal{H}_{01}}(\xi, \eta)\right\|_{s-s_{1}, 0} \leq C(a) \mu^{s_{1}}\|(\xi, \eta)\|_{s, 0}, \quad 0 \leq s_{1}<s-\frac{1}{2} \tag{3.65}
\end{equation*}
$$

Lemma 3.7. Assume $a<\frac{1}{3}$, then $\chi_{1}=\chi_{10}+\chi_{1 r}$ with

$$
\chi_{10}(\xi, \eta)=\frac{\alpha}{6 \sqrt{2}} \sum_{j}\left(\frac{1}{3} \xi_{j}^{3}-\frac{\mathrm{i}}{3} \eta_{j}^{3}+3 \xi_{j} \eta_{j}^{2}-3 \mathrm{i} \xi_{j}^{2} \eta_{j}\right)
$$

and there exists $C_{8}\left(a, G_{1}\right)$ such that

$$
\begin{equation*}
\left\|X_{\chi_{1 r}}(\xi, \eta)\right\|_{s-s_{1}, \sigma} \leq C_{8} \mu^{s_{1}}\|(\xi, \eta)\|_{s, \sigma}^{2} \tag{3.66}
\end{equation*}
$$

with

$$
\left\{\begin{array}{c}
0 \leq s_{1}<s-\frac{1}{2}<2, \sigma=0 \text { for } D B C \\
0 \leq s_{1}<s-\frac{1}{2}, s_{1} \leq 2 \sigma \geq 0 \text { for } P B C
\end{array}\right.
$$

Proof. According to (3.62), let's define

$$
\chi_{10}:=\mathcal{L}_{0}^{-1} H_{1}, \quad \quad \chi_{1 r}:=-\left(\mathcal{L}_{0}+\mathcal{L}_{1}\right)^{-1} \mathcal{L}_{1} \chi_{10}=-\left(L_{0}+L_{1}\right)^{-1} \mathcal{L}_{1} \chi_{10}
$$

Since $\chi_{10}$ solves the homological equation $\left\{\mathcal{H}_{00}, \chi_{10}\right\}=H_{1}$, it can be explicitly computed by

$$
\begin{aligned}
\chi_{10}(\xi, \eta) & =\int_{0}^{1} H_{1}\left(\Phi^{t}(\xi, \eta)\right) d t= \\
& =-\frac{\alpha}{6 \sqrt{2}} \sum_{j} s_{j}\left(-\frac{1}{3} \xi_{j}^{3}+\frac{\mathrm{i}}{3} \eta_{j}^{3}-3 \xi_{j} \eta_{j}^{2}+3 \mathrm{i} \xi_{j}^{2} \eta_{j}\right)
\end{aligned}
$$

which also implies

$$
\left|X_{\chi_{10}}\right|_{s, \sigma} \leq \frac{1}{2}\left|X_{H_{1}}\right|_{s, \sigma}
$$

The thesis follows from (3.28), (3.42) and (3.64).
We move to the second homological equation

$$
\begin{equation*}
\left\{\chi_{2}, H_{0}\right\}+\tilde{H}_{2}=Z \tag{3.67}
\end{equation*}
$$

where $\tilde{H}_{2}=H_{2}+\frac{1}{2}\left\{\chi_{1}, H_{1}\right\}$ can be split according to (3.62) into $\tilde{H}_{2}=\tilde{H}_{20}+\tilde{H}_{21}$ with

$$
\begin{equation*}
\tilde{H}_{20}:=H_{2}+\frac{1}{2}\left\{\chi_{10}, H_{1}\right\}, \quad \tilde{H}_{21}:=\frac{1}{2}\left\{\chi_{1 r}, H_{1}\right\} \tag{3.68}
\end{equation*}
$$

More explicitly, the leading term $\tilde{H}_{20}$ is composed of

$$
\begin{aligned}
\frac{1}{2}\left\{\chi_{10}, H_{1}\right\} & =\frac{\alpha^{2}}{24} \sum_{j}\left(\xi_{j}^{4}+4 \mathrm{i} \xi_{j}^{3} \eta_{j}+10 \xi_{j}^{2} \eta_{j}^{2}-4 \mathrm{i} \xi_{j} \eta_{j}^{3}+\eta_{j}^{4}\right) \\
H_{2} & =\frac{\beta}{16} \sum_{j}\left(\xi_{j}^{4}-4 \mathrm{i} \xi_{j}^{3} \eta_{j}-6 \xi_{j}^{2} \eta_{j}^{2}+4 \mathrm{i} \xi_{j} \eta_{j}^{3}+\eta_{j}^{4}\right)
\end{aligned}
$$

Before proceeding, it is useful to perform the change of variables

$$
\begin{equation*}
\hat{\psi}_{k}=\frac{\hat{p}_{k}+\mathrm{i} \hat{\mathrm{q}}_{k}}{\sqrt{2}}, \quad \psi_{j}=\sum_{k} \hat{\psi}_{k} \hat{e}_{k}(j) \tag{3.69}
\end{equation*}
$$

which puts the quadratic part into diagonal form. This implies a modification of $\tilde{H}_{20}$, which however is of higher order and therefore will be included into the remainder terms. Indeed, the Lemma below shows that the difference between $\xi$ and $\psi$ is small

Lemma 3.8. For any $2 \geq s_{1} \geq 0$ it holds true

$$
\begin{array}{r}
\|\xi-\psi\|_{s, \sigma} \leq a \mu^{s_{1}}\|\psi\|_{s+s_{1}, \sigma}, \quad\|\mathrm{i} \eta-\bar{\psi}\|_{s, \sigma} \leq a \mu^{s_{1}}\|\psi\|_{s+s_{1}, \sigma}  \tag{3.70}\\
s>\frac{1}{2}, \sigma \geq 0
\end{array}
$$

Proof. By definition

$$
\begin{aligned}
\|\xi-\psi\|_{s, \sigma}^{2} & =\sum_{k}[k]^{2 s} e^{2 \sigma k}\left(\sqrt{\omega}_{k}-1\right)^{2}\left(\frac{\left|\hat{\tilde{q}}_{k}\right|^{2}}{\omega_{k}}+\left|\hat{\tilde{p}}_{k}\right|^{2}\right) \leq \\
& \leq \sum_{k}[k]^{2 s} e^{2 \sigma k}\left(\sqrt{\omega}_{k}-1\right)^{2}\left(\left|\hat{\tilde{q}}_{k}\right|^{2}+\left|\hat{\tilde{p}}_{k}\right|^{2}\right)
\end{aligned}
$$

a Taylor expansion of the frequencies $\omega_{k}$ gives

$$
\left|\sqrt{\omega}_{k}-1\right|^{2} \leq \frac{1}{4} a^{2} 4 \sin ^{4}\left(\frac{k \pi}{2 N+2}\right) \leq C a^{2} \mu^{2 s_{1}} k^{2 s_{1}}
$$

which is the thesis.

Corollary 3.4. In terms of the variables $\psi, \bar{\psi}$ one has $\tilde{H}_{2}=H_{20}+H_{21}$ where

$$
\begin{align*}
H_{20}(\psi, \bar{\psi}) & :=\frac{\alpha^{2}}{24} \sum_{j}\left(\psi_{j}^{4}+4 \mathrm{i} \psi_{j}^{3} \bar{\psi}_{j}-10\left|\psi_{j}\right|^{4}+4 \mathrm{i} \psi_{j} \bar{\psi}_{j}^{3}+\bar{\psi}_{j}^{4}\right)+ \\
& +\frac{\beta}{16} \sum_{j}\left(\psi_{j}^{4}-4 \mathrm{i} \psi_{j}^{3} \bar{\psi}_{j}+6\left|\psi_{j}\right|^{4}-4 \mathrm{i} \psi_{j} \bar{\psi}_{j}^{3}+\bar{\psi}_{j}^{4}\right), \tag{3.71}
\end{align*}
$$

and there exists $C_{9}\left(a, G_{1}\right)$ such that

$$
\begin{equation*}
\left\|X_{H_{21}}(\psi, \bar{\psi})\right\|_{s-s_{1}, \sigma} \leq C_{9} \mu^{s_{1}}\|\psi\|_{s, \sigma}^{3} \tag{3.72}
\end{equation*}
$$

Just averaging (3.71) with respect to the flow $\Phi^{t}$ it is now immediate to get the following Corollary.

Corollary 3.5. The normal form $Z$ is composed of two terms, $Z=Z_{0}+Z_{r}$, where the leading term $Z_{0}$ is smooth and reads

$$
\begin{equation*}
Z_{0}(\psi)=\tilde{\gamma} \sum_{j}\left|\psi_{j}\right|^{4}, \quad \tilde{\gamma}:=\frac{3}{8}\left(\beta-\frac{10}{9} \alpha^{2}\right) \tag{3.73}
\end{equation*}
$$

while the remainder is small

$$
\left\|X_{Z_{r}}(\psi)\right\|_{s-s_{1}, \sigma} \leq C_{9} \mu^{s_{1}}\|\psi\|_{s, \sigma}^{3} \quad\left\{\begin{array}{c}
0 \leq s_{1}<s-\frac{1}{2}<2, \sigma=0 \text { for } D B C  \tag{3.74}\\
0 \leq s_{1}<s-\frac{1}{2}, s_{1} \leq 2, \sigma \geq 0 \text { for PBC }
\end{array}\right.
$$

Thus we have proved that the formula for $Z_{0}$ holds. The formula for $\chi_{10}$ implies that the canonical transformation has the structure (3.15) and this concludes the proof of Theorem 3.1.

## 4 Proof of Theorem 2.1

To discuss this issue we first write the equations of motion of the first part of the normal form, namely of $H_{0}+Z_{0}$, in the form

$$
\begin{equation*}
\mathrm{i} \dot{\psi}_{j}=(A \psi)_{j}-\tilde{\gamma} \psi_{j}\left|\psi_{j}\right|^{2} \tag{4.1}
\end{equation*}
$$

where $A$ is a linear operator which in the Fourier variables acts as a multiplier by $\omega_{k}=1+\frac{a}{2} \mu^{2} k^{2}+O\left(\mu^{4} k^{4}\right)$, namely

$$
\begin{equation*}
(\widehat{A \psi})_{k}=\omega_{k} \hat{\psi}_{k}=\left(1+\frac{a}{2} \mu^{2} k^{2}\right) \psi_{k}+\mathcal{O}\left(\mu^{4}\right) \equiv\left(\widehat{A_{N L S}}\right)_{k}+\mathcal{O}\left(\mu^{4}\right) \tag{4.2}
\end{equation*}
$$

Take now an interpolating function for $\psi$, in other words a function $u$ such that

$$
\begin{equation*}
\psi_{j}=\epsilon u(\mu j), \tag{4.3}
\end{equation*}
$$

where $\epsilon$ is a small parameter representing the amplitude. Then, up to corrections of higher order, $u$ fulfills the equation

$$
\begin{equation*}
-\mathrm{i} u_{t}=u+a \mu^{2} u_{x x}-\tilde{\gamma} \epsilon^{2} u|u|^{2}, \tag{4.4}
\end{equation*}
$$

which, up to a Gauge transformation and a scaling of the time introduced by

$$
\begin{equation*}
u(x, t)=e^{\mathrm{i} t} \varphi(x, \tau), \quad \tau:=a \mu^{2} t \tag{4.5}
\end{equation*}
$$

gives the NLS equation

$$
\begin{equation*}
\mathrm{i} \varphi_{\tau}=-\varphi_{x x}+\gamma \varphi|\varphi|^{2}, \quad \gamma:=\frac{\tilde{\gamma}}{a} \frac{\epsilon^{2}}{\mu^{2}} \tag{4.6}
\end{equation*}
$$

In order to get a bounded value of $\gamma$, from now on we take $\epsilon=\mu$.
We now compare an approximate solution constructed through NLS and the true solution of our Hamiltonian system. More explicitly, corresponding to a solution $\varphi^{a}(t)$ of the NLS with analytic initial data, we define an approximate solution $\psi^{a}$ of the original model by

$$
\begin{equation*}
\psi_{j}^{a}(t)=\mu e^{\mathrm{i} t} \varphi^{a}\left(\mu j, a \mu^{2} t\right) . \tag{4.7}
\end{equation*}
$$

We also consider the true solution $\psi(t)$ of the Hamilton equation of the original model, with initial datum $\psi_{j}^{0}=\mu \varphi^{a}(\mu j, 0)$.

From now on we will restrict to the case of DBC which is the complicate one since the smoothness is finite.

We first work in the variables in which $H$ is reduced to the normal form

$$
\begin{equation*}
H=H_{0}+Z_{0}+Z_{r}+\mathcal{R} . \tag{4.8}
\end{equation*}
$$

Lemma 4.1. Let $\psi$ be the solution of the equations of motion of (4.8) with initial datum $\psi(0)=\mathcal{T}^{-1}\left(\psi^{0}\right)$ and let $\psi^{a}$ be defined as in (4.7), then

$$
\psi=\psi^{a}+\psi_{1}
$$

with

$$
\left\|\psi_{1}(t)\right\|_{s, 0} \leq C \mu^{2}, \quad \frac{3}{2}<s<\frac{5}{2}, \quad|t| \leq \frac{T}{\mu^{2}} .
$$

Proof. Observe that the NLS equation for $\psi^{a}$ may be rewritten as

$$
\begin{equation*}
\dot{\psi}^{a}=X_{H_{N L S, 0}}\left(\psi^{a}\right)+X_{Z}\left(\psi^{a}\right)+X_{\mathcal{R}}\left(\psi^{a}\right)-X_{\mathcal{R}_{1}}\left(\psi^{a}\right) \tag{4.9}
\end{equation*}
$$

where

$$
\begin{aligned}
\mathcal{R}_{1} & :=\left(H_{0}-H_{N L S, 0}\right)+Z_{r}+\mathcal{R} \\
H_{N L S, 0}(\hat{\psi}) & :=\sum_{k}\left(1+a \frac{1}{2} \mu^{2} k^{2}\right)\left|\hat{\psi}_{k}\right|^{2},
\end{aligned}
$$

so that $X_{\mathcal{R}_{1}}$ fulfills the estimate

$$
\begin{aligned}
\left\|X_{\mathcal{R}_{1}}\left(\psi^{a}\right)\right\|_{s, 0} & \leq C_{1} \mu^{4}\left\|\psi^{a}\right\|_{s+4,0}+C_{r} \mu^{s_{1}}\left\|\psi^{a}\right\|_{s+s_{1}, 0}^{3}+C_{\mathcal{R}}\left\|\psi^{a}\right\|_{s, 0}^{4} \leq \\
& \leq C_{4} \mu^{4}, \quad \frac{1}{2}<s<\frac{5}{2} .
\end{aligned}
$$

We compare $\psi^{a}$ with the full solution $\psi$ of the equation

$$
\dot{\psi}=X_{H_{0}}(\psi)+X_{Z}(\psi)+X_{\mathcal{R}}(\psi)
$$

with initial datum $\psi_{0}=\mathcal{T}^{-1}\left(\psi^{0}\right)$, whose difference from $\psi^{0}$ (initial datum for $\psi^{a}$ ) is controlled by

$$
\left\|\psi_{1}(0)\right\|_{s, 0}=\left\|\psi^{0}-\mathcal{T}^{-1}\left(\psi^{0}\right)\right\|_{s, 0} \leq C_{\mathcal{T}}\left\|\psi^{0}\right\|_{s, 0}^{2} \leq C_{\mathcal{T}} \mu^{2} .
$$

So we apply the Gronwall lemma (see Lemma A.3) with

$$
A:=X_{H_{0}}, \quad P=X_{Z}+X_{\mathcal{R}}, \quad R=X_{\mathcal{R}_{1}},
$$

obtaining that the error $\psi_{1}:=\psi-\psi^{a}$ from the NLS dynamics satisfies

$$
\begin{equation*}
\dot{\psi}_{1}=A \psi_{1}+\left[P\left(\psi^{a}+\psi_{1}\right)-P\left(\psi^{a}\right)\right]+X_{\mathcal{R}_{1}}\left(\psi^{a}\right) \tag{4.10}
\end{equation*}
$$

and is estimated by

$$
\begin{equation*}
\left\|\psi_{1}(t)\right\|_{s, \sigma^{\prime}} \leq C_{\mathcal{T}} \mu^{2} e^{C_{6} \mu^{2} t}+\frac{C_{4} \mu^{4}}{C_{6} \mu^{2}}\left(e^{C_{6} \mu^{2} t}-1\right) \leq C_{7} \mu^{2}, \quad|t| \leq T / \mu^{2} \tag{4.11}
\end{equation*}
$$

where $C_{6}:=6 C_{Z}$.
When we go back to the original variables, the solution $z$ may be split as

$$
z=\mathcal{T}(\psi)=\mathcal{T}\left(\psi^{a}+\psi_{1}\right)=\mu z^{a}+\mu^{2} z_{1}+\mu^{3} z_{2}
$$

where we have defined

$$
\begin{equation*}
z^{a}:=\frac{\psi^{a}}{\mu}, \quad z_{1}:=\frac{\psi_{1}+X_{\chi_{10}}\left(\psi^{a}\right)}{\mu^{2}}, \quad \quad z_{2}:=\frac{z-\mu z^{a}-\mu^{2} z_{1}}{\mu^{3}} . \tag{4.12}
\end{equation*}
$$

More precisely, we claim that it holds
Lemma 4.2. We have

$$
\left\|z_{1}\right\|_{s, 0} \leq C_{1}, \quad\left\|z_{2}\right\|_{s, 0} \leq C_{2}
$$

up to times s.t. $|t| \leq \frac{T}{\mu^{2}}$.

Proof. The first inequality comes directly from the Lemma 4.1. Concerning the second one, we remark that

$$
\begin{aligned}
z & =\mathcal{T}\left(\psi^{a}+\psi_{1}\right)=\psi^{a}+\psi_{1}+\left[\mathcal{T}\left(\psi^{a}+\psi_{1}\right)-\left(\psi^{a}+\psi_{1}\right)\right]= \\
& =\psi^{a}+\psi_{1}+X_{\chi_{1}}\left(\psi^{a}+\psi_{1}\right)+\mathcal{O}\left(\left\|\psi^{a}+\psi_{1}\right\|_{s, 0}^{3}\right)= \\
& =\psi^{a}+\psi_{1}+X_{\chi_{1}}\left(\psi^{a}\right)+\mathcal{O}\left(\left\|\psi_{1}\right\|_{s, 0}\left\|\psi^{a}\right\|_{s, 0}+\left\|\psi^{a}+\psi_{1}\right\|_{s, 0}^{3}\right)
\end{aligned}
$$

(by differentiability of $X_{\chi_{1}}$ and Lagrange mean value theorem). Finally from (3.66) with $s_{1}=1$ we have

$$
X_{\chi_{1}}\left(\psi^{a}\right)=X_{\chi_{10}}\left(\psi^{a}\right)+\mathcal{O}\left(\mu\left\|\psi^{a}\right\|_{s+1,0}^{2}\right)
$$

This concludes the proof of Theorem 2.1.
Proof of Theorem 2.2. We analyze the first correction $z_{1}$. To this end we analyze separately its two terms.

First remark that, from (4.10) one has $\psi_{1}=\psi_{10}+\mathcal{O}\left(|t|\left\|\psi^{a}\right\|_{s, 0}^{3}\right)$, where $\psi_{10}$ solves the equation $\dot{\psi}_{10}=A \psi_{10}$ with initial datum $\mathcal{T}^{-1}\left(\psi^{0}\right)-\psi^{0}$. Thus we have

$$
\begin{equation*}
\psi_{10}=\mathrm{e}^{A t}\left(\mathcal{T}^{-1}\left(\psi^{0}\right)-\psi^{0}\right)=-\mathrm{e}^{A t} X_{\chi_{10}}\left(\psi^{0}\right)+\mathcal{O}\left(\mu\left\|\psi^{0}\right\|_{s+1,0}^{2}\right) \tag{4.13}
\end{equation*}
$$

We now analyze the other term. To this end, with the aim of considering the short time dynamics, we rewrite the equation (4.9) as

$$
\dot{\psi}^{a}=i \psi^{a}+\mathcal{O}\left(\mu^{3}\right) \quad \Longleftrightarrow \quad \psi^{a}=\mathrm{e}^{\mathrm{i} t} \psi^{0}+\mathcal{O}\left(\mu^{3}|t|\right) .
$$

Thus exploiting the differentiability of $X_{\chi_{10}}$ we have

$$
\begin{equation*}
\mu^{2} z_{1}=-\mathrm{e}^{A t} X_{\chi_{10}}\left(\psi^{0}\right)+X_{\chi_{10}}\left(\mathrm{e}^{\mathrm{i} t} \psi^{0}\right)+\mathcal{O}\left(\mu^{3}|t|\right) \tag{4.14}
\end{equation*}
$$

Since

$$
\begin{aligned}
\mathrm{e}^{A t} X_{\chi_{10}}\left(\psi^{0}\right) & =-\frac{\alpha}{6 \sqrt{2}}\left[3 e^{A t} \psi_{0}^{2}+6 \mathrm{i} e^{A t}\left|\psi_{0}\right|^{2}+e^{A t} \bar{\psi}_{0}^{2}\right] \\
X_{\chi_{10}}\left(\mathrm{e}^{\mathrm{i} t} \psi^{0}\right) & =-\frac{\alpha}{6 \sqrt{2}}\left[3 \psi_{0}^{2} e^{2 \mathrm{i} t}+6 \mathrm{i}\left|\psi_{0}\right|^{2}+e^{-2 \mathrm{i} t} \bar{\psi}_{0}^{2}\right]
\end{aligned}
$$

which yields to
$\mu^{2} z_{1}=-\frac{\alpha}{6 \sqrt{2}}\left[3\left(e^{A t}-e^{2 \mathrm{i} t}\right) \psi_{0}^{2}+6 \mathrm{i}\left(e^{A t}-1\right)\left|\psi_{0}\right|^{2}+\left(e^{A t}-e^{-2 \mathrm{i} t}\right) \bar{\psi}_{0}^{2}\right]+\mathcal{O}\left(\mu^{3}|t|\right)$.
In the case of $\psi_{0}=\mathrm{i} \mu z_{0}$ (zero velocity initial datum) we have

$$
z_{1}=\frac{\alpha}{6 \sqrt{2}}\left[4 e^{A t}-3 e^{2 \mathrm{it} t}-e^{-2 \mathrm{i} t}-6 \mathrm{i} e^{A t}+6 \mathrm{i}\right] z_{0}^{2}+\mathcal{O}(\mu|t|)
$$

which gives immediately the thesis.

## A Appendix: a few technical lemmas.

Lemma A.1. Let $u \in H^{r, \sigma}$ and $v \in H^{s, \sigma}$ with $s>\frac{1}{2}$ and $s \geq r \geq 0, \sigma \geq 0$. Then there exists $C=C(r, s)$ such that the following inequality holds

$$
\begin{equation*}
\|u v\|_{r, \sigma} \leq C\|u\|_{r, \sigma}\|v\|_{s, \sigma} \tag{A.1}
\end{equation*}
$$

Proof. In this proof it is useful to use the expansion of $u$ and $v$ on the complex exponentially. Thus we will write $u(x)=\sum_{k \in \mathbb{Z}} \hat{u}_{k} \mathrm{e}^{\mathrm{i} k x} / \sqrt{2 \pi}$, and remark that if in the definition of the norm cf. (2.14) we substitute such coefficients to the coefficients on the real Fourier basis, nothing changes. This is due to the fact that both the basis of the complex exponentials and the real Fourier basis are orthonormal. The advantage is that in terms of the complex exponentials the product is mapped into the convolution of the Fourier coefficients, thus we have simply to estimate the norm of the function whose Fourier coefficients are

$$
\begin{equation*}
(\hat{u} * \hat{v})_{k}=\sum_{j} \hat{u}_{j-k} \hat{v}_{k} . \tag{A.2}
\end{equation*}
$$

As a preliminary fact we define the quantities

$$
\gamma_{j, k}=\frac{[j-k][k]^{\frac{s}{r}}}{[j]},
$$

and prove that there exists a constant $C(s, r)$ such that

$$
\begin{equation*}
\sum_{k} \frac{1}{\gamma_{j, k}^{2 r}}<C \tag{A.3}
\end{equation*}
$$

To obtain (A.3) we need some preliminary inequalities. For any positive $a$ and $b$ one has

$$
\begin{equation*}
(a+b)^{2 r} \leq 2^{2 r} \max \{a ; b\}^{2 r}<4^{r}\left(a^{2 r}+b^{2 r}\right) \tag{A.4}
\end{equation*}
$$

and for any $j$ and $k$ in $\mathbb{Z}$

$$
\begin{equation*}
\frac{1}{[j-k]^{2 r}[k]^{2 s-2 r}}<\frac{1}{(\min \{[j-k],[k]\})^{2 s}}<\frac{1}{[j-k]^{2 s}}+\frac{1}{[k]^{2 s}} \tag{A.5}
\end{equation*}
$$

From (A.4), (A.5) and $[j]<[j-k]+[k]$ it follows

$$
\begin{aligned}
\frac{1}{\gamma_{j, k}^{2 r}} & \leq\left(\frac{[j-k]+[k]}{[j-k][k]^{\frac{s}{r}}}\right)^{2 r} \leq\left(\frac{1}{[k]^{\frac{s}{r}}}+\frac{1}{[j-k][k]^{\frac{s}{r}-1}}\right)^{2 r} \leq \\
& \leq 4^{r}\left(\frac{1}{[k]^{2 s}}+\frac{1}{[j-k]^{2 r}[k]^{2 s-2 r}}\right) \leq \\
& \leq 4^{r}\left(\frac{1}{[k]^{2 s}}+\frac{1}{[j-k]^{2 s}}+\frac{1}{[k]^{2 s}}\right)
\end{aligned}
$$

which gives (A.3) with

$$
C=3 \times 4^{r} \times \sum_{k \in \mathbb{Z}} \frac{1}{[k]^{2 s}}
$$

Hence

$$
\begin{aligned}
\|u v\|_{r, \sigma}^{2} & =\sum_{j}[j]^{2 r} e^{2 \sigma|j|}\left|\sum_{k} \hat{u}_{j-k} \hat{v}_{k}\right|^{2} \leq \\
& \leq \sum_{j}[j]^{2 r} e^{2 \sigma|j|}\left(\sum_{k} \frac{1}{\gamma_{j, k}^{2 r}}\right)\left(\sum_{k} \gamma_{j, k}^{2 r}\left|\hat{u}_{j-k} \hat{v}_{k}\right|^{2}\right) \leq \\
& \leq C^{2} \sum_{j, k}[j-k]^{2 r} e^{2 \sigma|j-k|}\left|\hat{u}_{k-j}\right|^{2}[k]^{2 s} e^{2 \sigma|k|}\left|\hat{v}_{k}\right|^{2} \leq \\
& \leq C^{2}\left(\sum_{l}[l]^{2 r} e^{2 \sigma|l|}\left|\hat{u}_{l}\right|^{2}\right)\left(\sum_{k}[k]^{2 r} e^{2 \sigma|k|}\left|\hat{u}_{k}\right|^{2}\right),
\end{aligned}
$$

which concludes the proof.

We state here a version of the Gronwall Lemma which is suited for our estimates. First we recall the following lemma.

Lemma A.2. Let $x:[0, T] \rightarrow \mathcal{P}$ be a differentiable function and $\mathcal{P}$ a Banach space. Assume that $\forall t \in[0, T]$ it fulfills the integral inequality

$$
\begin{equation*}
\|x(t)\| \leq K+\int_{0}^{t}(a\|x(s)\|+b) d s \tag{A.6}
\end{equation*}
$$

with $a, b$ real and non negative parameters, then

$$
\begin{equation*}
\|x(t)\| \leq e^{a t} K+\frac{b}{a}\left(e^{a t}-1\right) \tag{A.7}
\end{equation*}
$$

The lemma we use in sect. 4 is the following one.
Lemma A.3. Let $z(t), z^{a}(t) \in \mathcal{P}, t \in[-T, T]$ be respectively the solutions of

$$
\left\{\begin{array}{l}
\dot{z}=A z+P(z), \\
z(0)=z_{0}
\end{array}, \quad\left\{\begin{array}{l}
\dot{z}^{a}=A z^{a}+P\left(z^{a}\right)-R\left(z^{a}\right), \\
z^{a}(0)=z_{0}^{a}
\end{array}\right.\right.
$$

where $A$ is the generator of a unitary group in $\mathcal{P}$, and $\left\|z^{a}(t)\right\| \leq C$. Assume also that the non-linearity $P$ has a zero of third order at the origin and that for all $t \in[-T, T]$ and all $z$ with $\|z\| \leq 2 C$

$$
\|P(z)\| \leq \rho_{1}\|z\|^{3}, \quad\|d P(z)\| \leq 3 \rho_{1}\|z\|^{2}
$$

and the remainder $R$ is estimated by

$$
\left\|R\left(z^{a}(t)\right)\right\| \leq \rho_{2}, \quad \forall t \in[-T, T]
$$

Let $\delta:=z-z^{a}$, then the following estimate holds

$$
\begin{equation*}
\|\delta(t)\| \leq\|\delta(0)\| e^{\rho_{1} t}+\frac{\rho_{2}}{\rho_{1}}\left(e^{\rho_{1} t}-1\right), \quad t \in[-T, T] \tag{A.8}
\end{equation*}
$$

Proof. The difference $\delta(t)$ is solution of the differential equation

$$
\dot{\delta}=A \delta+\left(P\left(z^{a}(t)+\delta\right)-P\left(z^{a}(t)\right)\right)+R\left(z^{a}(t)\right)
$$

by Duhamel formula one has

$$
\delta(t)=e^{A t} \delta(0)+e^{A t} \int_{0}^{t} e^{-A s}\left[\left(P\left(z^{a}(s)+\delta\right)-P\left(z^{a}(s)\right)\right)+R\left(z^{a}(s)\right)\right] d s
$$

Using Lagrange mean value theorem to estimate $P\left(z^{a}(s)+\delta\right)-P\left(z^{a}(s)\right)$ and the fact that $A$ is unitary one has

$$
\|\delta(t)\| \leq\|\delta(0)\|+\int_{0}^{t}\left[3 \rho_{1}\|\delta(s)\|+\rho_{2}\right] d s
$$

which fulfills (A.6), from which the thesis follows.

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[^0]:    ${ }^{1}$ However our normal form holds in the region of the phase points with small energy density $\epsilon^{2}$, independently of N . The limitation $\epsilon \sim \mu$ comes from the fact that we are only able to study the dynamics of the NLS in this situation.

[^1]:    ${ }^{2}$ Actually we plot only modes with odd index, since, as shown in [BMP07] the dynamics involves only modes with odd index $k$.

