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The quantum Fermi Pasta Ulam problem

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Abstract

In this work we consider the quantum version of the classical Fermi-Pasta-Ulam problem, i.e. we study the quantum dynamics of a one-dimensional chain of particles interacting through nonlinear forces. Using the quantum analogue of the classical Hamiltonian perturbation theory, in the Heisenberg picture, we eliminate through a canonical transformation the nonresonant anharmonic terms, computing the quantum version of the Birkhoff normal form to second order. Such a normal form is shown to display small divisors for large size systems, being thus useless to describe anharmonic lattice vibrations. We then show that, for the initial excitation of long wavelength modes (acoustic modes), which is the case of low temperature lattices in thermal equilibrium, the dynamics of the system is close to that of the quantum Korteweg-de Vries equation.

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Introduction

The aim of this work is to study the dynamics of a one-dimensional anharmonic chain of bosons with fixed boundary conditions, which is the quantum equivalent of one of the classical problems of statistical physics of the last century classically known as the Fermi-Pasta-Ulam (in the following FPU) problem [1]. The FPU problem was intended to describe the relaxation towards the thermodynamical equilibrium of a solid: the dynamics of a classical one dimensional chain of particles with anharmonic interaction were studied (numerically, initially, and then also analytically) and no thermalisation was found. Motivated by the idea that a consistent model of a solid must be a quantum one, we believe that it is important to study the out of equilibrium dynamics of this quantum system. However, the ergodic and thermalisation properties of closed quantum systems are still an open and complex subject of study (for example, a review of the recent theoretical achievements can be found in [4]), so we do not enter in such a treatment; but we want to emphasize that this type of problems is receiving much attention in the last years. In fact such a system is already experimentally studied in [3], where a preparation of out-of-equilibrium arrays of trapped one dimensional Bose gases, containing from 40 to 250 ^{87}Rb atoms, is reported. Like the classical Fermi-Pasta-Ulam system, no thermalisation is found. A more recent experiment is reported in [5], where local emergence of thermal correlations of a one-dimensional Bose gas are studied.

We gave mainly two original contributions. We constructed the second-order non resonant normal form of the quantum Fermi-Pasta-Ulam system using the tools of Hamiltonian perturbation theory for the Heisenberg picture of Quantum Mechanics, and calculated the shift of the energy levels due to the non-linearity of the forces. These are results that can be experimentally verified. Moreover, we built a connection between the dynamics of the acoustic modes of the system and the so-called quantum Korteweg-de Vries equation, i.e. if $a_k^\dagger$, $k = 1, \dots, N-1$ are the creation operators of the quantum Fermi-Pasta-Ulam system, then the Heisenberg equations for this operators are equivalent to the Fourier-Galerkin truncation to the first $N-1$ modes of the equation

$$\psi_t = \frac{1}{24}\psi_{xxx} + \frac{\alpha}{2\sqrt{2}}(\psi\psi_x + \psi_x\psi), \qquad [\psi(x), \psi(y)] = i\delta_x(x-y).$$

where $\alpha \in \mathbb{R}$ and ψ is a $2N$-periodic hermitian quantum field. Thus, the dynamics of the acoustic modes of the system can be mapped, for a period of time increasing with the number of particles, in the dynamics given by this quantum field equation, which is already known in literature. For example, in [6] this equation is proven to be integrable, admitting an infinity of commuting conserved quantities; this equation is

also studied in Conformal Field Theory, for example in [9]. We remark that we have constructed a strong and clear connection, which as far as we are aware was absent, between this known equation and this physical system. The work is organized in the following way:

1. In the first chapter we provide a general overview of the Hamiltonian Mechanics tools which will be used in the following. We also include some elements of ergodic theory to understand the connection between integrability and lack of thermalisation.

2. In the second chapter we describe the Hamiltonian formulation of infinite dimensional systems. A particular importance is given to Quantum Mechanics.

3. In the third chapter we provide the classical construction of the Fermi-Pasta-Ulam model and its normal modes of oscillation and we canonically quantize the system.

4. In the fourth chapter we provide one of the formulations of Hamiltonian perturbation theory an the mean principle, for the classical and the quantum case.

5. In the fifth chapter we build the second order non-resonant normal form for the quantum case.

6. In the sixth chapter we explain the so-called small divisors problem in our system of interest, which leads us to consider the first order resonant Birkhoff normal form for the acoustic modes. We also prove that the Heisenberg equation for the creation operator of this normal form is equivalent to what is known in literature as the *quantum Korteweg-de Vries* equation.

CHAPTER 1

Hamiltonian Mechanics

In this first chapter we will provide the basic tools of Hamiltonian mechanics introducing the concept of Poisson algebras, a mathematical environment which generalize the elementary Hamiltonian systems.

1.1 Poisson algebras and Hamiltonian systems

Definition 1.1 (Poisson brackets)**.** Let Γ be a differentiable manifold and $\mathscr{A}(\Gamma)$ the algebra of real smooth functions defined on it. A function $\{\ ,\ \} : \mathscr{A}(\Gamma) \times \mathscr{A}(\Gamma) \to \mathscr{A}(\Gamma)$ is called a *Poisson bracket* on Γ if it satisfies the following properties:

1. $\{F, G\} = -\{G, F\} \quad \forall F, G \in \mathscr{A}(\Gamma)$ (skew-symmetry);
2. $\{\alpha F + \beta G, H\} = \alpha\{F, H\} + \beta\{G, H\} \quad \forall \alpha, \beta \in \mathbb{R}$ and $\forall F, G, H \in \mathscr{A}(\Gamma)$ (left linearity);
3. $\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0 \quad \forall F, G, H \in \mathscr{A}(\Gamma)$ (Jacobi identity);
4. $\{FG, H\} = F\{G, H\} + \{F, H\}G \quad \forall F, G, H \in \mathscr{A}(\Gamma)$ (Leibniz rule).

Remark 1.1. Properties 1 and 2 imply right linearity, so the Poisson brackets are in fact bilinear, as properties 1 and 4 imply the right Leibniz rule.

One can see that the Poisson brackets known from elementary Hamiltonian mechanics, i.e., if $(q, p) \in \Gamma$, $\forall F, G \in \mathscr{A}(\Gamma)$

$$\{F, G\} := \sum_i \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right)$$

are included in this definition, and one clearly has

$$\{q_i, q_j\} = 0, \qquad \{p_i, p_j\} = 0, \qquad \{q_i, p_j\} = \delta_{i,j},$$

where $\delta_{i,j}$ is the standard Kronecker delta.

Definition 1.2 (Poisson algebra)**.** The pair $\{\mathscr{A}(\Gamma), \{\ ,\ \}\}$, where $\{\ ,\ \}$ is a Poisson bracket on Γ is called a *Poisson algebra*.

Remark 1.2. A Poisson algebra is a Lie algebra, with an additional property of the product (the Leibniz Rule).

Definition 1.3 (Hamiltonian system)**.** Given a differentiable manifold Γ and a Poisson algebra $\{\mathscr{A}(\Gamma), \{\ ,\ \}\}$, a dynamical system $\dot{x} = u(x)$, $u(x) \in T_x\Gamma$, is a *Hamiltonian system*, if there exists $H \in \mathscr{A}(\Gamma)$, called the *Hamiltonian* of the system, such that

$$u_i(x) = [X_H(x)]_i := \{x_i, H\}.$$

X_H is called the *Hamiltonian vector field* of H.

Again, this is a generalization of the elementary Hamiltonian systems, namely systems whose dynamics satisfy the Hamilton equations

$$\dot{q} = \frac{\partial H}{\partial p}. \qquad \dot{p} = -\frac{\partial H}{\partial q}$$

where $(q, p) \in \Gamma = \mathbb{R}^{2n}$ and $H(q, p)$ is the Hamiltonian of the system. If $\{\ ,\ \} := \sum_{i=1}^{n}(\frac{\partial}{\partial q_i}\frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_j}\frac{\partial}{\partial q_i})$ is the elementary Poisson bracket, one in fact has

$$\dot{q}_i = \{q_i, H\} = \sum_{j=1}^{n}\left(\frac{\partial q_i}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial q_i}{\partial p_j}\frac{\partial H}{\partial q_j}\right) = \sum_{j=1}^{n}\delta_{ij}\frac{\partial H}{\partial p_j} = \frac{\partial H}{\partial p_i}$$

and, with an analogous computation $\{p_i, H\} = -\frac{\partial H}{\partial q_i}$.

Remark 1.3. Hamiltonian systems are often introduced by means of *symplectic geometry*, introducing a differentiable manifold and defining a *symplectic form* on it. Although this approach is the most mathematically precise one, we choose to present Hamiltonian systems in a more physical way, as it is more fitting to the calculations we are going to perform.

At this point one can see that the elementary Poisson brackets can be written in matricial form, namely $\forall F, G \in \mathscr{A}(\Gamma)$

$$\{F, G\} = \nabla F \cdot \mathbb{J}\nabla G, \qquad \mathbb{J} = \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ -\mathbb{1} & \mathbb{0} \end{pmatrix}_{2n\times 2n}$$

and $\mathbb{J}$ is called *symplectic matrix* or *standard Poisson tensor*, in a sense that will be clarified below. It is useful to extend these notions from elementary Hamiltonian mechanics to the general environment.

Proposition 1.1. *A skew-symmetric, bilinear Leibniz bracket* $\{\ ,\ \}$ *on a differentiable manifold* Γ *is such that*

$$\{F, G\} = \nabla F \cdot J\nabla G := \sum_{j,k}\frac{\partial F}{\partial x_j}J_{jk}(x)\frac{\partial G}{\partial x_k}, \tag{1.1}$$

$\forall F, G \in \mathscr{A}(\Gamma)$, *where*

$$J_{jk}(x) := \{x_j, x_k\} \qquad \forall j, k. \tag{1.2}$$

This bracket satisfies the Jacobi identity (i.e. it is a Poisson bracket) if and only if $J(x)$ is such that

$$\sum_s \left(J_{is}\frac{\partial J_{jk}}{\partial x_s} + J_{js}\frac{\partial J_{ki}}{\partial x_s} + J_{ks}\frac{\partial J_{ij}}{\partial x_s} \right) = 0 \qquad \forall j,k. \tag{1.3}$$

Now we can give a general definition of Poisson tensors, and see that the symplectic matrix $\mathbb{J}$ is in fact a particular case.

Definition 1.4 (Poisson tensor)**.** Given a Poisson algebra $\{\mathscr{A}(\Gamma), \{\ ,\ \}\}$, a *Poisson tensor* is a function operator $J_{ij}(x) = \{x_i, x_j\}\ \forall x \in \Gamma$, skew symmetric and satisfying

$$\sum_s \left(J_{is}\frac{\partial J_{jk}}{\partial x_s} + J_{js}\frac{\partial J_{ki}}{\partial x_s} + J_{ks}\frac{\partial J_{ij}}{\partial x_s} \right) = 0 \qquad \forall j,k.$$

Remark 1.4. This is clearly a generalization of the symplectic matrix $\mathbb{J}$, in fact it is easily verified that any constant skew-symmetric tensor is a Poisson tensor.

Remark 1.5. Thanks to proposition 1.1, there is a one-to-one correspondence between Poisson brackets and Poisson tensors. Therefore in the following we will denote a Poisson algebra indiscriminately by $\{\mathscr{A}(\Gamma), \{\ ,\ \}\}$ (when we want to stress the algebraic valence) and $\{\mathscr{A}(\Gamma), J\}$, where $\{\ ,\ \}$ and J are linked by the relation $J(x) = \{x_i, x_j\}$.

We have seen that every Poisson brackets can be written in the form (1.1), where $J(x)$ is a Poisson tensor. This leads to the fact that every Hamiltonian vector field $X_H(x)$ can be written as a function of the Poisson tensor, in fact

$$[X_H(x)]_i = \{x_i, H(x)\} = \sum_{jk} \frac{\partial x_i}{\partial x_j} J_{jk}(x) \frac{\partial H(x)}{\partial x_k} = \sum_k J_{ik}(x) \frac{\partial H(x)}{\partial x_k} = [J(x)\nabla H(x)]_i$$

which is clearly a generalization of the standard Hamiltonian vector field $\mathbb{J}\nabla H(x)$.

It is possible to extend to the general environment the equations of evolutions of observables, i.e. $\forall F \in \mathscr{A}(\Gamma)$, given a solution of the Hamilton equations $\dot{x} = J(x)\nabla H(x)$, $t \mapsto x(t)$

$$\frac{d}{dt}F(x(t)) = \sum_i \frac{\partial F(x(t))}{\partial x_i}\frac{dx_i}{dt} = \sum_{i,j} \frac{\partial F(x(t))}{\partial x_i} J_{ij}(x) \frac{\partial H(x(t))}{\partial x_j} = \{F, H\}$$

so that $\frac{dF}{dt} = \{F, H\}$. This equation will be the most general form of time evolution equation for a Hamiltonian system, and will be particularly interesting for our work when extended to the quantum mechanics environment.

1.2 Change of coordinates and canonical transformations

Of course, one is interesting in performing change of coordinates. In fact, a dynamical system might appear obscure written as it is, but a change of variables allows us to see it in a different light, highlighting some of its qualities. This is indeed the concept of *Liouville integrability*, which we will see in the following chapters. For Lagrangian systems, adapted to working on constrained systems,

only a particular set of change of coordinates is allowed, in which the change of velocities is bounded in a precise way to the change of positions. When Hamiltonian systems are introduced in the most elementary way, i.e. the Legendre transform of a Lagrangian system, one learns that the transformations of the momenta and the transformations of the positions are no longer bounded but, again, only a particular set of change of coordinates are allowed, often called *symplectomorphisms* of *symplectic transformations*. In the general environment of Poisson algebras we will learn that *every change of coordinates maps Hamiltonian systems into Hamiltonian systems*, at the cost of changing the Poisson tensor.

Proposition 1.2 (Change of variables)**.** *Let $\dot{x} = J(x)\nabla_x H(x)$, $x \in \Gamma$ a Hamiltonian system, and $f : x \mapsto y = f(x)$ a change of variables with inverse $g := f^{-1} : y \mapsto x = g(x)$. Then, the first Hamiltonian system is conjugated by f to*

$$\dot{y} = J^\sharp(y)\nabla_y \widetilde{H}(y) \tag{1.4}$$

where $\widetilde{H} = H \circ g$ and

$$J^\sharp(y) = \left[\frac{\partial f}{\partial x}\right] J(x) \left[\frac{\partial f}{\partial x}\right]^T |_{x=g(y)} = \left[\frac{\partial g}{\partial y}\right]^{-1} J(x) \left[\frac{\partial g}{\partial y}\right]^{-T}. \tag{1.5}$$

Proof. The proof is straightforward starting from the identities

$$\frac{\partial}{\partial x_i} = \sum_j \frac{\partial y_i}{\partial x_i}\frac{\partial}{\partial y_j}, \qquad \frac{\partial f}{\partial x}(g(y)) = \left[\frac{\partial g}{\partial y}\right]^{-1},$$

so that $y = f(x)$ implies $\dot{y} = \frac{\partial f}{\partial x}\dot{x}|_{x=g(y)} = \left[\frac{\partial f}{\partial x}\right] J(x) \left[\frac{\partial f}{\partial x}\right]^T \nabla_y H|_{x=g(y)}$. □

At this point, one might ask if the system (1.4) is still Hamiltonian. The answer is given by the following proposition, which implies that a dynamical system is Hamiltonian independently of the coordinates chosen (that, one can say, is the true strength of the Hamiltonian formalism).

Proposition 1.3. *Poisson brackets are characterized by coordinate-independent properties.*

Proof. Given a Poisson bracket $\{F, G\}(x) = \nabla F(x) \cdot J(x) \nabla G(x)$ we want to show that it transforms into another Poisson bracket under any change of variables $f \colon x \mapsto y$, with inverse $g = f^{-1}$. We will denote with a tilde composition with the inverse, namely $\widetilde{F}(y) := F(g(y))$. By means of (1.5) one finds

$$\begin{aligned}
\widetilde{\{F, G\}}(y) &= \left[\left(\frac{\partial f}{\partial x}\right)^T \nabla_y F\right] \cdot J(x) \left(\frac{\partial f}{\partial x}\right) \nabla_y G|_{x=g(y)} = \\
&= \nabla_y \widetilde{F}(y) \cdot \left[\left(\frac{\partial g}{\partial y}\right)^{-1} J(g(y)) \left(\frac{\partial g}{\partial y}\right)^{-T}\right] \nabla_y \widetilde{G}(y) = \\
&= \nabla_y \widetilde{F}(y) \cdot J^\sharp(y) \nabla_y \widetilde{G}(y) := \{\widetilde{F}, \widetilde{G}\}_\sharp(y).
\end{aligned}$$

Equivalently, with notation independent of coordinates, one has

$$\widetilde{\{F, G\}} = \{\widetilde{F}, \widetilde{G}\}_\sharp \quad \iff \quad \{F, G\} \circ g = \{F \circ g, G \circ g\}_\sharp.$$

We must show thaat the bracket $\{\widetilde{F},\widetilde{G}\}_\sharp$, formally defined above, is an actual Poisson bracket on the algebra of the transformed functions. To this end, we observe that skew-symmetry, bi-linearity and Leibniz property follow directly from those of $\{\ ,\ \}$. The validity of the Jacobi identity can be shown by the repeated use of the latter relation

$$\begin{aligned}0 &= \{F,\widetilde{\{G,H\}}\}+\{G,\widetilde{\{H,F\}}\}+\{H,\widetilde{\{F,G\}}\}=\\ &=\{\widetilde{F},\widetilde{\{G,H\}}\}_\sharp+\{\widetilde{G},\widetilde{\{H,F\}}\}_\sharp+\{\widetilde{H},\widetilde{\{F,G\}}\}_\sharp=\\ &=\{\widetilde{F},\{\widetilde{G},\widetilde{H}\}_\sharp\}_\sharp+\{\widetilde{G},\{\widetilde{H},\widetilde{F}\}_\sharp\}_\sharp+\{\widetilde{H},\{\widetilde{F},\widetilde{G}\}_\sharp\}_\sharp.\end{aligned}$$

Thus, the change of variables f transforms Poisson brackets into Poisson brackets. □

Remark 1.6. A convenient way to characterize the transformation of a Poisson tensor under a given change of variables is that $\{y_i,y_j\}_\sharp=\{f_i,f_j\}\circ g$ holds for any change of variables $f: x\mapsto y$.

Given the Hamiltonian dynamical system $\dot{x}=J(x)\nabla_x H(x)$, $x\in\Gamma$, among all the possible changes of variables concerning it, a privileged role is played by those leaving the Poisson tensor and the Hamilton equations invariant in form, i.e. mapping the equation $\dot{x}=J(x)\nabla_x H(x)$ into the equation $\dot{y}=J(y)\nabla_y\widetilde{H}(y)$ *for any particular Hamiltonian*. Such particular changes of variables are the so-called *canonical transformation* of the given Poisson structure and are characterized by the following equivalent conditions:

$$\begin{gathered}J^\sharp(y)=J(y);\\ \{y_i,y_j\}=\{f_i,f_j\}\circ g;\\ \{F\circ g,G\circ g\}=\{F,G\}\circ g\ \forall F,G.\end{gathered}$$

Definition 1.5 (Canonical transformation)**.** Given a Poisson algebra $\{\mathscr{A}(\Gamma),J\}$, a *canonical transformation* is a change of coordinates $\mathscr{C}:\Gamma\to\Gamma$, $x\mapsto y$ such that for any Hamiltonian H, it conjugates the Hamiltonian system $\dot{x}=J(x)\nabla_x H(x)$ into

$$\dot{y}=J(y)\nabla_y\widetilde{H}(y)$$

where $\widetilde{H}=H\circ\mathscr{C}^{-1}$.

Remark 1.7. The set of all the canonical transformation of a given Poisson structure has a natural group structure with respect to composition (they are actually a subgroup of all the change of variables).

If $x=(q,p)\in\mathbb{R}^{2n}$ and $J(x)=\mathbb{J}_{2n}$, then a direct computation shows that a canonical transformation $f: x\mapsto y=(Q,P)$,

$$\mathbb{J}_{2n}=\left[\frac{\partial(Q,P)}{\partial(q,p)}\right]\mathbb{J}_{2n}\left[\frac{\partial(Q,P)}{\partial(q,p)}\right]^T,\qquad \frac{\partial(Q,P)}{\partial(q,p)}=\frac{\partial f}{\partial x}.$$

preserves the Poisson brackets, i.e.

$$\{Q_i,Q_j\}(q,p)=0,\qquad \{P_i,P_j\}(q,p)=0,\qquad \{Q_i,P_j\}(q,p)=\delta_{i,j}$$

where we have stressed the fact that Q and P are functions of (q,p).

A very convenient way of performing canonical transformations is to do it through Hamiltonian flows. To such a purpose, let us consider a Hamiltonian $H(x)$ and its associated Hamilton equations $\dot{x} = X_H(x)$. Let ϕ_G^s denote the flow of H at time s, so that $\phi_H^s(\xi)$ is the solution of the Hamilton equations at time s corresponding to the initial condition ξ at $s = 0$. We also denote by

$$L_H := \{\ , H\} = (J\nabla H) \cdot \nabla = X_H \cdot \nabla$$

the *Lie derivative* along the Hamiltonian vector field X_H.

Lemma 1.1. *For any function F one has*

$$F \circ \phi_G^s = e^{sL_G} F.$$

Proposition 1.4. *If H is independent of the time, the change of variables $x \mapsto y = \phi_H^s(x)$ defined by its flow at time s constitutes a one-parameter group of canonical transformation.*

As we have seen, a canonical transformation $(q, p) \mapsto (Q, P) = (\alpha q, \beta p)$, $\alpha, \beta \in \mathbb{R} \setminus \{0\}$ must preserve the Poisson brackets, so if the initial Poisson tensor is $\mathbb{J}_{2n}$, the canonicity of the transformation is assured if $\alpha\beta = 1$, as

$$\{Q_i, P_j\}(q, p) = \alpha\beta\delta_{i,j}.$$

However, one can relax the notion of canonical transformation to a transformation which involves not only the coordinates, but also the Hamiltonian and the time itself, $(q, p, H, t) \mapsto (Q, P, K, T)$ which preserves just the Hamilton equations. Such a transformation will be called a *non-univalent canonical transformation*. In literature, the canonical transformations are often called *symplectic* transformation, and the non-univalent canonical transformations are called simply canonical. In this work, since the difference between the two is very little, we will call all of them *canonical* or *symplectic* indiscriminately. In this way, in a canonical transformation $(q, p, H, t) \mapsto (Q, P, K, T) = (\alpha q, \beta p, \gamma H, \delta t)$ the extra factor $\alpha\beta \neq 1$ gained by the Poisson tensor can be re-absorbed by a rescaling of the Hamiltonian and the time. The new equations then will be

$$\frac{dQ}{dT} = \frac{\partial K}{\partial P}, \qquad \frac{dP}{dT} = -\frac{\partial K}{\partial Q}, \qquad \Longleftrightarrow \qquad \alpha\beta = \gamma\delta.$$

At this point, we can easily see an application of the canonical transformation formalism which will be useful in the following, i.e. the so called *Birkhoff coordinates* (or *complex coordinates*) for the harmonic oscillator. Suppose we have a standard Hamiltonian system, $(q, p) \in \mathbb{R}^2$ with Hamiltonian

$$H(q, p) = \frac{1}{2}(p^2 + \omega^2 q^2).$$

The Hamilton equations read

$$\dot{q} = p. \qquad \dot{p} = -\omega^2 q.$$

This system physically refers to a one-dimensional Harmonic oscillator with unitary mass and frequency ω. One can operate a change of coordinates $\mathbb{R}^2 \to \mathbb{C}^2$, $(q,p) \mapsto (z,z^*)$ where

$$z = \frac{\omega q + ip}{\sqrt{2\omega}}, \qquad z^* = \frac{\omega q - ip}{\sqrt{2\omega}}.$$

The resulting system is of course Hamiltonian, with Hamiltonian

$$K = \omega |z|^2$$

with $|z|^2 = zz^*$, but the transformation is not canonical. In fact, the new Poisson tensor is

$$\begin{pmatrix} \sqrt{\frac{\omega}{2}} & \frac{i}{\sqrt{2\omega}} \\ \sqrt{\frac{\omega}{2}} & -\frac{i}{\sqrt{2\omega}} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{\omega}{2}} & \sqrt{\frac{\omega}{2}} \\ \frac{i}{\sqrt{2\omega}} & -\frac{i}{\sqrt{2\omega}} \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_2$$

where we have introduced the second *Pauli matrix*. The new Hamilton equations read

$$\dot{z} = -i\omega z, \qquad \dot{z}^* = i\omega z^*,$$

so that, the solutions of the Cauchy problem with initial datum z_0 is $z(t) = e^{-i\omega t} z_0$: in this new coordinates, the solution rotates in the complex plane with frequency ω. These coordinates were initially introduced in classical mechanics, but they find a strong application in quantum mechanics as they are the equivalent of the creation and annihilation operators, which are used in the description of the quantum harmonic oscillators and many-body systems.

Remark 1.8. Sometimes, instead of performing the change of variables written above, two different steps are used. The first is a canonical rescaling $(q,p) \mapsto (q',p')$ such that $q = \frac{q'}{\sqrt{\omega}}$ and $p = \sqrt{\omega} p'$ which conjugates the harmonic oscillator Hamiltonian to

$$\frac{\omega}{2}(q'^2 + p'^2),$$

and then pass to complex coordinates

$$z = \frac{q' + ip'}{\sqrt{2}}, \quad z^* = \frac{q' - ip'}{\sqrt{2}}.$$

The two methods are of course equivalent, and transform the standard Poisson tensor $\mathbb{J}_2$ into σ_2.

1.3 Integrability of Hamiltonian systems

Among all the possible Hamiltonian systems, it is interesting to study a particular (and very special) class of them, i.e. the so-called *integrable* systems. Although there are several (and somehow almost equivalent) concepts of integrability of a dynamical system, the most common one concerns the *quasi-periodicity* of its solutions. It is nonetheless important, however, to recall that initially the integrability of a certain differential equation indicated that it can be solved exactly, explicitly or *by quadrature*. As we will see, there is a strong connection between these two conceptions.

In order to talk about Hamiltonian integrability we need to introduce its basilar element, and its connection to the presence of symmetries of the given dynamical system.

Definition 1.6 (First Integral)**.** A function $I \in \mathscr{A}(\Gamma)$ endowed with the Poisson brackets $\{\ ,\ \}$ is a *first integral* of the Hamiltonian $H \in \mathscr{A}(\Gamma)$ if

$$\{I, H\} = 0.$$

Definition 1.7 (Involution)**.** Two first integrals I_1 and I_2 of the same Hamiltonian system are *in involution* if

$$\{I_1, I_2\} = 0.$$

Keeping in mind the time evolution equation for Hamiltonian systems $\dot{I} = \{I, H\}$, we understand that a first integral of a Hamiltonian system is a function on the phase space which doesn't change along the flow of the system. It is easy to notice that, due to the skew-symmetry of the Poisson brackets, any Hamiltonian system admits at least a first integral which is the Hamiltonian itself.

Proposition 1.5. *If the Hamiltonian H is invariant with respect to the Hamiltonian flow of the Hamiltonian K, i.e. $H \circ \phi_K^s = H\ \forall s \in \mathbb{R}$, then K is a first integral of H.*

This last proposition is the Hamiltonian version of the Nöther theorem: for a Hamiltonian system, a dynamical symmetry *always* produces a conserved quantity (a first integral). Of course, when a first integral is present, a particular initial data must evolve under the flow of the Hamilton equations on the level sets of this first integral, which under the suitable assumptions are differentiable manifolds: the effective phase space accessible to the dynamical system is smaller. If two symmetries, and thus two first integrals are present, the initial data must evolve under the flow on the intersection of the level sets of the two integrals, which (again, under some assumptions) is a smaller differentiable manifold. One can imagine, then, that if there exists a sufficient number of first integrals the motion becomes so constrained that in some coordinates the flow becomes trivial, and thus exactly solvable. All this is formalized by the celebrated *Liouville-Arnol'd theorem*, which regards the so-called *Liouville integrability*

Definition 1.8. Given a $2n$-dimensional Hamiltonian system, we say that it is *integrable in the sense of Liouville* if it admits n first integrals in involution.

The importance of this type of integrability resides in the fact that it was proven that a Hamiltonian system which is integrable in the sense of Liouville is also integrable by quadrature. Morevoer, it was proven that if the $2n$-dimensional system is integrable and $I_1, \dots, I_n$ are n first integrals of the system, it is possible to perform a canonical transformation $f\colon (q, p) \to (\phi, I)$ such that the Hamiltonian depends only by the momenta I, and the transformed equations of motion are, for some $\omega(I)$

$$\dot{\phi} = \omega(I), \qquad \dot{I} = 0.$$

Trivially, their solution is $I(t) = I_0$ and $\phi(t) = \phi_0 + \omega(I_0)t$. If the level sets of the n first integrals are *compact*, then the motion is periodic and the phase space is

foliated in *invariant tori* endowed with coordinates ϕ and radius dependent on I: if we choose an initial data on a torus the flow remains on the same torus forever.

This is surely the case of the n-dimensional harmonic oscillator. As we have seen for the one-dimensional case, one can introduce the Birkhoff variables z_k and z_k^*, $k = 1, \ldots, n$, so that the Hamiltonian is conjugated to $\sum_k \omega_k |z_k|^2$ and the motion is trivial: $z_k(t) = z_k(0) \exp(-i\omega_k t)$. This system surely has n first integrals in involution, which are the modules $|z_k|$, while the phases evolve periodically in time: the n-dimensional harmonic oscillator is an integrable system.

Although the integrable case is an exceptional one, it regards some of the most significant problems in the history of physics, like the harmonic chain, the Euler rigid body, or the Kepler problem. For these systems, the Hamiltonian environment must not be seen as a tool to solve the equations of motion, but to give a deep look into the geometric structure of the problem, and to understand the very interesting but difficult case of systems next to the integrable ones: a system of masses bounded by slightly non-linear forces, a rigid body in a weak force field, or two or more weakly coupled Kepler problems. For this type of problems, like ours, one must turn to the Hamiltonian *perturbation theory* which gives very useful tools.

1.4 Elements of ergodic theory

The integrability of a system has deep consequences on its *thermalisation* properties. In the following we will give a general idea of ergodic theory, providing the main definitions and concepts and omitting the proofs in order to emphasize the physical sense of the problem. We will follow [18].

Ergodic theory is a mathematical field which started with the works by Von Neumann and Birkhoff at the end of the twenties. The fundamental ideas come from Boltzmann and Gibbs, who laid the foundations of Statistical Mechanics and introduced the fundamental notion of *ensembles* to describe a macroscopic state of a system with many degrees of freedom. Statistical mechanics was born for understanding the macroscopic behaviour of a thermodynamic system starting from its microscopic structure, using probability theory as a fundamental tool. We will start by introducing Boltzmann's and Gibbs's points of view of Statistical Mechanics, which affect deeply the basic notions of ergodic theory.

Let us consider a thermodynamic system constituted by a big number N of identical subsystems, each of them having l degrees of freedom; the complete system then will have $n = lN$ degrees of freedom. The $2l$-dimensional phase space of the single subsystem is traditionally denoted by μ, and by $\Gamma = \mu^N$, $\dim\Gamma = 2n$ the phase space of the whole system. Denoting with $x^{(i)} = (p^{(i)}, q^{(i)}) \in \mu$ the canonical coordinates of the i-th subsystem, then the *microscopic state* of the system is represented by a ordered N-tuple of points $x^{(i)}$ in μ, or equivalently by a point $x = (q, p)$ in Γ. The microscopic evolution then appears indistinctly as a motion in Γ or a N-tuple of motions in μ. The motion in Γ is solution of the microscopic differential equations: we suppose them to be Hamiltonian, with some Hamiltonian of the kind

$$H(q,p) = \sum_{i=1}^{N} h(p^{(i)}, q^{(i)}) + V(q), \qquad (p,q) \in \Gamma$$

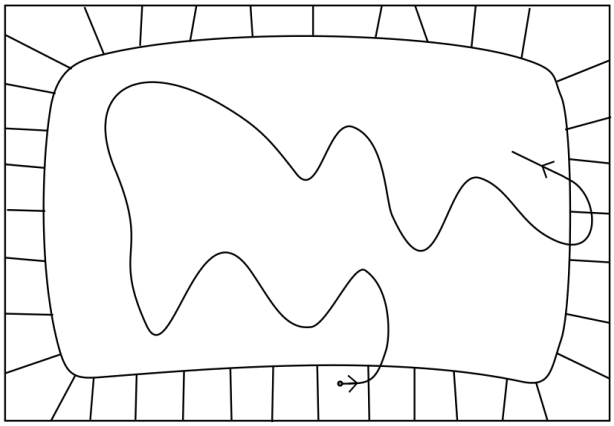

Figure 1.1: The Maxwell-Boltzmann state W^* dominates $\Gamma_{E\pm\Delta E}$.

where h is the Hamiltonian of the single subsystem, and it is identical for each of them, while V is a suitable interaction potential between the subsystems. The presence of V is essential for the subsystems to interact and for the system to evolve in a significant way: it is assumed, on the other hand, that V is considerably smaller then the first term, and approximately irrelevant when it comes to compute the energy.

The core of Bolzmann's idea consists of dividing the μ space into small cells ω_j with the same volume ω. To every choice of the occupation numbers of the cells N_j corresponds a set $W(N_1, N_2, \ldots)$ in Γ, arranged in a thin layer $\Gamma_{E\pm\Delta E}$ around the constant energy surface Σ_E. For the effect of the dynamics the occupation numbers change in time but for the energy conservation the motion is constrained to the layer $\Gamma_{E\pm\Delta E}$ which represents the true phase space of the system. The central idea of Boltzmann's work is that, unless the system enters in very special regions, with an extremely little volume, the points in μ evolve maintaining the densities f_j constant, and the macroscopic state with them. One finds that almost the totality of the accessible phase space corresponds to well defined densities, with irrelevant fluctuations. One in fact finds that

$$W(N_1, N_2, \ldots) = \frac{N!}{N_1! N_2! \ldots} \omega^N$$

and that the maximum W^* of W, with E and N fixed is for $N_j = N_j^*$ with

$$N_j^* = CN\omega e^{-\beta\varepsilon_j}, \qquad C^{-1} = \sum_j e^{-\beta\varepsilon_j}\omega,$$

so $f_j = f_j^* = Ce^{-\beta\varepsilon_j}$, where β is a Lagrange multiplier. This is called *Maxwell-Boltzmann state.*

At this point Boltzmann introduced a fundamental dynamical hypothesis, known as *ergodic hypothesis*: the microscopic dynamics is such that the point $x \in \Gamma$, representative of the microscopic state of the system, wanders through all the layer $\Gamma_{E\pm\Delta E}$ and spends in each volume W a time proportional to W itself. So, if the system is observed in a random instant (chosen in long period of time) the probability

of finding the system in a generic set coincides with its volume W. This interpretation of volume in the phase space as a probability *a priori* of a set of microscopic states is commonly called *principle of equiprobability of the microscopic states*, on which the whole statistical mechanics is built: the ergodic hypothesis represents a possible dynamic justification of it.

Boltzmann's conclusion is that no matter how the system is prepared, even in condition which are far from the thermodynamic equilibrium, the microscopic dynamics will push the system into W^*, and in this set it will spend the majority of its time, up to extremely rare fluctuations.

Gibbs's notion of macroscopic state is different from the one of Boltzmann's, the probability playing a more essential role. While Boltzmann thinks at the μ space, and associates the macroscopic state to a distribution f of the subsystems in the μ space where each of them is defined, Gibbs works directly in Γ, and identifies the macroscopic state as a probability distribution ρ in this space; the interpretation of ρ is that for a generic $W \subset \Gamma$ the *a priori* probability that one of the microscopic states $x \in W$ is realized is

$$P(W) = \int_W \rho \, dV,$$

where dV is the volume in Γ. Every macroscopic state is then a measure in Γ, with density ρ. Gibbs then considers at each time a family or *ensemble* of systems in evolution, independent mental replicas of the same physical system in different microscopic states, distributed in Γ with a suitable probability density ρ. The idea is that in every experiment the preparation of the system at $t = 0$ determines a initial distribution ρ_0 in Γ; under the dynamics each initial condition evolves independently, determining at each instant a suitable distribution ρ_t. From the volume conservation in the phase space follows the evolution equation for ρ_t

$$\rho_t(x) = \rho_0(\phi^{-t}(x)), \qquad x \in \Gamma,$$

denoting with $x \mapsto \phi^t(x)$ the microscopic evolution. The search for equilibrium states, the ones in which $\rho_t(x)$ in each point x does not depend on t, becomes natural. An example of equilibrium distribution is obtained for each $\Gamma_{E\pm\Delta E}$ as

$$\rho^*(x) = \begin{cases} \text{const} & \text{in } \Gamma_{E\pm\Delta E} \\ 0 & \text{elsewhere} \end{cases}.$$

The situation of equiprobability of the microscopic states is then, in Gibbs's view, an equilibrium state. It is clear that such a state is not unique: in fact, every

$$\rho^*(x) = F(H(x)),$$

where $F\colon \mathbb{R} \to \mathbb{R}^*$ is arbitrary and H is the Hamiltonian, is an equilibrium state. Indeed, the dynamics preserves the energy, so one must work in a constant energy surface Σ_E instead of the whole phase space Γ. One finds that the volume conservation in the phase space induces a conserved measure μ on each constant energy surface Σ_E. At this point one can introduce, instead of the density ρ in Γ, a superficial

density in Σ_E, which we keep on calling ρ, and attribute to each set $A \subset \Sigma_E$ the probability

$$P(A) = \int_A \rho(x) d\mu$$

with the same evolution equation.

Our aim is now to give the idea of a dynamical justification of these statistical assumptions. We will just enter the problem, giving the most basilar definitions and results, avoiding every kind of technical details.

Definition 1.9. For every function $f\colon M \to \mathbb{R}$, the function $\overline{f}\colon M \to \mathbb{R}$ defined by

$$\overline{f}(x) := \lim_{t\to\infty} \frac{1}{t} \sum_{s=0}^{t-1} f(\phi^s(x))$$

or in the continuous case

$$\overline{f}(x) := \lim_{t\to\infty} \frac{1}{t} \int_0^t f(\phi^s(x))\, ds$$

is called, if it exists, the *time average* of f.

For example, the average time of visit of an orbit in a measurable set A

$$\tau_A(x) := \lim_{t\to\infty} \frac{1}{t} \tau_A(x,t), \qquad \tau_A(x,t) := \int_0^t \chi_A(\phi^s(x))\, ds,$$

where χ_A is the characteristic function of A, is precisely the time average of χ_A. The time average of a function f, is itself a function $\overline{f}$; it is instead a number the *phase average* $\langle f \rangle$ of f, defined for every $f \in L_1(M,\mu)$, by

$$\langle f \rangle := \int_M f\, d\mu.$$

Theorem 1.1 (Ergodic theorem of Birkhoff-Kinchin)**.** *Let (M,μ,ϕ) a discrete dynamical system, and be $f\colon M \to \mathbb{R}$ in L_1. Then the limit*

$$\overline{f}(x) = \lim_{t\to\infty} \frac{1}{t} \sum_{s=0}^{t-1} f(\phi^s(x)),$$

exists almost everywhere in M, and one has

$$\overline{f}(\phi(x)) = \overline{f}(x), \qquad \langle \overline{f} \rangle = \langle f \rangle.$$

If the system is invertible, then the limit

$$\overline{f}_-(x) = \lim_{t\to\infty} \frac{1}{t} \sum_{s=0}^{t-1} f(\phi^{-s}(x))$$

exists almost everywhere, and almost everywhere coincides with $\overline{f}$

Definition 1.10 (Ergodic system)**.** The dynamical system (M,μ,ϕ) is said *ergodic* if one of the following equivalent properties is satisfied:

1. For every summable function $f\colon M \to \mathbb{R}$, time average and phase average coincide:
$$\overline{f}(x) = \langle f \rangle \qquad \text{almost everywhere in } M;$$

2. For every measurable set $A \subset M$ the average time of visit is equal to the measure of A:
$$\tau_A(x) = \mu(A) \qquad \text{almost everywhere in } M;$$

3. There are no summable non-trivial integrals of motion:
$$f(\phi^t(x)) = f(x) \quad \forall t \quad \text{almost everywhere in } M \quad \Longrightarrow \quad f \text{ constant in } M$$
for every $f\colon M \to \mathbb{R}$.

The first property is the most classical one, and is at the basis of the definition of ergodicity in different textbooks of statistical mechanics; it corresponds to the practical idea of substituting phase averages to time averages, which are in general difficult to compute. The second property formalize to the idea by Boltzmann that in an observation made in a casual time corresponds a probability of finding the microscopic state of the system in A equal to the measure of A: in this way, for an ergodic system, the volume assumes the meaning of probability. The third property, finally, corresponds to the uniqueness of the equilibrium in Gibbs's sense: if the macroscopic state ρ_t evolves with
$$\rho_t(x) = \rho_t(\phi^{-t}(x))$$
then the only equilibrium state, such that $\rho_t = \rho_0$ for every t is the uniform one $\rho(x) = 1$ almost everywhere.

Clearly, every Hamiltonian system with one degree of freedom, on a constant surface energy Σ_E compact connected and with no singular point, is ergodic. It is ergodic, then, the single harmonic oscillator $H(q,p) = \frac{1}{2}(p^2 + \omega^2 q^2)$ on each of the constant energy curves. It is not ergodic instead, on the constant energy surface, a system of two or more harmonic oscillators, $H = \frac{1}{2}\sum_{i=1}^{n}(p_i^2 + \omega_i^2 q_i^2)$, or more generally a system like
$$H(q,p) = \sum_{i=1}^{n} h_i(q_i, p_i);$$
in fact, the energies of the single components are first integrals, thus going against the third property. An integrable system with $n \geq 2$ degrees of freedom is not ergodic, since it admits n non-trivial first integrals. Systems like these prompt us to put a very natural question: what happens if one includes a small coupling between the oscillators? This is exactly the question to which Fermi, Pasta and Ulam tried to answer in the celebrated work [1], that is the starting point of this work.

CHAPTER 2

Infinite dimensional systems

Let $L_2(\Lambda)$ be the space of real-valued square integrable function on a one dimensional differentiable manifold Λ with norm

$$\langle f, g \rangle = \int_\Lambda dx\ f(x)g(x) \qquad \forall f, g \in L_2(\Lambda).$$

In the following we will denote partial derivatives with a subscript, for example $\frac{\partial \psi}{\partial t} = \psi_t$.

We would like to give an Hamiltonian structure to an infinite dimensional system, namely a PDE system in the form

$$\psi_t = f(\psi, \psi_x, \psi_{xx}, \ldots), \qquad \psi \in L_2(\Lambda).$$

In this work, in fact, we will use the Heisenberg picture of Quantum Mechanics and its Hamiltonian properties in order to understand the dynamics of the particular quantum system which is the quantum equivalent of the classical Fermi-Pasta-Ulam system [1]. With the tools provided by this theory of infinite dimensional systems we will formulate Quantum Mechanics in an Hamiltonian environment, providing an Hamiltonian formulation for the Schrödinger picture, and seeing its isomorphism (in the algebraic sense) with the Heisenberg picture. Thanks to the Poisson structure of Quantum Mechanics we will in fact extend the theorems known in the classical environment and perform calculations that allows us to keep in close contact to the well studied classical case.

2.1 Lagrangian formulation

We will introduce the Hamiltonian structure of an infinite dimensional system starting by the Lagrangian formulation, and then pass to the Hamiltonian formulation performing the Legendre transform. In analogy with the finite dimensional case, the Lagrangian will be a real functional $L(\psi, \psi_t)$. Instead of the sum over the discrete indices in the finite dimensional case, we have now a integral over Λ of a function

$\mathscr{L}(\psi, \psi_x, \psi_t)$ called *Lagrangian density*

$$L(\psi, \psi_t) = \int_\Lambda \mathscr{L}(\psi, \psi_x, \psi_t)\, dx.$$

The *action* is the integral over the time of this quantity

$$S(\psi) = \int_{\mathbb{R}} L(\psi, \psi_t)\, dt = \int_R \int_\Lambda \mathscr{L}(\psi, \psi_x, \psi_t)\, dx\, dt$$

We would like to apply the *principle of least action*, i.e. find the equations of motion by searching the critical points of the action functional S, but to perform such task we need first of all to define differentiation in the infinite dimensional space L_2. In the finite dimensional case, for a function $f\colon \mathbb{R}^n \to \mathbb{R}$, $x \mapsto f(x)$ we have

$$df(x) = \frac{d}{d\varepsilon} f(x + \varepsilon h)|_{\varepsilon=0} = \nabla f(x) \cdot h.$$

In the infinite dimensional case we define the *weak differential* of a functional $F(\psi_1, \dots, \psi_n)$ along the direction $(h_1, \dots, h_n)$, with $h_i|_{\partial\Lambda} = 0\ \forall i = 1, \dots, n$

$$dF(\psi_1, \dots \psi_n) = \frac{d}{d\varepsilon} F(\psi_1 + \varepsilon h_1, \dots, \psi_n + \varepsilon h_n)|_{\varepsilon=0}$$

and the *L_2-gradients* $\nabla_{\psi_i} F$ such that

$$dF = \sum_{i=1}^{n} \langle \nabla_{\psi_i} F, h_i \rangle.$$

We now calculate the L_2-gradients of L along the directions h, h_t

$$\begin{aligned} dL(\psi.\psi_t) &= \int_\Lambda \frac{d}{d\varepsilon} \mathscr{L}(\psi + \varepsilon h, \psi_x + \varepsilon h_x, \psi_t + \varepsilon h_t)|_{\varepsilon=0}\, dx \\ &= \int_\Lambda (\frac{\partial \mathscr{L}}{\partial \psi} h + \frac{\partial \mathscr{L}}{\partial \psi_x} h_x + \frac{\partial \mathscr{L}}{\partial \psi_t} h_t)\, dx \\ &= \int_\Lambda \left((\frac{\partial \mathscr{L}}{\partial \psi} - \frac{d}{dx} \frac{\partial \mathscr{L}}{\partial \psi_x}) h + \frac{\partial \mathscr{L}}{\partial \psi_t} h_t \right)\, dx \end{aligned}$$

so that

$$dL = \langle \frac{\partial \mathscr{L}}{\partial \psi} - \frac{d}{dx} \frac{\partial \mathscr{L}}{\partial \psi_x}, h \rangle + \langle \frac{\partial \mathscr{L}}{\partial \psi_t}, h_t \rangle.$$

The L_2-gradients of L are then

$$\nabla_\psi L = \frac{\partial \mathscr{L}}{\partial \psi} - \frac{d}{dx} \frac{\partial \mathscr{L}}{\partial \psi_x}, \qquad \nabla_{\psi_t} L = \frac{\partial \mathscr{L}}{\partial \psi_t}.$$

The principle of least action reads $dS(\psi) = 0$, so

$$\begin{aligned} dS(\psi) &= \int_{\mathbb{R}} dL(\psi, \psi_t)\, dt \\ &= \int_{\mathbb{R}} (\langle \nabla_\psi L, h \rangle + \langle \nabla_{\psi_t} L, h_t \rangle)\, dt \\ &= \int_{\mathbb{R}} \int_\Lambda (\nabla_\psi L - \frac{d}{dt} \nabla_{\psi_t} L) h\, dx\, dt \\ &\equiv \langle \nabla_\psi S, h \rangle. \end{aligned}$$

The equation of motion are then

$$\nabla_\psi S = \nabla_\psi L - \frac{d}{dt}\nabla_{\psi_t} L = 0 \quad \Longrightarrow \quad \frac{\partial \mathscr{L}}{\partial \psi} - \frac{d}{dx}\frac{\partial \mathscr{L}}{\partial \psi_x} - \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \psi_t} = 0$$

which are the *Euler-Lagrange equations* for the Lagrangian density $\mathscr{L}$.

Remark 2.1. In theoretical physics a slightly different notation is used, which we will use in the following. The weak differential

$$dF(\psi) := \delta F(\psi)$$

is called *Gateaux differential* while $h =: \delta\psi$ so that

$$\delta F(\psi) = \frac{d}{d\varepsilon} F(\psi + \varepsilon\delta\psi)|_{\varepsilon=0}.$$

The L_2-gradient are called *functional derivative* $\nabla_\psi F =: \frac{\delta F}{\delta \psi}$ so that

$$\delta F(\psi) = \langle \frac{\delta F}{\delta \psi}, \delta\psi \rangle.$$

The Euler-Lagrange equation thus reads

$$\frac{d}{dt}\frac{\delta L}{\delta \psi_t} - \frac{\delta L}{\delta \psi} = 0. \tag{2.1}$$

2.2 Hamiltonian formulation

In analogy to the well known finite dimensional case, we define the *momentum*

$$\pi = \frac{\delta L}{\delta \psi_t}.$$

Suppose the above relation is invertible, i.e. it exists a smooth function $\mathscr{F}$ such that

$$\psi_t = \mathscr{F}(\psi, \pi).$$

This hypothesis is verified, for example, if L is convex in ψ_t, but it is not if the dependence is linear. Starting from a Lagrangian functional L we can now define the *Hamiltonian* as its Legendre transform

$$H(\psi, \pi) = \left(\langle \pi, \psi_t \rangle - L(\psi, \psi_t)\right)|_{\psi_t = \mathscr{F}(\psi,\pi)}$$

which can be written as a function of a *Hamiltonian density* $\mathscr{H}$ as $H = \int_\Lambda \mathscr{H}\, dx$ where

$$\mathscr{H} = (\pi\psi_t - \mathscr{L}(\psi, \psi_x, \psi_t))|_{\psi_t = \mathscr{F}(\psi,\pi)}.$$

In the following we will understand the evaluation of ψ_t in $\mathscr{F}(\psi, \pi)$. The action functional is $S(\psi, \pi) = \int (\langle \pi, \psi_t \rangle - H(\psi, \pi))\, dt$. A direct computation shows that the least action principle implies the Hamilton equations for ψ and π, i.e.

$$\psi_t = \frac{\delta H}{\delta \pi}, \qquad \pi_t = -\frac{\delta H}{\delta \psi}.$$

In this way we have seen that ψ and π defined as above are a infinite dimensional Hamiltonian system, with the standard Poisson tensor $\mathbb{J}$ and the standard partial derivative substituted by functional derivatives

$$\begin{pmatrix} \psi_t \\ \pi_t \end{pmatrix} = \mathbb{J} \begin{pmatrix} \frac{\delta H}{\delta \psi} \\ \frac{\delta H}{\delta \pi} \end{pmatrix}.$$

Moreover, the algebra of real-valued, square-integrable functions of ψ and π together with the Poisson tensor $\mathbb{J}$ form a Poisson algebra, which can be object of changes of variables and canonical transformations as described in the previous section.

2.3 Quantum mechanics

2.3.1 Hamiltonian structure of the Schrödinger equation

Let us consider the Schrödinger equation for the wave function $\psi\colon \Lambda \times \mathbb{R} \to \mathbb{C}$, $x \mapsto \psi(x,t)$, of a single particle with mass $m > 0$ and position x in some d-dimensional differentiable manifold[1] Λ in a potential $V(x)$

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi = -\frac{\hbar^2}{2m}\Delta\psi + V\psi. \tag{2.2}$$

Our aim is to look for an Hamiltonian formulation of this equation, i.e. look for an Hamiltonian, function of $\psi(x,t)$, whose Hamilton equations are precisely the Schrödinger equation (and its complex conjugate). Of course this whole construction can be extended to the many-particle case.

First of all we want to formulate the problem in a Lagrangian environment. The Schrödinger equation and its complex conjugate are the Euler-Lagrange equations for the Lagrangian density

$$\mathscr{L}(\psi, \psi^*, \psi_t, \psi_t^*) = \frac{i\hbar}{2}(\psi^*\psi_t - \psi\psi_t^*) - V|\psi|^2 - \frac{\hbar^2}{2m}|\nabla\psi|^2 \tag{2.3}$$

and $L = \int_\Lambda \mathscr{L}\, dx$. In fact, the Euler-Lagrange equation for ψ^* are

$$\frac{d}{dt}\frac{\delta L}{\delta \psi_t^*} = \frac{\delta L}{\delta \psi^*} \qquad \Longrightarrow \qquad \frac{d}{dt}(-i\hbar\psi) = -V\psi - \sum_{j=1}^{d} \frac{d}{dx_j}(-\frac{\hbar^2}{2m}\frac{\partial \psi}{\partial x_j})$$

which is of course (2.2). One would like to apply the Legendre transform in order to pass to the Hamiltonian formulation, but as L is linear in ψ_t and ψ_t^*, the change of variables

$$\pi = \frac{\delta L}{\delta \psi_t}$$

is not invertible, and the whole construction of the Legendre transform theory cannot be applied. However, if we define ψ as the "coordinate" and $i\hbar\psi^*$ as the "momentum" and use the standard Poisson tensor $\mathbb{J}_2$, we have a Hamiltonian system of Hamiltonian

$$H = \int_\Lambda \mathscr{H}\, dx, \qquad \mathscr{H} = \frac{\hbar^2}{2m}|\nabla\psi|^2 + V|\psi|^2.$$

[1] Common choices for Λ are $\mathbb{R}^d$, or the torus $\mathbb{T}^d \equiv (\mathbb{R}/l\mathbb{Z})^d$ for some $l > 0$, for $d = 1, 2, 3$.

In fact, the Hamilton equations are

$$\psi_t = \frac{\delta H}{\delta \pi} = \frac{1}{i\hbar}\frac{\delta H}{\delta \psi^*} = \frac{1}{i\hbar}\left(\frac{\partial \mathscr{H}}{\partial \psi^*} - \nabla \cdot \frac{\hbar^2}{2m}\frac{\partial |\nabla \psi|^2}{\partial \nabla \psi^*}\right) = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\Delta\psi + V\psi\right)$$

which is (2.2), and

$$\pi_t = i\hbar\psi_t^* = -\frac{\delta H}{\delta \psi}$$

which gives its complex conjugate. One can also use the so called *Birkhoff structure*, which is a more symmetric Poisson structure where ψ is the coordinate and ψ^* is the momentum. In these coordinates, the Poisson tensor is $\frac{\sigma_2}{\hbar}$, in fact the Hamilton equations are

$$\begin{pmatrix} \psi_t \\ \psi_t^* \end{pmatrix} = \frac{1}{\hbar}\begin{pmatrix} -i\frac{\delta H}{\delta \psi^*} \\ i\frac{\delta H}{\delta \psi} \end{pmatrix} = \frac{1}{i\hbar}\mathbb{J}_2 \begin{pmatrix} \frac{\delta H}{\delta \psi} \\ \frac{\delta H}{\delta \psi^*} \end{pmatrix}$$

and $\frac{1}{i}\mathbb{J}_2 = \sigma_2$. Observe that, in this Poisson algebra, the Poisson bracket of two functions $F(\psi, \psi^*)$ and $G(\psi, \psi^*)$ is given by

$$\{F, G\} = \frac{1}{i\hbar}\int_\Lambda \left(\frac{\delta F}{\delta \psi}\frac{\delta G}{\delta \psi^*} - \frac{\delta F}{\delta \psi^*}\frac{\delta G}{\delta \psi}\right) dx.$$

Remark 2.2. The Hamiltonian $H(\psi, \psi^*)$, namely

$$H(\psi, \psi^*) = \int_\Lambda \left(\frac{\hbar^2}{2m}|\nabla\psi|^2 + V|\psi|^2\right) dx = \int_\Lambda \psi^* \hat{H}\psi \, dx = \langle \psi, \hat{H}\psi \rangle$$

is the quadratic (Hermitian) form associated to $\hat{H}$ (the Hamiltonian operator) computed in ψ.

2.3.2 Schrödinger and Heisenberg pictures as Poisson algebras

We have just shown that the Schrödinger equation admits a Hamiltonian formulation in terms of the Poisson bracket

$$\{F, G\} = \frac{1}{i\hbar}\int_\Lambda \left(\frac{\delta F}{\delta \psi}\frac{\delta G}{\delta \psi^*} - \frac{\delta F}{\delta \psi^*}\frac{\delta G}{\delta \psi}\right) dx$$

with Hamiltonian $H(\psi, \psi^*) = \langle \psi, \hat{H}\psi \rangle$. Here the phase space of the system is the space L_2 of complex valued, square-integrable wave-functions, and the Poisson Algebra is the algebra of real functions $F(\psi, \psi^*)$ endowed with the bracket $\{\ ,\ \}$ defined above. In this picture, called *Schrödinger picture*, the wave function evolves in time, and the functions defined on the phase space evolve as a consequence.

$$\begin{array}{ccc} \psi(0) & \longrightarrow & \psi(t) \\ \downarrow & & \downarrow \\ F(\psi(0), \psi^*(0)) & \longrightarrow & F(\psi(t), \psi^*(t)) \end{array}$$

An alternative formulation of quantum mechanics is the following. First, the flow of the Schrödinger equation is explicitly introduced, in the form of a unitary time-evolution operator $\hat{U}(t)$ solution of

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{H}\hat{U}(t), \qquad \hat{U}(0) = \mathbb{1}.$$

One easily checks that, due to the above equation and initial condition, $\hat{U}^\dagger(t)\hat{U}(t) = \mathbb{1}$ $\forall t \in \mathbb{R}$. For the sake of simplicity $\hat{H}$ and all the other self-adjoint operators are supposed to be independent of time. One then finds

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t} := \sum_{j\geq 0} \frac{1}{j!}(-\frac{i}{\hbar}\hat{H}t)^j.$$

Second, it is postulated that the relevant physical quantities that are measurable, i.e. the so-called *observables*, correspond to the quadratic (Hermitian) forms associated to certain self-adjoint linear operatos, computed in $\psi(t)$, namely

$$\langle \psi(t), \hat{A}\psi(t)\rangle, \qquad \text{where} \quad \hat{A}^\dagger = \hat{A}.$$

The above quadratic form is called the *quantum expectation* of the operator $\hat{A}$ at time t. Now, one has

$$\langle \psi(t), \hat{A}\psi(t)\rangle = \langle \psi(0), \hat{A}_H(t)\psi(0)\rangle$$

where $\hat{A}_H(t) := \hat{U}^\dagger(t)\hat{A}\hat{U}(t)$. In other words, the quantum expectation of the time-independent operator $\hat{A}$ a time t equals the quantum expectation of the time dependent operator $\hat{A}_H(t)$ at time $t = 0$. One can thus think of the wave function as fixed to its initial value, letting the operators evolve in time. This is the so-called *Heisenberg picture*. In such a picture the operators evolve according to the similarity transformation $\hat{A} \to \hat{U}^\dagger(t)\hat{A}\hat{U}(t) =: \hat{A}_H(t)$. One easily finds that

$$\frac{d}{dt}\hat{A}_H(t) = \frac{1}{i\hbar}[\hat{A}_H(t), \hat{H}(t)]$$

called the *Heisenberg equation of motion* for $\hat{A}_H(t)$. Observe that the bracket $\frac{1}{i\hbar}[\ ,\ ]$ is a bilinear, skew-symmetric, Jacobi and Leibniz product in the space of self-adjoint operators: a Poisson bracket on the algebra of linear self-adjoint operatos acting on L_2, which then becomes a Poisson algebra.

In order to compare the Poisson algebra of the Schrödinger picture to that of the Heisenberg picture, one has to restrict the algebra of the functions in the former pictures to that of the real quadratic functions. Thus, to any such function $\mathscr{F}(\phi, \phi^*)$ there correspond a linear self-adjoint operator $\hat{F}$ such that $\mathscr{F}(\psi, \psi^*) = \langle \psi, \hat{F}\psi\rangle$, and such a correspondence is a bijection. Now, given $\mathscr{F}(\psi, \psi^*) = \langle \psi, \hat{F}\psi\rangle$ and $\mathscr{G}(\psi, \psi^*) = \langle \psi, \hat{G}\psi\rangle$, one has

$$\begin{aligned}
\{\mathscr{F}, \mathscr{G}\} &= \frac{1}{i\hbar}\int_\Lambda (\frac{\delta\mathscr{F}}{\delta\psi}\frac{\delta\mathscr{G}}{\delta\psi^*} - \frac{\delta\mathscr{F}}{\delta\psi^*}\frac{\delta\mathscr{G}}{\delta\psi})\, dx \\
&= \frac{1}{i\hbar}\int_\Lambda [(\hat{F}\psi^*)\hat{G}\psi - (\hat{F}\psi)\hat{G}\psi^*]\, dx \\
&= \frac{1}{i\hbar}[\langle \psi, \hat{F}\hat{G}\psi\rangle - \langle \psi, \hat{G}\hat{F}\psi\rangle] \\
&= \langle \psi, \frac{1}{i\hbar}[\hat{F}, \hat{G}]\psi\rangle
\end{aligned}$$

i.e.

$$\{\langle \psi, \hat{F}\psi\rangle, \langle \psi, \hat{F}\psi\rangle\} = \langle \psi, \frac{1}{i\hbar}[\hat{F}, \hat{G}]\psi\rangle.$$

Such a relation shows that the Poisson algebras of the Schrödinger and of the Heisenberg picture are isomorphic. More precisely, the map

$$Q\colon \hat{F} \mapsto \mathscr{F} = Q(F) := \langle \psi, \hat{F}\psi \rangle$$

that associates linear self-adjoint operators to their quadratic forms, (elements of the Heisenberg algebra to elements of the Schrödinger algebra) is a bijection and preserves the product

$$\{Q(\hat{F}), Q(\hat{G})\} = Q(\frac{1}{i\hbar}[\hat{F}, \hat{G}]).$$

Thus Q is a isomorphism between the two algebras.

CHAPTER 3

The classical FPU problem and its quantization

After World War II, Fermi became interested in the development and potentialities of the electronic computing machines, trying a selection of problems for heuristic work where in absence of closed analytic solutions experimental work on a computing machine would perhaps contribute to the understanding of properties of solutions, for example regarding long-time behaviour of non-linear physical systems. In particular, the first of these work was the study of the ergodic properties of a one-dimensional anharmonic chain, which was the simplest non-linear model for a metal, expecting the thermalisation to show. In particular:

- A chain of 64 particles with fixed boundary conditions was considered, the force between the particles satisfying the Hooke Law, plus weak non-linear corrections;
- The equations of motion were resolved numerically;
- The results were analysed in Fourier components and plotted against time.

The initial data were chosen by setting all the energy in the first Fourier component and the program was let run, waiting for an *energy equipartition* state, in which all the Fourier components had approximately the same amount of energy.

The results, shown in figure 3.1 were quite surprising, and became known as the *Fermi-Pasta-Ulam paradox*: instead of the energy equipartition, a recurrent meta-state was found in which the energy is exchanged by the lower Fourier modes only, and after some time the system recurs to the initial data, the $\sim 97\%$ of the energy returning to the first Fourier component. These results were one of the first intimations that the prevalent (at those times) beliefs in the universality of mixing and thermalisation in non-linear systems may not be always justified.

The solution of the paradox can be seen in multiple equivalent ways, one of them being the existence and stability of *solitons* for the Korteweg-de Vries equation

$$U_t = aU_{xxx} + bUU_x.$$

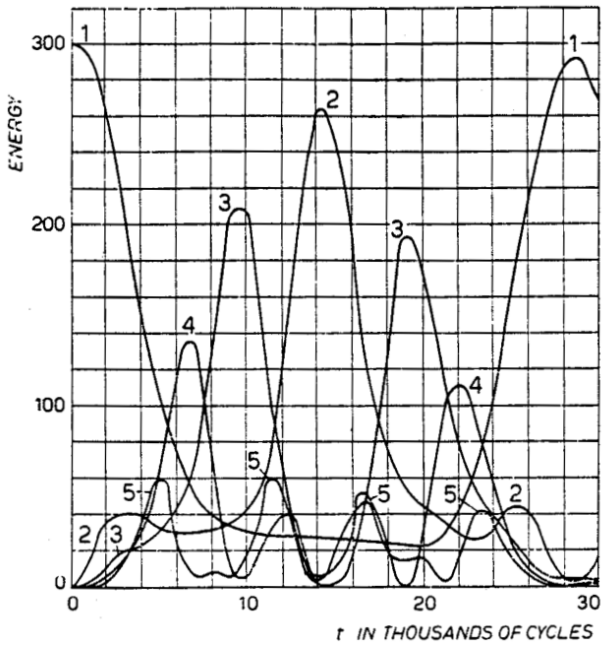

Figure 3.1: The recurrence results of the original work [1]. As one can see, the energy returns almost completely to the first Fourier component.

In 1965 in fact, using the continuum limit, Zabusky and Kruskal [2], were able to relate the periodic behaviour of the FPU system to the dynamics of localized excitations, nowadays known as *solitons*, of this equation. Moreover, in [11] it was found that the continuum limit of the Hamilton equations for the acoustic modes (i.e. long wavelength modes) was equivalent to the Korteweg-de Vries equation, which admits an infinite number of conserved quantities in involution, and thus is integrable. Applying the ergodic theory, it is clear that a system described by this equation cannot show any thermalisation property. However, the equivalence of the Fermi-Pasta-Ulam system with the Korteweg-de Vries equation is obtained in a perturbative way, therefore it holds only for a long, but finite, period of time. The perturbative approach and the integrability of the Korteweg-de Vries equation explains the meta-stability of the Fermi-Pasta-Ulam recurrence state.

In this chapter we will construct the traditionally called $\alpha+\beta$ FPU model, starting from the physical system of particles with equal masses and a certain interaction. Then we will pass to the normal modes of oscillation, which is the starting point for the canonical quantization of the system. Then we will canonically quantize the system and pass to a set of coordinates particularly useful in our work, which are the creation and annihilation operators.

3.1 Construction of the model

Let us consider a one dimensional chain of length L of $N+1$ particles with mass m, $x_n \in \mathbb{R}$ $n = 0, \dots, N$ being the coordinate of the n-th particle, with the analytical interaction potential energy $\phi(x_{n+1} - x_n)$. We denote the momentum of the n-th particle by $y_n \in \mathbb{R}$. In the following we will often denote by (x, y) the coordinates of

the whole phase space. Here we will consider fixed boundary conditions, i.e.

$$x_0 = 0, \quad x_N = L, \quad y_0 = 0, \quad y_N = 0. \tag{3.1}$$

The Hamiltonian of the system will then be

$$K = \sum_{n=1}^{N-1} \frac{y_n^2}{2m} + \sum_{n=0}^{N-1} \phi(x_{n+1} - x_n). \tag{3.2}$$

Since the Hamilton equations are

$$\dot{y}_k = -\frac{\partial K}{\partial x_k} = \phi'(x_{k+1} - x_k) - \phi'(x_k - x_{k-1})$$
$$\dot{x}_k = \frac{\partial K}{\partial y_k} = \frac{y_k}{m},$$

the system surely has (at least) the equilibrium (x^{eq}, y^{eq}) such that

$$y_n^{eq} = 0, \quad x_{n+1}^{eq} - x_n^{eq} = x_n^{eq} - x_{n-1}^{eq} \qquad \forall n. \tag{3.3}$$

This physically corresponds to a state where all the particles stay still and equally distant from one another. Denoting with a the interspacing between the particles in the equilibrium configuration one has

$$x_0^{eq} = 0, \quad x_1^{eq} = a, \quad x_2^{eq} = 2a, \quad \dots \quad , \quad x_n^{eq} = na, \quad \dots, \quad x_N^{eq} = Na,$$

so, given the boundary conditions, surely $Na = L$, which is the classic crystal configuration.

Now we want to change coordinates, putting us in a frame where only small deviations from the equilibrium are considered. Moreover, we want to deal only with non dimensional quantities. With this in mind we will operate the change of coordinates $(x_n, y_n) \mapsto (q_n, p_n)$ and the reparametrization of the time $T \mapsto t$ that conjugates K to H, where

$$\begin{gathered} x_n = na + aq_n, \quad y_n = \tfrac{ma}{\tau} p_n \\ T = \tau t, \quad K = \tfrac{ma^2}{\tau^2} H. \end{gathered} \tag{3.4}$$

Remark that we denoted with T the old dimensional time, t the new non dimensional time, and $\tau \in \mathbb{R}$ a parameter yet to be specified. With the rescaling of the Hamiltonian and the time, this transformation is canonical. The boundary conditions 3.1 become

$$q_0 = p_0 = q_N = p_N = 0. \tag{3.5}$$

With this new coordinates the Hamiltonian K 3.2 becomes (yet to be rescaled according to 3.4)

$$K = \sum_{n=1}^{N-1} \frac{ma^2}{\tau} \frac{p_n^2}{2} + \sum_{n=0}^{N-1} \phi(a + a(q_{n+1} - q_n)).$$

In the same frame of mind, denoting $\delta_n q := q_{n+1} - q_n$, and being the interaction potential energy analytic, we can expand it in Taylor expansion around the point a, obtaining

$$\phi(a + a\delta_n q) = \sum_{s\geq 0} \frac{\phi^{(s)}(a)}{s!} a^s (\delta_n q)^s.$$

The potential energy will be

$$\sum_{s\geq 0} \frac{\phi^{(s)}(a)}{s!} a^s \sum_{n=0}^{N-1} (\delta_n q)^s = \\ \phi(a)N + \phi'(a) \sum_{n=0}^{N-1} (q_{n+1} - q_n) + \sum_{s\geq 2} \frac{\phi^{(s)}(a)}{s!} a^s \sum_{n=0}^{N-1} (q_{n+1} - q_n)^s.$$

Being $\sum_{n=0}^{N-1}(q_{n+1} - q_n) = 0$ (it is easy to verify keeping in mind the fixed boundary conditions), and eliminating the constant term, one can write the potential energy

$$\frac{\phi^{(2)}(a)a^2}{2} \sum_{n=0}^{N-1} (q_{n+1} - q_n)^2 + \frac{\phi^{(3)}(a)a^3}{3!} \sum_{n=0}^{N-1} (q_{n+1} - q_n)^3 + \\ + \frac{\phi^{(4)}(a)a^4}{4!} \sum_{n=0}^{N-1} (q_{n+1} - q_n)^4 + \dots$$

Remark that by assuming that the equilibrium is stable, one must require that $\phi^{(2)}(a) > 0$.

The new Hamiltonian is

$$H = \sum_{n=1}^{N-1} \frac{p_n^2}{2} + \sum_{s\geq 2} \frac{\phi^{(s)}(a) a^{s-2} \tau^2}{ms!} \sum_{n=0}^{N-1} (q_{n+1} - q_n)^s, \tag{3.6}$$

still containing the arbitrary parameter τ, which will be chosen by setting the coefficient of the quadratic term of the Taylor expansion $\tau^2 \frac{\phi^{(2)}(a)}{m} = 1$, that is

$$\tau = \sqrt{\frac{m}{\phi^{(2)}(a)}}.$$

With this choice of τ, the following coefficients are

$$\alpha := \frac{\phi^{(3)}(a)a}{2\phi^{(2)}(a)}, \\ \beta := \frac{\phi^{(4)}(a)a^2}{6\phi^{(2)}(a)}, \\ \gamma := \frac{\phi^{(5)}(a)a^3}{24\phi^{(2)}(a)}, \quad \dots$$

so that the Hamiltonian has the traditional form of the *Fermi-Pasta-Ulam Model* (also known as *FPU*)

$$H = \sum_{n=1}^{N-1} \frac{p_n^2}{2} + \sum_{n=0}^{N-1} \left[\frac{1}{2}(q_{n+1} - q_n)^2 + \frac{\alpha}{3}(q_{n+1} - q_n)^3 + \frac{\beta}{4}(q_{n+1} - q_n)^4 + \dots \right]. \tag{3.7}$$

Remark 3.1. The non-dimensional parameters τ, α, β, ecc... are obtainable from the physical potential ϕ, the number of particles N and the length of the chain L. Some examples of these parameters for various potentials are found in [20].

Remark 3.2. If $\alpha \neq 0$ one can set $\alpha = 1$, by means of the canonical transformation $q_n \mapsto q'_n$ and a reparametrization of the time $t \mapsto t'$ that conjugates H to H' such that

$$q_n = \frac{q'_n}{\alpha}, \quad p_n = \frac{p'_n}{\alpha}$$
$$t = t', \quad H = \frac{H'}{\alpha^2},$$

and then redefining $\beta' = \beta/\alpha^2$, $\gamma' = \gamma/\alpha^3$, ...

Remark 3.3. Here we use fixed boundary conditions, which are a particular case of the periodic ones, in the following sense. Given a FPU system with $M = 2N$ particles with periodic boundary conditions, i.e.

$$q_{j+M} = q_j, \quad p_{j+M} = p_j \qquad \forall j,$$

one can find a particular set of initial data whose evolution is precisely the evolution of a FPU system with N particles and fixed boundary conditions. In fact, suppose that the Hamiltonian for $2N$ particle with periodic boundary condition is

$$H(q,p) = \sum_{n=-N+1}^{N-1} \frac{p_n^2}{2} + \sum_{n=-N+1}^{N-1} u(q_{m+1} - q_n)$$

and suppose we take a set of initial data which satisfy to the condition

$$q_n = -q_{-n}, \quad p_n = -p_{-n}, \quad \forall n.$$

Denoting $z = (q,p)$ this condition can be written in a matrix form as $Tz_0 =: z'_0 = z_0$, with

$$T := \begin{pmatrix} & & & & & & & -1 & & & & & & & \\ & & & & & & \iddots & & & & & & & & \\ & & & & & -1 & & & & & & & & & \\ & & & & \iddots & & & & & & & & & & \\ -1 & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & & -1 \\ & & & & & & & & & & & & & \iddots & \\ & & & & & & & & & & & & -1 & & \\ & & & & & & & & & & & \iddots & & & \\ & & & & & & & & & & -1 & & & & \end{pmatrix}$$

It is easy to verify that the transformation $z \mapsto z' = Tz$ is canonical, and that $H \circ T = H$. Thus, supposing z_t is the solution of the Hamilton equations $\dot{z}_t = X_H(z_0)$ for the initial data $z'_0 = z_0$ we have (since the transformation is canonical)

$$\dot{z}'_t = X_{H\circ T}(z'_0) = X_H(z_0).$$

So Tz_t and z_t are solutions of the same differential equation with the same initial data, and for the Cauchy–Lipschitz theorem they are the same solution, $z_t = Tz_t$. Physically, for such initial data the dynamics maintain the condition

$$q_n = -q_{-n}, \quad p_n = -p_{-n}, \quad \forall n$$

true: the motion is then symmetric, the coordinates with positive n mirroring the ones with negative n, while $(q_0, p_0) = (q_N, p_N) = 0$. It is exactly the dynamics of a N particle system with fixed boundary condition.

3.2 Normal modes

From now on we shall consider only FPU models (3.7) truncated up the 4-th order, called $\alpha + \beta$ models. Let us now introduce the *normal modes* of oscillation of the FPU chain, i.e. a canonical transformation

$$\mathscr{N} : (q, p)_n \mapsto (Q, P)_k \tag{3.8}$$

such that, defining $\phi_k(n) := \sqrt{\frac{2}{N}} \sin \frac{\pi k n}{N}$, one has

$$\mathscr{N} : \begin{cases} Q_k = \sum_{n=1}^{N-1} q_n \phi_k(n) \\ P_k = \sum_{n=1}^{N-1} p_n \phi_k(n) \end{cases}$$

and on the other hand

$$\mathscr{N}^{-1} : \begin{cases} q_n = \sum_{k=1}^{N-1} Q_k \phi_k(n) \\ p_n = \sum_{k=1}^{N-1} P_k \phi_k(n) \end{cases}$$

Remark 3.4. One has $\sum_{n=1}^{N-1} \phi_k(n)\phi_{k'}(n) = \delta_{k,k'}$ (see lemma 3.2).

Proposition 3.1. *This change of variables conjugates the Hamiltonian 3.7 to the Hamiltonian*[1] $H := H \circ \mathscr{N}^{-1}$

$$H(Q, P) = \sum_{k=1}^{N-1} \frac{P_k^2 + \omega_k^2 Q_k^2}{2} + \sum_{D>2} \frac{g_D}{D(2N)^{D/2-1}} \sum_{k_1,\dots,k_D}^{N-1} \Delta_D(k_1, \dots, k_D) \prod_{s=1}^{D} \omega_{k_s} Q_{k_s} \tag{3.9}$$

where

$$\omega_k := 2 \sin \frac{\pi k}{2N}, \quad k = 1, \dots, N-1$$

are the frequencies and

$$\Delta_D(k_1, \dots, k_D) := \frac{1}{2} \sum_{\sigma \in \mathscr{S}^D} \delta_{\sigma \cdot k, 0} + \sum_{\sigma \in \mathscr{S}^D} \sum_{l \geq 1} (-1)^l \delta_{\sigma \cdot k, 2lN}$$

are called selectors*, where* $\mathscr{S} = \{-1, 1\}$.

Now we show how we got to (3.9).

[1] In order to avoid heavy notations, we will use the same symbol for conjugated Hamiltonians.

Lemma 3.1. $\sum_{n=0}^{N-1} \cos \frac{\pi k n}{N} = \sum_{s\in\mathbb{Z}} (N\delta_{k,2sN} + \delta_{k,2s+1})$

Proof. Let us begin by calculating the quantity $\sum_{n=0}^{N-1} e^{i\frac{\pi k n}{N}}$ (the result will be its real part). Note that if $k \in 2\mathbb{Z}N$ then the result is simply N.

$$\sum_{n=0}^{N-1} e^{i\frac{\pi k n}{N}} = \frac{1-e^{i\pi k}}{1-e^{i\frac{\pi k}{N}}} = \frac{e^{i\pi k}-1}{e^{i\frac{\pi k}{2N}}(e^{i\frac{\pi k}{2N}} - e^{-i\frac{\pi k}{2N}})} = \frac{e^{-i\frac{\pi k}{2N}}((-1)^k-1)}{2i\sin\frac{\pi k}{2N}}.$$

Now we take the real part:

$$\mathrm{Re}\sum_{n=1}^{N-1} e^{i\frac{\pi k n}{N}} = \mathrm{Re}\left(\frac{e^{-i\frac{\pi k}{2N}}((-1)^k-1)}{2i\sin\frac{\pi k}{2N}}\right) = \frac{1}{2}(1-(-1)^k) = \begin{cases} 0 & \text{if } k \text{ is even} \\ 1 & \text{if } k \text{ is odd} \end{cases} \qquad \square$$

Lemma 3.2. $\sum_{n=1}^{N-1} \phi_n(k)\phi_n(k') = \delta_{k,k'}$

Proof. Using the prosthaphaeresis formula $\sin\alpha\sin\beta = \frac{1}{2}(\cos(\alpha-\beta) - \cos(\alpha+\beta))$, one finds that

$$\sum_{n=1}^{N-1} \phi_n(k)\phi_n(k') = \frac{1}{N}\sum_{n=1}^{N-1}(\cos\frac{\pi(k-k')n}{N} - \cos\frac{\pi(k+k')n}{N}).$$

Now we use Lemma 3.1 and find

$$\frac{1}{2}\sum_{s\in\mathbb{Z}}[N(\delta_{k-k',2sN} - \delta_{k+k',2sN}) + (\delta_{k-k',2s+1} - \delta_{k+k',2s+1})].$$

Now, $1 \le k, k' \le N-1$, so $2 \le k+k' \le 2N-2$ and $2-N \le k-k' \le N-2$: the first term is non zero only if $k-k'=0$; besides, if $k+k'$ is odd $k-k'$ is also odd: the second term is always zero. The result is then $\frac{1}{N}N\delta_{k-k',0} = \delta_{k,k'}$. $\square$

By using Lemma 3.2 one can easily see that the kinetic part of (3.7) becomes

$$\sum_{n=1}^{N-1} \frac{p_n^2}{2}|_{p_n=\sum_{k=1}^{N-1} P_k\phi_k(n)} = \sum_{k=1}^{N-1} \frac{P_k^2}{2}.$$

Now we will show how to compute the perturbation part, i.e.

$$\sum_{n=0}^{N-1} U(q_{n+1}-q_n)|_{q_n=\sum_{k=1}^{N-1} Q_k\phi_k(n)},$$

where

$$U(x) = \sum_{D\ge 2} \frac{g_D}{D}x^D.$$

Note that $g_2 = 1$, $g_3 = \alpha$, $g_4 = \beta$ and so on. First of all let us compute the difference $q_{n+1}-q_n$ for a generic $n = 0, \dots, N-1$. One has

$$\begin{aligned} q_{n+1}-q_n &= \sum_{k=1}^{N-1} Q_k(\phi_{n+1}(k) - \phi_n(k)) \\ &= \sum_{k=1}^{N-1} Q_k\sqrt{\frac{2}{N}}(\sin\frac{\pi k(n+1)}{N} - \sin\frac{\pi k n}{N}) \\ &= \sum_{k=1}^{N-1} \omega_k Q_k\sqrt{\frac{2}{N}}\cos\frac{\pi k(2n+1)}{2N}. \end{aligned}$$

So, the D-degree perturbation energy will be

$$\frac{g_D}{D}\sum_{n=0}^{N-1}(q_{n+1}-q_n)^D = \frac{g_D}{D}\left(\frac{2}{N}\right)^{D/2}\sum_{k_1,\dots,k_D=1}^{N-1}\prod_{s=1}^{D}\omega_{k_s}Q_{k_s}\sum_{n=0}^{N-1}\prod_{s=1}^{D}\cos\frac{\pi k_s(2n+1)}{2N}.$$

In order to do this computation, a general formula for the product of cosines will be useful.

Lemma 3.3. *$\forall D\in\mathbb{N}$, let be $\theta^{(D)}=(\theta_1,\dots,\theta_D)$ and $\mathscr{S}=\{-1,1\}$. Then,*

$$\prod_{s=1}^{D}\cos\theta_s = \frac{1}{2^D}\sum_{\sigma\in\mathscr{S}^D}\cos(\sigma\cdot\theta^{(D)}).$$

Proof. We will proceed by induction. The formula is trivially true for $D=1$. Suppose it is true for a generic D. Then,

$$\begin{aligned}\prod_{s=1}^{D+1}\cos\theta_s &= \frac{1}{2^D}\sum_{\sigma\in\mathscr{S}^D}\cos(\sigma\cdot\theta^{(D)})\cos\theta_{D+1}\\ &= \frac{1}{2^{D+1}}\sum_{\sigma\in\mathscr{S}^D}[\cos(\sigma\cdot\theta^{(D)}+\theta_{D+1})+\cos(\sigma\cdot\theta^{(D)}-\theta_{D+1})\\ &= \frac{1}{2^{D+1}}\sum_{\sigma\in\mathscr{S}^{D+1}}\cos(\sigma\cdot\theta^{(D+1)}) \qquad \square\end{aligned}$$

Using Lemma 3.3 the D-degree perturbation energy becomes

$$\frac{g_D}{D}\sum_{n=0}^{N-1}(q_{n+1}-q_n)^D = \frac{g_D}{D}\left(\frac{2}{N}\right)^{D/2}\frac{1}{2^D}\sum_{k_1,\dots,k_D=1}^{N-1}\prod_{s=1}^{D}\omega_{k_s}Q_{k_s}\sum_{n=0}^{N-1}\sum_{\sigma\in\mathscr{S}^D}\cos\left(\frac{\pi(2n+1)}{2N}k\cdot\sigma\right),$$

where $k=(k_1,\dots,k_D)$.

Lemma 3.4. *If $k\in\mathbb{Z}$ one has*

$$\sum_{n=0}^{N-1}\cos\frac{\pi k(2n+1)}{2N} = \sum_{s\in\mathbb{Z}}(-1)^s N\delta_{k,2sN}.$$

Proof. First of all we compute $\sum_{n=0}^{N-1}e^{i\frac{\pi k(2n+1)}{2N}}$, and the result will be its real part. One can see that, if $k=2sN$, $s\in\mathbb{Z}$, then the result is $(-1)^sN$. Otherwise one has

$$\begin{aligned}\sum_{n=0}^{N-1}e^{i\frac{\pi k(2n+1)}{2N}} &= e^{i\frac{\pi k}{2N}}\sum_{n=0}^{N-1}e^{i\frac{\pi kn}{N}}\\ &= e^{i\frac{\pi k}{2N}}\frac{e^{-i\frac{\pi k}{2N}}((-1)^k-1)}{2i\sin(\frac{\pi k}{2N})}\\ &= \frac{i}{2}\frac{1-(-1)^k}{\sin(\frac{\pi k}{2N})}.\end{aligned}$$

So in this case $\mathrm{Re}(\sum_{n=0}^{N-1}e^{i\frac{\pi k(2n+1)}{2N}})=0$. $\square$

Let us now define the *selector*

$$\Delta_D(k_1,\dots,k_D) := \frac{1}{2}\sum_{\sigma\in\mathscr{S}^D}\sum_{l\in\mathbb{Z}}(-1)^l\delta_{\sigma\cdot k,2lN}. \tag{3.10}$$

An alternative but completely equivalent form of the selector is

$$\Delta_D(k_1,\dots,k_D) = \frac{1}{2}\sum_{\sigma\in\mathscr{S}^D}\delta_{\sigma\cdot k,0} + \sum_{\sigma\in\mathscr{S}^D}\sum_{l\geq 1}(-1)^l\delta_{\sigma\cdot k,2lN}. \tag{3.11}$$

By means of this definition and of Lemma 3.4 one can see that the D-degree perturbation energy can be written in a more compact way

$$\left[\frac{g_D}{D}\left(\frac{2}{N}\right)^{D/2}\frac{N}{2^{D-1}}\right]\sum_{k_1,\dots,k_D=1}^{N-1}\Delta_D(k_1,\dots,k_D)\prod_{s=1}^{D}\omega_{k_s}Q_{k_s} \tag{3.12}$$

For example, let us write the selectors of degree two, three, and four. For $D=2$

$$\Delta_2(k_1,k_2) = \delta_{k_1,k_2}.$$

For $D=3$

$$\Delta_3(k_1,k_2,k_3) = \delta_{k_1+k_2,k_3} + \delta_{k_2+k_3,k_1} + \delta_{k_3+k_1,k_2} - \delta_{k_1+k_2+k_3,2N}. \tag{3.13}$$

For $D=4$,

$$\begin{aligned}\Delta_4(k_1,k_2,k_3,k_4) = {}& \delta_{k_1+k_2+k_3,k_4} + \delta_{k_2+k_3+k_4,k_1} + \delta_{k_3+k_4+k_1,k_2} + \delta_{k_4+k_1+k_2,k_3} + \\ & + \delta_{k_1+k_2,k_3+k_4} + \delta_{k_1+k_3,k_2+k_4} + \delta_{k_1+k_4,k_2+k_3} + \\ & - \delta_{k_1+k_2+k_3,k_4+2N} - \delta_{k_1+k_2+k_4,k_3+2N} - \delta_{k_1+k_3+k_4,k_2+2N} + \\ & - \delta_{k_2+k_3+k_4,k_1+2N} - \delta_{k_1+k_2+k_3+k_4,2N}.\end{aligned} \tag{3.14}$$

In this way, one can compute explicitly the Hamiltonian (3.9), and find

$$H = \sum_{k=1}^{N-1}\frac{P_k^2+\omega_k^2Q_k^2}{2} + \sum_{D=3,4}\frac{g_D}{D(2N)^{D/2-1}}\sum_{k_1,\dots,k_D}^{N-1}\Delta_D(k_1,\dots,k_D)\prod_{s=1}^{D}\omega_{k_s}Q_{k_s}$$

Remark 3.5. $H_2 = \sum_{k=1}^{N-1}\frac{P_k^2+\omega_k^2Q_k^2}{2}$ is precisely the Hamiltonian of $N-1$ non coupled harmonic oscillators, so, in a sense, is *integrable*. Thus here we are considering $N-1$ coupled oscillators with cubic and quartic interaction.

One can now perform a canonical rescaling, namely a symplectic change of coordinates $(Q,P)\mapsto(Q',P')$ such that

$$Q_k = \frac{Q'_k}{\sqrt{\omega_k}}, \quad P_k = \sqrt{\omega_k}P'_k, \quad k=1,\dots,N-1$$

which conjugates the Hamiltonian (3.9) to

$$\begin{aligned}H(Q',P') = {}& \sum_{k=1}^{N-1}\omega_k\frac{P'^2_k+Q'^2_k}{2} \\ & + \sum_{D\geq 3}\frac{g_D}{D(2N)^{D/2-1}}\sum_{k_1,\dots,k_D}^{N-1}\Delta_D(k_1,\dots,k_D)\prod_{s=1}^{D}\sqrt{\omega_{k_s}}Q'_{k_s}.\end{aligned} \tag{3.15}$$

In order to perform quantization, it is useful to pass to *complex coordinates*, i.e.

$$z_k := \frac{Q'_k + iP'_k}{\sqrt{2}}, \quad z_k^* := \frac{Q'_k - iP'_k}{\sqrt{2}} \qquad k : 1, \dots, N-1. \tag{3.16}$$

This conjugates (3.15) to

$$H(z, z^*) = \sum_{k=1}^{N-1} \omega_k |z_k|^2 + \sum_{D\geq 3} \frac{g_D}{DN^{D/2-1}2^{D-1}} \sum_{k_1,\dots,k_D}^{N-1} \Delta_D(k_1, \dots, k_D) \prod_{s=1}^{D} \sqrt{\omega_{k_s}}(z_{k_s} + z_{k_s}^*). \tag{3.17}$$

Remark 3.6. The change of coordinates (3.16) is not symplectic, so it does not preserve the poisson structure. One can easily see with a direct computation that the new Poisson structure is

$$\{z_k, z_{k'}^*\} = -i\delta_{k,k'}$$

so that the ODEs related to H are

$$\dot{z}_k = -i\frac{\partial H}{\partial z_k^*} = -i\omega_k z_k + \dots$$

and its complex conjugate for $\dot{z}_k^*$.

The Hamiltonian (3.17) is the starting point of the analysis in [11], in which it was found that the Hamilton equations for the first modes z_k, $k \ll N$ are, in a certain way that will be specified in the following, equivalent to the Korteweg-de Vries equation. Our aim is to quantize this system, and find out which equation is the quantum equivalent of the KdV, using the tool of the Hamiltonian theory of perturbations. We will write the calculations for the quantum case, while, since the computations are very similar and differ only for the commutativity of products, we only report the results for the classical case.

3.3 Canonical quantization of the FPU problem

In order to quantize the FPU problem, one can proceed in two different, but as we will show, completely equivalent ways.

The first is to start from the "physical" Hamiltonian (3.2), rescale the momenta and the positions to obtain non dimensional quantities, and then pass to the normal modes of oscillation (Q, P). Finally quantize the momenta, namely substitute P_k and Q_k, $\forall k = 1, \dots, N-1$, with hermitian non dimensional operators $\hat{P}_k$ and $\hat{Q}_k$ such that

$$\hat{P}_k = -i\frac{\partial}{\partial \hat{Q}_k} \quad \forall k.$$

The second is to start from the "physical" Hamiltonian (3.2) and canonically quantize the momenta y_n and coordinates x_n, namely substitute y_n, and x_n $\forall n = 1, \dots, N-1$, with hermitian dimensional operators $\hat{y}_n$ and $\hat{x}_n$ such that

$$\hat{y}_n = -i\hbar\frac{\partial}{\partial \hat{x}_n} \quad \forall n.$$

Then, rescale $(\hat{x}, \hat{y})$ in order to obtain non dimensional quantities $(\hat{q}, \hat{p})$ such that

$$\hat{p}_n = -i\frac{\partial}{\partial \hat{q}_n} \quad \forall n,$$

and then pass to the normal modes of oscillation $(\hat{Q}, \hat{P})$, and find again

$$\hat{P}_k = -i\frac{\partial}{\partial \hat{Q}_k} \quad \forall k.$$

The first way is the continuation of what we did in the previous sections. Here we will proceed with the second alternative method, and show its equivalence with the first.

Consider a quantum Hamiltonian operator

$$\hat{K} = \sum_{n=1}^{N-1} \frac{\hat{y}_n^2}{2m} + \sum_{n=0}^{N-1} \phi(\hat{x}_{n+1} - \hat{x}_n), \qquad \hat{y}_n = -i\hbar\frac{\partial}{\partial \hat{x}_n} \quad \forall n = 1, N-1.$$

This is a Hamiltonian system in the Poisson algebra of the Heisenberg picture, so all the notions from Hamiltonian mechanics are well defined. We look for a canonical non univalent transformation $(\hat{x}, \hat{y}, \hat{K}, T) \mapsto (\hat{q}, \hat{p}, \hat{H}, t)$ of the form

$$\hat{x}_n = na + \alpha\hat{q}_n, \quad \hat{y}_n = \beta\hat{p}_n$$

$$\hat{K} = \gamma\hat{H}, \quad T = \tau t$$

which conjugates $\hat{K}$ to

$$\hat{H} = \sum_{n=1}^{N-1} \frac{\hat{p}_n^2}{2} + \sum_{n=0}^{N-1} \left[\frac{(\hat{q}_{n+1} - \hat{q}_n)^2}{2} + \alpha\frac{(\hat{q}_{n+1} - \hat{q}_n)^3}{3} + \beta\frac{(\hat{q}_{n+1} - \hat{q}_n)^4}{4} + \dots \right]$$

such that:

1. $\alpha\beta = \gamma\tau$;
2. in order to "normalize" the kinetic energy $\beta^2 = \gamma m$;
3. in order to "normalize" the quadratic term of the potential energy $\phi^{(2)}(a)\alpha^2 = \gamma$;
4. $\hat{p}_n = -i\frac{\partial}{\partial \hat{q}_n}$.

The last condition is satisfied if and only if

$$\alpha\beta = \hbar.$$

We have four equations for four parameters. The solution is

$$\alpha = \frac{\sqrt{\hbar}}{(m\phi^{(2)}(a))^{1/4}}, \quad \beta = \sqrt{\hbar}(m\phi^{(2)}(a))^{1/4}, \quad \gamma = \hbar\sqrt{\frac{\phi^{(2)}(a)}{m}}, \quad \tau = \sqrt{\frac{m}{\phi^{(2)}(a)}}.$$

When passing to the normal modes of oscillation

$$\begin{cases} \hat{q}_n = \sum_k \hat{Q}_k \phi_k(n) \\ \hat{p}_n = \sum_k \hat{P}_k \phi_k(n) \end{cases}, \qquad \begin{cases} \hat{Q}_k = \sum_n \hat{q}_n \phi_k(n) \\ \hat{P}_k = \sum_n \hat{p}_n \phi_k(n) \end{cases},$$

where $\phi_k(n) = \sqrt{\frac{2}{N}} \sin\left(\frac{\pi k n}{N}\right)$, the condition $\hat{P}_k = -i\frac{\partial}{\partial \hat{Q}_k}$ is automatically satisfied. In fact, being

$$\frac{\partial}{\partial \hat{q}_n} = \sum_k \frac{\partial \hat{Q}_k}{\partial \hat{q}_n} \frac{\partial}{\partial \hat{Q}_k} = \sum_k \phi_k(n) \frac{\partial}{\partial \hat{Q}_k},$$

one has

$$\hat{P}_k = \sum_n \phi_k(n)(-i\frac{\partial}{\partial \hat{q}_n}) = \sum_n \sum_{k'} \phi_k(n)\phi_{k'}(n)(-i\frac{\partial}{\partial \hat{Q}_{k'}}) = -i\frac{\partial}{\partial \hat{Q}_k}.$$

Remark 3.7. It is easy to verify that the operators $\hat{Q}_k$ and $\hat{P}_k$ satisfy the commutation rule

$$[\hat{Q}_k, \hat{P}_{k'}] = i\delta_{k,k'}.$$

We have shown that one can obtain in two different but equivalent ways the quantum Hamiltonian operator for the FPU problem, as a function of the normal modes of oscillation $\hat{Q}_k, \hat{P}_k$, as in 3.9:

$$\hat{H}(\hat{Q}, \hat{P}) = \sum_{k=1}^{N-1} \frac{\hat{P}_k^2 + \omega_k^2 \hat{Q}_k^2}{2} + \sum_{D \leq 2} \frac{g_D}{D(2N)^{D/2-1}} \sum_{k_1,\ldots,k_D}^{N-1} \Delta_D(k_1, \ldots, k_D) \prod_{s=1}^{D} \omega_{k_s} \hat{Q}_{k_s}.$$

As we did in the previous section, one can now perform a canonical rescaling, namely a symplectic change of coordinates $(\hat{Q}, \hat{P}) \mapsto (\hat{Q}', \hat{P}')$ such that

$$\hat{Q}_k = \frac{\hat{Q}'_k}{\sqrt{\omega_k}}, \quad \hat{P}_k = \sqrt{\omega_k}\hat{P}'_k, \quad k = 1, \ldots, N-1$$

which conjugates the previous Hamiltonian to

$$\hat{H}(\hat{Q}', \hat{P}') = \sum_{k=1}^{N-1} \omega_k \frac{\hat{P}'^2_k + \hat{Q}'^2_k}{2} + \sum_{D \geq 3} \frac{g_D}{D(2N)^{D/2-1}} \sum_{k_1,\ldots,k_D}^{N-1} \Delta_D(k_1, \ldots, k_D) \prod_{s=1}^{D} \sqrt{\omega_{k_s}} \hat{Q}'_{k_s}. \quad (3.18)$$

At this point, it is useful to introduce the *annihilation and creation operators*[2] a_k and $a_k^\dagger$ which are the analogous of the complex coordinates introduced in the previous chapter. We define

$$a_k = \frac{\hat{Q}'_k + i\hat{P}'_k}{\sqrt{2}}, \qquad a_k^\dagger = \frac{\hat{Q}'_k - i\hat{P}'_k}{\sqrt{2}}.$$

[2]Since the symbols a and $a^\dagger$ will be used only to indicate these operators, the circumflex will be omitted.

They inherit the commutation rule from the one of $\hat{Q}'_k$ and $\hat{P}'_k$: being $[\hat{Q}'_k, \hat{P}'_q] = i\delta_{k,q}$ one obtains

$$[a_k, a_q^\dagger] = \frac{\delta_{k,q}}{2} + \frac{\delta_{k,q}}{2} = \delta_{k,q}$$

while the other mixed commutators are always zero. This conjugates the Hamiltonian operator 3.18 to

$$\hat{H}(a, a^\dagger) = \sum_{k=1}^{N-1} \omega_k a_k^\dagger a_k + \sum_{D\geq 3} \frac{g_D}{DN^{D/2-1}2^{D-1}} \sum_{k_1,\ldots,k_D=1}^{N-1} \Delta_D(k_1, \ldots, k_D) \prod_{s=1}^{D} \sqrt{\omega_{k_s}}(a_{k_s} + a_{k_s}^\dagger), \quad (3.19)$$

and we will call

$$\hat{V}(a, a^\dagger) = \sum_{D\geq 3} \frac{g_D}{DN^{D/2-1}2^{D-1}} \sum_{k_1,\ldots,k_D}^{N-1} \Delta_D(k_1, \ldots, k_D) \prod_{s=1}^{D} \sqrt{\omega_{k_s}}(a_{k_s} + a_{k_s}^\dagger)$$

the *perturbation term*. We will call in the following the Hamiltonian operator (3.19) the *quantum Fermi-Pasta-Ulam* (or *qFPU*) Hamiltonian. It is important to notice that we arrived to this formulation of the quantum problem simply starting from the canonical quantization of the physical Hamiltonian, so the only physical assumption that we made is the validity of the canonical quantization, i.e. to substitute to the momentum y_n an operator

$$\hat{y}_n = -i\hbar \frac{\partial}{\partial \hat{x}_n}.$$

3.4 Normal Ordering

Here we will show the normal ordering of the Hamiltonian of the $\alpha + \beta$ model. First of all we need to define it.

Definition 3.1. Given A a product of any number of operators a_k and $a_k^\dagger$, $\forall k$, we define

- $N[A]$ is the product of the same operators in A rearranged in a way such as all the $a^\dagger$ operators are to the left, taking into account the commutation rule $[a_k, a_q^\dagger] = \delta_{k,q}$: $N[A]$ is said the *normal ordering* of A;
- $:A:$ is the product of the same operators in A rearranged in a way such as all the $a^\dagger$ operators are to the left, without taking into account the commutation rule $[a_k, a_q^\dagger] = \delta_{k,q}$ (so treated as if they were commuting real numbers);

Remark 3.8. $N[A]$ and A are the same operator: only its functional form changes. $:A:$ and A instead are two different operators.

So, for example, given $A = a_k a_q^\dagger$

$$N[A] = a_q^\dagger a_k + \delta_{k,q}, \qquad :A: = a_q^\dagger a_k.$$

The normal ordering of

$$\prod_{s=1}^{2}(a_{k_s}+a_{k_s}^\dagger)=a_{k_1}a_{k_2}+a_{k_1}a_{k_2}^\dagger+a_{k_1}^\dagger a_{k_2}+a_{k_1}^\dagger a_{k_2}^\dagger.$$

is more complicated. The first, third and fourth term are already ordered normally, so we just have to rearrange the second term replacing $a_{k_1}a_{k_2}^\dagger$ with $a_{k_2}^\dagger a_{k_1}+\delta_{k_1,k_2}$. So one has

$$:\prod_{s=1}^{2}(a_{k_s}+a_{k_s}^\dagger):\ =a_{k_1}a_{k_2}+a_{k_2}^\dagger a_{k_1}+a_{k_1}^\dagger a_{k_2}+a_{k_1}^\dagger a_{k_2}^\dagger,$$

$$N\left[\prod_{s=1}^{2}(a_{k_s}+a_{k_s}^\dagger)\right]=a_{k_1}a_{k_2}+a_{k_2}^\dagger a_{k_1}+a_{k_1}^\dagger a_{k_2}+a_{k_1}^\dagger a_{k_2}^\dagger+\delta_{k_1,k_2}.$$

The normal ordering of terms like $\prod_{s=1}^{D}(a_{k_s}+a_{k_s}^\dagger)$ grows exponentially with the degree D, so one can imagine that normal ordering this kind of quantities becomes more and more complicated.

Our aim is to normal order the qFPU Hamiltonian operator(3.19) for the $\alpha+\beta$ model, namely

$$\hat{H}(a,a^\dagger)=\sum_{k=1}^{N-1}\omega_k a_k^\dagger a_k + \sum_{D=3,4}\frac{g_D}{DN^{D/2-1}2^{D-1}}\sum_{k_1,\dots,k_D}^{N-1}\Delta_D(k_1,\dots,k_D)\prod_{s=1}^{D}\sqrt{\omega_{k_s}}(a_{k_s}+a_{k_s}^\dagger),$$

where the $\{a_{k_s}\}$ and $\{a_{k_s}^\dagger\}$ are called respectively *annihilation operators* and *creation operators*, and where we dropped out the constant term $\sum_k \frac{\omega_k}{2}$ (which refers to the vacuum energy). This manipulation of the Hamiltonian operator will be useful when we will apply the perturbation theory. The quadratic term is already normal ordered, so we will start by normal ordering the perturbation term. We will denote by $\hat{H}_3$ and $\hat{H}_4$ the cubic and quartic term of the Hamiltonian, i.e.

$$\hat{H}_3(a,a^\dagger)=\frac{\alpha}{12\sqrt{N}}\sum_{k_1,k_2,k_3=1}^{N-1}\Delta_3(k_1,k_2,k_3)\prod_{s=1}^{3}\sqrt{\omega_{k_s}}(a_{k_s}+a_{k_s}^\dagger) \tag{3.20}$$

$$\hat{H}_4(a,a^\dagger)=\frac{\beta}{32N}\sum_{k_1,k_2,k_3,k_4=1}^{N-1}\Delta_4(k_1,k_2,k_3,k_4)\prod_{s=1}^{4}\sqrt{\omega_{k_s}}(a_{k_s}+a_{k_s}^\dagger). \tag{3.21}$$

We will need to compute quantities like

$$\sum_{k_1,\dots,k_D=1}^{N-1}\Delta_D(k_1,\dots,k_D)N\left[\prod_{s=1}^{D}\sqrt{\omega_{k_s}}(a_{k_s}+a_{k_s}^\dagger)\right],$$

where ω_k and Δ_D are defined in the previous sections, for $D=3,4$, where the products are made with increasing s (remind that products of operators do not commute) Let

us forget about the frequencies for the moment (they are real commuting numbers). Let us start to compute

$$N\left[\prod_{s=1}^{D}(a_{k_s}+a_{k_s}^\dagger)\right].$$

For $D=3$ one has

$$N\left[\prod_{s=1}^{3}(a_{k_s}+a_{k_s}^\dagger)\right]=$$
$$:\prod_{s=1}^{3}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_1,k_2}(a_{k_3}+a_{k_3}^\dagger)+\delta_{k_1,k_3}(a_{k_2}+a_{k_2}^\dagger)+\delta_{k_2,k_3}(a_{k_1}+a_{k_1}^\dagger), \quad (3.22)$$

while for $D=4$

$$N\left[\prod_{s=1}^{4}(a_{k_s}+a_{k_s}^\dagger)\right]=$$
$$:\prod_{s=1}^{4}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_1,k_2}:\prod_{s=3,4}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_1,k_3}:\prod_{s=2,4}(a_{k_s}+a_{k_s}^\dagger):+$$
$$+\delta_{k_1,k_4}:\prod_{s=2,3}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_2,k_3}:\prod_{s=1,4}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_2,k_4}:\prod_{s=1,3}(a_{k_s}+a_{k_s}^\dagger):+$$
$$+\delta_{k_3,k_4}:\prod_{s=1,2}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_1,k_2}\delta_{k_3,k_4}+\delta_{k_1,k_3}\delta_{k_2,k_4}+\delta_{k_1,k_4}\delta_{k_2,k_3}. \quad (3.23)$$

Now consider

$$\sum_{k_1,\dots,k_D=1}^{N-1}\Delta_D(k_1,\dots,k_D)N\left[\prod_{s=1}^{D}\sqrt{\omega_{k_s}}(a_{k_s}+a_{k_s}^\dagger)\right]$$

for $D=3$. When we apply the selector $\Delta_3(k_1,k_2,k_3)=\delta_{k_1+k_2,k_3}+\delta_{k_3+k_1,k_2}+\delta_{k_2+k_3,k_1}-\delta_{k_1+k_2+k_3,2N}$ and sum over $k_1,k_2,k_3=1\dots,N-1$ some terms are vanishing. Look for example at the first term of the selector $\delta_{k_1+k_2,k_3}$ applied to $\delta_{k_1,k_3}(a_{k_2}+a_{k_2}^\dagger)$ and to $\delta_{k_2,k_3}(a_{k_1}+a_{k_1}^\dagger)$: $k_3=k_1+k_2$ can be equal neither to k_1 nor to k_2, as they are never zero, so they will not contribute. The same is valid for the other terms of the selector. One finally has

$$\sum_{k_1,k_2,k_3=1}^{N-1}\Delta_3(k_1,k_2,k_3)N\left[\prod_{s=1}^{3}(a_{k_s}+a_{k_s}^\dagger)\right]=$$
$$\sum_{k_1,k_2,k_3=1}^{N-1}\Big[\Delta_3(k_1,k_2,k_3):\prod_{s=1}^{3}(a_{k_s}+a_{k_s}^\dagger):+\delta_{k_1+k_2,k_3}\delta_{k_1,k_2}(a_{k_3}+a_{k_3}^\dagger)+$$
$$+\delta_{k_2+k_3,k_1}\delta_{k_2,k_3}(a_{k_1}+a_{k_1}^\dagger)+\delta_{k_3+k_1,k_2}\delta_{k_3,k_1}(a_{k_2}+a_{k_2}^\dagger)+$$
$$-\delta_{k_1+k_2+k_3,2N}(\delta_{k_1,k_2}(a_{k_3}+a_{k_3}^\dagger)+\delta_{k_1,k_3}(a_{k_2}+a_{k_2}^\dagger)+\delta_{k_2,k_3}(a_{k_1}+a_{k_1}^\dagger))\Big]$$

If we sum over k_1, k_2, k_3 we can rename the $\{k_s\}$ in a suitable way so that some contributions to the sum are equal. So one obtains

$$\sum_{k_1,k_2,k_3=1}^{N-1} \Delta_3(k_1,k_2,k_3) N \left[\prod_{s=1}^{3}(a_{k_s}+a_{k_s}^\dagger)\right] =$$
$$\sum_{k_1,k_2,k_3=1}^{N-1} \Big[\Delta_3(k_1,k_2,k_3)\colon \prod_{s=1}^{3}(a_{k_s}+a_{k_s}^\dagger)\colon + 3(\delta_{k_1+k_2,k_3}-\delta_{k_1+k_2+k_3,2N})\delta_{k_1,k_2}(a_{k_3}+a_{k_3}^\dagger)\Big]$$

One can see that $N[\hat{H}_3]$ contains terms of the third order in a and $a^\dagger$ that will be denoted by $\hat{H}_3^{(3)}$, and terms of the first order, that will be denoted by $\hat{H}_3^{(1)}$. One finds that

$$\hat{H}_3^{(3)}(a,a^\dagger) = \frac{\alpha}{12\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}}$$
$$\Delta_3(k_1,k_2,k_3)[a_{k_1}a_{k_2}a_{k_3} + 3a_{k_1}^\dagger a_{k_2}a_{k_3} + 3a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} + a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger]. \quad (3.24)$$

In general one finds that

$$\hat{H}_D^{(D)}(a,a^\dagger) =$$
$$\frac{g_D}{DN^{D/2-1}2^{D-1}} \sum_{k_1,\ldots,k_D=1}^{N-1} \prod_{s=1}^{D} \sqrt{\omega_{k_s}}\Delta_D(k_1,\ldots,k_D) \sum_{d=0}^{D} \binom{D}{d} \prod_{t=1}^{D-d} a_{k_t}^\dagger \prod_{t=D-d+1}^{D} a_{k_t}. \quad (3.25)$$

One also finds

$$\hat{H}_3^{(1)}(a,a^\dagger) = \frac{\alpha}{4\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}}(\delta_{k_1+k_2,k_3} - \delta_{k_1+k_2+k_3,2N})\delta_{k_1,k_2}(a_{k_3}+a_{k_3}^\dagger)$$
$$= \frac{\alpha}{4\sqrt{N}}\Big\{ \sum_{k_2,k_3=1}^{N-1} \omega_{k_2}\sqrt{\omega_{k_3}}\delta_{2k_2,k_3}(a_{k_3}+a_{k_3}^\dagger) - \sum_{k_2,k_3=1}^{N-1} \omega_{k_2}\sqrt{\omega_{k_3}}\delta_{2k_2+k_3,2N}(a_{k_3}+a_{k_3}^\dagger)\Big\}$$
$$= \frac{\alpha}{4\sqrt{N}}\Big\{ \sum_{k=1}^{B_1(N)} \omega_k\sqrt{\omega_{2k}}(a_{2k}+a_{2k}^\dagger) - \sum_{k=B_2(N)}^{N-1} \omega_k\sqrt{\omega_{2N-2k}}(a_{2N-2k}+a_{2N-2k}^\dagger)\Big\}$$

where

$$B_1(N) = \begin{cases} \frac{N-1}{2} & \text{if } N \text{ is odd} \\ \frac{N-2}{2} & \text{if } N \text{ is even} \end{cases} \qquad B_2(N) = \begin{cases} \frac{N+1}{2} & \text{if } N \text{ is odd} \\ \frac{N+2}{2} & \text{if } N \text{ is even} \end{cases}.$$

By sending $2N-2k$ to $2k$ in the second sum one obtains

$$\hat{H}_3^{(1)}(a,a^\dagger) = \frac{\alpha}{4\sqrt{N}} \sum_{k=1}^{B_1(N)} \sqrt{\omega_{2k}}(\omega_k - \omega_{N-k})(a_{2k}+a_{2k}^\dagger). \quad (3.26)$$

Remark 3.9. The coefficient $\omega_k - \omega_{N-k}$ is non zero for every $k = 1, \ldots, B_1(N)$. In fact it vanishes if and only if $k = N/2 > B_1(N)$.

Consider now $D = 4$. We recall the selector, which is (3.14)

$$\begin{aligned}\Delta_4(k_1,k_2,k_3,k_4) = &\delta_{k_1+k_2+k_3,k_4} + \delta_{k_2+k_3+k_4,k_1} + \delta_{k_3+k_4+k_1,k_2} + \delta_{k_4+k_1+k_2,k_3} + \\ &+ \delta_{k_1+k_2,k_3+k_4} + \delta_{k_1+k_3,k_2+k_4} + \delta_{k_1+k_4,k_2+k_3} + \\ &- \delta_{k_1+k_2+k_3,k_4+2N} - \delta_{k_1+k_2+k_4,k_3+2N} - \delta_{k_1+k_3+k_4,k_2+2N} + \\ &- \delta_{k_2+k_3+k_4,k_1+2N} - \delta_{k_1+k_2+k_3+k_4,2N}.\end{aligned}$$

When we apply Δ_4 to (3.23) and sum over $k_1, k_2, k_3, k_4 = 1 \ldots, N-1$ some terms are vanishing. For example, let us consider the term in (3.23)

$$: \prod_{s=3,4} (a_{k_s} + a^\dagger_{k_s}) : \delta_{k_1,k_2}.$$

When multiplied by, for instance, $\delta_{k_2+k_3+k_4,k_1}$, and summed over $k_1, k_2, k_3, k_4 = 1 \ldots, N-1$ it is non zero if and only if

$$\begin{cases} k_1 = k_2 \\ k_2 + k_3 + k_4 = k_1 \end{cases} \qquad \Longrightarrow \qquad k_3 + k_4 = 0$$

which never happens. The same is true for $\delta_{k_3+k_4+k_1,k_2}$, $\delta_{k_1+k_3,k_2+k_4}$ and $\delta_{k_1+k_4,k_2+k_3}$. Now consider the selector term $\delta_{k_1+k_3+k_4,k_2+2N}$. If $k_1 = k_2$ its contribution is zero, because $k_3 + k_4 \leq 2N - 2 < 2N$. So we can state that when we have something in (3.23) multiplied by δ_{k_i,k_j}, for some i, j, the terms inside the selector with k_i and k_j in the two different "sides" of the delta do not contribute.

Because of this we can also state that the terms with two deltas in (3.23), of the form $\delta_{k_i,k_j}\delta_{k_l,k_m}$, contribute only when multiplied by $\delta_{k_1+k_2+k_3+k_4,2N}$.
Finally one has

$$\begin{aligned}&\sum_{k_1,k_2,k_3,k_4=1}^{N-1} \Delta_4(k_1,k_2,k_3,k_4) N \big[\prod_{s=1}^{4} (a_{k_s} + a^\dagger_{k_s}) \big] = \\ &\sum_{k_1,k_2,k_3,k_4=1}^{N-1} \big[\Delta_4(k_1,k_2,k_3,k_4) : \prod_{s=1}^{4} (a_{k_s} + a^\dagger_{k_s}) : + \\ &+ \delta_{k_1,k_2} : \prod_{s=3,4} (a_{k_s} + a^\dagger_{k_s}) : (\delta_{k_1+k_2+k_3,k_4} + \delta_{k_1+k_2+k_4,k_3} + \delta_{k_1+k_2,k_3+k_4} + \\ &- \delta_{k_1+k_2+k_3,k_4+2N} - \delta_{k_1+k_2+k_4,k_3+2N} - \delta_{k_1+k_2+k_3+k_4,2N}) + \\ &+ \delta_{k_2,k_3} : \prod_{s=1,4} (a_{k_s} + a^\dagger_{k_s}) : (\delta_{k_1+k_2+k_3,k_4} + \delta_{k_2+k_3+k_4,k_1} + \delta_{k_1+k_4,k_2+k_3} + \\ &- \delta_{k_1+k_2+k_3,k_4+2N} - \delta_{k_2+k_3+k_4,k_1+2N} - \delta_{k_1+k_2+k_3+k_4,2N}) + \\ &+ \ldots + \\ &- (\delta_{k_1,k_2}\delta_{k_3,k_4} + \delta_{k_1,k_3}\delta_{k_2,k_4} + \delta_{k_1,k_4}\delta_{k_2,k_3})\delta_{k_1+k_2+k_3+k_4,2N}) \big]\end{aligned}$$

where in $\ldots$ we omit the other contributions, which one can obtain from the other by simply rearranging k_1, k_2, k_3, k_4 in the other possible ways. Now we can rename

the $\{k_s\}$ in a suitable way and find

$$\sum_{k_1,k_2,k_3,k_4=1}^{N-1} \Delta_4(k_1,k_2,k_3,k_4) N\big[\prod_{s=1}^{4}(a_{k_s}+a_{k_s}^\dagger)\big] =$$
$$\sum_{k_1,k_2,k_3,k_4=1}^{N-1} \big[\Delta_4(k_1,k_2,k_3,k_4) : \prod_{s=1}^{4}(a_{k_s}+a_{k_s}^\dagger) : +$$
$$+ 6\delta_{k_1,k_2} : \prod_{s=3,4}(a_{k_s}+a_{k_s}^\dagger) : (\delta_{k_1+k_2+k_3,k_4} + \delta_{k_1+k_2+k_4,k_3} + \delta_{k_1+k_2,k_3+k_4} +$$
$$- \delta_{k_1+k_2+k_3,k_4+2N} - \delta_{k_1+k_2+k_4,k_3+2N} - \delta_{k_1+k_2+k_3+k_4,2N}) +$$
$$- 3\delta_{k_1,k_2}\delta_{k_3,k_4}\delta_{k_1+k_2+k_3+k_4,2N}\big]$$

From the normal ordering of $\hat{H}_4$ one obtains

$$N[\hat{H}_4] = \frac{\beta}{32N} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \Delta_4(k_1,k_2,k_3,k_4) \prod_{s=1}^{4}\sqrt{\omega_{k_s}}\big\{ : \prod_{s=1}^{4}(a_{k_s}+a_{k_s}^\dagger) : +$$
$$+ 6\delta_{k_1,k_2} : \prod_{s=3,4}(a_{k_s}+a_{k_s}^\dagger) : + 3\delta_{k_1,k_2}\delta_{k_3,k_4}\big\}.$$

Like the cubic term of the perturbation, the normal ordering of the quartic term also contains non quartic terms $\hat{H}_4^{(2)}$ and $\hat{H}_4^{(0)}$, while the quartic term $\hat{H}_4^{(4)}$ can be obtained by the general formula (3.25) and is

$$\hat{H}_4^{(4)}(a,a^\dagger) = \frac{\beta}{32N} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}}\Delta_4(k_1,k_2,k_3,k_4)$$
$$[a_{k_1}a_{k_2}a_{k_3}a_{k_4} + 4a_{k_1}^\dagger a_{k_2}a_{k_3}a_{k_4} + 6a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}a_{k_4} + 4a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger a_{k_4} + a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger a_{k_4}^\dagger]. \tag{3.27}$$

Consider the constant term $\hat{H}_4^{(0)}$, which reads

$$\begin{aligned}\hat{H}_4^{(0)} &= -\frac{3\beta}{32N} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}}\delta_{k_1,k_2}\delta_{k_3,k_4}\delta_{k_1+k_2+k_3+k_4,2N} \\ &= -\frac{3\beta}{32N} \sum_{k_1,k_3=1}^{N-1} \omega_{k_1}\omega_{k_3}\delta_{2k_1+2k_3,2N} \\ &= -\frac{3\beta}{32N} \sum_{k=1}^{N-1} \omega_k\omega_{N-k}.\end{aligned}$$

Being $\omega_k = 2\sin\frac{\pi k}{2N}$, a direct computation shows that the constant term is

$$\hat{H}_4^{(0)} = -\frac{3\beta}{16N}\cot\frac{\pi}{2N}.$$

Remark 3.10. In the thermodynamic limit $N\to\infty$ this term converges to $-\frac{3\beta}{8\pi}$.

The quadratic term $\hat{H}_4^{(2)}$ instead reads

$$\hat{H}_4^{(2)}(a,a^\dagger) = \frac{3\beta}{16N} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \prod_{s=1}^{4} \sqrt{\omega_{k_s}} \Delta_4(k_1,k_2,k_3,k_4) \delta_{k_1,k_2} (a_{k_3} a_{k_4} + 2a_{k_3}^\dagger a_{k_4} + a_{k_3}^\dagger a_{k_4}^\dagger).$$

Writing explicitly the selector Δ_4 and repeating the same arguments in the previous section one finds

$$\begin{aligned}\hat{H}_4^{(2)}(a,a^\dagger) = \frac{3\beta}{16N} \sum_{k_1,k_3,k_4=1}^{N-1} & \omega_{k_1} \sqrt{\omega_{k_3}\omega_{k_4}} \\ & (2\delta_{2k_1+k_3,k_4} + \delta_{2k_1,k_3+k_4} - 2\delta_{2k_1+k_3,k_4+2N} - \delta_{2k_1+k_3+k_4,2N}) \\ & (a_{k_3} a_{k_4} + 2a_{k_3}^\dagger a_{k_4} + a_{k_3}^\dagger a_{k_4}^\dagger).\end{aligned}$$

CHAPTER 4

Perturbation theory

4.1 Classical perturbation theory and mean principle

Let us suppose to have an Hamiltonian, defined in some phase space Λ,

$$H_\lambda = h + \sum_n \lambda^n P_n,$$

where h is *integrable*, so we know its hamiltonian flow ϕ_h^t, ans λ is a small parameter. We call $\sum_n \lambda^n P_n$ the *perturbation* of H_λ and h the *unperturbed part* of H_λ. Our aim is to look for a new set of coordinates such that the Hamiltonian, written in these new coordinates, is integrable up to a certain order r. One might ask if a canonical transformation $\mathscr{C}_\lambda : x \mapsto y$ such that $H \circ \mathscr{C}_\lambda^{-1} = h + \lambda^r \dots$ exists, that is a set of coordinates which eliminates completely the perturbation at the r-th order in λ. Such a transformation, sadly, doesn't generally exists up to any order, as stated by Poincaré's *little theorem*.

Instead we look for a less restrictive transformation, a canonical transformation

$$\mathscr{C}_\lambda : x \mapsto y$$

λ-close to the identity, i.e. $\|\mathscr{C}_\lambda - \mathrm{Id}\| = O(\lambda)$, and regular in λ, such that

$$H_\lambda \circ \mathscr{C}_\lambda^{-1} = h + \lambda S_1 + \lambda^2 S_2 + \dots, \quad \text{and} \quad \{S_i, h\} = 0 \quad \forall i = 1, \dots, r.$$

so that it conjugates the perturbation to a collection of *first integrals* of the unperturbed part h, up to a certain order r. An Hamiltonian in this form is said to be the *r-th order Birkhoff normal form* of H_λ. In the following we will construct such a transformation for $r = 2$, noticing that the construction for any order r can be done in an analogous way.

We will proceed by the so called *Lie method*, i.e. searching for a canonical transformation such that $\mathscr{C}_\lambda^{-1} := f_\lambda = \phi_{G_2}^{\lambda^2} \circ \phi_{G_1}^{\lambda}$, where G_1 and G_2 are two unknown Hamiltonians, called *generatrices*. From the identity

$$F \circ \phi_{G_i}^s = e^{sL_i} F$$

for any $F : \Lambda \to \mathbb{R}$ and where $L_i = \{\cdot, G_i\}$, $i = 1, 2$, one obtains

$$H \circ f_\lambda = h + \lambda(L_1 h + P_1) + \lambda^2(L_2 h + \frac{1}{2} L_1^2 h + L_1 P_1 + P_2) + \ldots = h + \lambda S_1 + \lambda^2 S_2 + \ldots. \tag{4.1}$$

We will start by the first order, i.e. by finding one or more Hamiltonians G_1 (as we will see, there will be an infinite number of them) such that $\{S_1, h\} = 0$. This will be done by the so called *mean principle* or *averaging method*, which is by averaging the perturbation along the flow of the unperturbed part h.

Definition 4.1 (Average)**.** For any $F : \Lambda \to \mathbb{R}$ we define its *average along the flow of* h, or simply *average*, the function

$$\bar{F} = \lim_{t\to\infty} \frac{1}{t} \int_0^t F \circ \phi_h^s ds.$$

With the following lemma one can understand why the average along the flow of h produces a first integral.

Lemma 4.1. *For any* $F : \Lambda \to \mathbb{R}$, $\bar{F} \circ \phi_h^u = \bar{F}$ $\forall u \in \mathbb{R}$.

Proof.

$$\bar{F} \circ \phi_h^u = \left(\lim_{t\to\infty} \frac{1}{t} \int_0^t F \circ \phi_h^s ds \right) \circ \phi_h^u$$

Using the group property of the flow $\phi_h^s \circ \phi_h^u = \phi_h^{s+u}$ one obtains

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t F \circ \phi_h^{s+u} ds$$

and by denoting $v = s + u$

$$\lim_{t\to\infty} \frac{1}{t} \int_u^{u+t} F \circ \phi_h^v dv = \lim_{t\to\infty} \frac{1}{t} \int_u^0 F \circ \phi_h^v dv + \lim_{t\to\infty} \frac{1}{t} \int_0^t F \circ \phi_h^v dv + \lim_{t\to\infty} \frac{1}{t} \int_t^{u+t} F \circ \phi_h^v dv.$$

In the $t \to \infty$ limit only the second term survives, leading to $\bar{F}$. □

From (4.1) we can read an equation for S_1 and G_1

$$S_1 = L_1 h + P_1 \tag{4.2}$$

which we will solve with the following proposition.

Proposition 4.1 (First order mean principle)**.** *If* ϕ_h^t *is limited in* t*, then*

$$S_1 = \bar{P}_1 = \lim_{t\to\infty} \frac{1}{t} \int_0^t P_1 \circ \phi_h^s ds \tag{4.3}$$

and

$$G_1 = \mathscr{G}_1 + \lim_{t\to\infty} \frac{1}{t} \int_0^t (s - t)(P_1 - \bar{P}_1) \circ \phi_h^s ds \tag{4.4}$$

where $\mathscr{G}_1$ *is any function such that* $\{\mathscr{G}_1, h\} = 0$.

Proof. Our aim is to find a function S_1 such that $S_1 \circ \phi_h^s = S_1$, or equivalently $e^{sL_h} S_1 = S_1$, $\forall s$. So we have

$$S_1 = e^{sL_h} S_1 = e^{sL_h} P_1 + e^{sL_h} L_1 h = e^{sL_h} P_1 - e^{sL_h} L_h G_1 = e^{sL_h} P_1 - \frac{d}{ds} e^{sL_h} G_1.$$

Now, integrating both sides of the last equation in ds from 0 to t and diving by t we have, $\forall t$

$$S_1 = \frac{1}{t} \int_0^t ds e^{sL_h} P_1 - \frac{e^{tL_h} G_1 - G_1}{t}.$$

Now, sending $t \to \infty$ and using the fact that ϕ_h^t is limited the second term vanishes and

$$S_1 = \lim_{t\to\infty} \frac{1}{t} \int_0^t ds e^{sL_h} P_1 = \bar{P}_1.$$

Now we find an expression for G_1. Starting from $S_1 = P_1 - L_h G_1 = \bar{P}_1$ we get $L_h G_1 = P_1 - \bar{P}_1$. So, one has

$$\int_0^t (s-t) e^{sL_h} (P_1 - \bar{P}_1) ds = \int_0^t (s-t) e^{sL_h} L_h G_1 ds = \int_0^t (s-t) \frac{d}{ds} e^{sL_h} G_1 ds.$$

Integrating by parts we have

$$\int_0^t (s-t) e^{sL_h} (P_1 - \bar{P}_1) ds = tG - \int_0^t G_1 \circ \phi_h^s ds,$$

and thus, sending $t \to \infty$,

$$G_1 = \lim_{t\to\infty} \frac{1}{t} \int_0^t G_1 \circ \phi_h^s ds + \lim_{t\to\infty} \frac{1}{t} \int_0^t (s-t)(P_1 - \bar{P}_1) \circ \phi_h^s ds.$$

The first term, being the average of G_1 along the flow of h, $\bar{G}_1$, is a first integral of h, so we have the thesis. □

Now we proceed to the construction of the second order normal form. From (4.1) we find

$$S_2 = L_2 h + \frac{1}{2} L_1^2 h + L_1 P_1 + P_2, \tag{4.5}$$

which is an equation for S_2 and G_2 with the same form as (4.2), and thus it will be solved likewise.

Proposition 4.2 (Second order mean principle)**.** *If ϕ_h^t is limited in t, then, denoting $P_2' = \frac{1}{2} L_1^2 h + L_1 P_1 + P_2$,*

$$S_2 = \lim_{t\to\infty} \frac{1}{t} \int_0^t P_2' \circ \phi_h^s ds \tag{4.6}$$

and

$$G_2 = \mathscr{G}_2 + \lim_{t\to\infty} \frac{1}{t} \int_0^t (s-t)(P_2' - \bar{P}'_2) \circ \phi_h^s ds \tag{4.7}$$

where $\mathscr{G}_2$ is any function such that $\{\mathscr{G}_2, h\} = 0$.

At this point, the generalization for the construction of the r-th order Birkhoff normal form for any r is straightforward. For the n-th order we will have an equation of the form

$$S_n = L_n h + P'_n$$

for some P'_n, which will contain the P_i for $i \leq n$, h, and G_i for $i < n$, which leads us to

$$S_n = \bar{P'}_n.$$

G_n will be found solving the so called *homological equation*

$$L_h G_n = \widetilde{P'}_n \tag{4.8}$$

where, for any $F : \Lambda \to \mathbb{R}$, $\widetilde{F} := F - \bar{F}$ is the fluctuation of F around its average.

4.2 Quantum perturbation theory

In this section we will discuss perturbation theory in a quantum environment, proceeding in analogy with the classical case thanks to the Poisson structure of the algebra of hermitian operators in the Heisenberg picture. Given an Hamiltonian operator $\hat{h}$, we say that an hermitian operator $\hat{A}_H$ is in the Heisenberg picture if its evolution satisfies the so called *Heisenberg equation*

$$\frac{d}{dt}\hat{A}_H(t) = \frac{1}{i\hbar}[\hat{A}_H(t), \hat{h}]. \tag{4.9}$$

The Heisenberg equation (4.9) can be solved, at least formally, and

$$\hat{A}_H(t) = \hat{U}_h^\dagger(t)\hat{A}\hat{U}_h(t)$$

where $\hat{A} = \hat{A}_H(0)$ is the operator in the Schrödinger picture, and

$$\hat{U}_h(t) = e^{-\frac{i}{\hbar}t\hat{h}}$$

is the time-evolution operator. We now define the *Lie derivative*

$$\mathscr{L}_{\hat{h}} = \frac{1}{i\hbar}[\quad, \hat{h}]$$

so that we can write (4.9) as

$$\frac{d}{dt}\hat{A}_H(t) = \mathscr{L}_{\hat{h}}\hat{A}_H(t).$$

The equivalence between these two forms of the Heisenberg equation leads us to the identity

$$\hat{U}_h^\dagger(t)\hat{A}\hat{U}_h(t) = e^{t\mathscr{L}_{\hat{h}}}\hat{A}. \tag{4.10}$$

Equation (4.10) will be used to map the formulas in the previous section to the quantum environment, in order to perform quantum perturbation theory. We will proceed by computing the first order normal form for a general Hamiltonian operator. In particular, suppose we have a quantum Hamiltonian operator

$$\hat{H} = \hat{h} + \lambda\hat{P}_1 + \lambda^2\hat{P}_2 + \dots$$

Our aim is to look for a unitary transformation, generated by an unknown Hamiltonian operator $\hat{G}_1$ at the time $\lambda \in \mathbb{R}$, such that $\hat{H}$ is conjugated to

$$\hat{U}_1^\dagger(\lambda)\hat{H}\hat{U}_1(\lambda) = e^{\lambda \mathscr{L}_1}\hat{H} = \hat{h} + \lambda \hat{S}_1 + \dots, \qquad \text{such that} \quad [\hat{S}_1, \hat{h}] = 0,$$

where $\hat{U}_1(\lambda) = e^{-\frac{i}{\hbar}\lambda \hat{G}_1}$ and $\mathscr{L}_1 = \frac{1}{i\hbar}[\quad, \hat{G}_1]$.
This problem is formally equivalent to the classical one, up to the different meaning of the Lie derivative which, in the quantum mechanics case, is given by (4.10). At this point one can write the formulas for $\hat{S}_1$ and $\hat{G}_1$ without proving them, thanks to the formal equivalence of the two problems given by their Poisson structures:

$$\hat{S}_1 = \overline{\hat{P}}_1 = \lim_{t\to\infty} \frac{1}{t} \int_0^t \hat{U}_h^\dagger(s)\hat{P}_1\hat{U}_h(s)ds \tag{4.11}$$

and

$$\hat{G}_1 = \lim_{t\to\infty} \frac{1}{t} \int_0^t (s-t)\hat{U}_h^\dagger(s)(\hat{P}_1 - \overline{\hat{P}}_1)\hat{U}_h(s)ds + \hat{\mathscr{G}}_1 \tag{4.12}$$

where $\hat{\mathscr{G}}_1$ is any hermitian operator such that $[\hat{\mathscr{G}}_1, \hat{h}] = 0$. The second order normal form can be obtained by means of a second generatrix $\hat{G}_2$, in the same way of the classical case, and it is given by

$$\hat{S}_2 = \overline{\hat{P}'_2}$$

where $\hat{P}'_2 = \hat{P}_2 + \mathscr{L}_1\hat{P}_1 + \frac{1}{2}\mathscr{L}_1^2\hat{P}_1$. One can see that, if $\hat{S}_1 = 0$ (which, as we will find, is our case), then

$$\hat{S}_2 = \overline{\hat{P}}_2 + \frac{1}{2i\hbar}\overline{[\hat{P}_1, \hat{G}_1]}. \tag{4.13}$$

CHAPTER 5

Second order non-resonant Birkhoff normal form

We will use quantum perturbation theory developed in the previous chapter to eliminate the perturbation, as much as possible, from the Hamiltonian operator of the $\alpha+\beta$ quantum Fermi-Pasta-Ulam model up to quartic terms. An analysis similar to the one treated in this work was made by Herbert Fröhlich in 1952 (see [15]), were a unitary transformation was applied to a superconductive system, in order to eliminate the interaction of the electrons with the lattice vibrations. For the classical case, the second order Birkhoff normal form of the $\alpha+\beta$ FPU model was computed by Henrici and Kappeler in [10] for periodic boundary conditions.

5.1 Construction of the quantum normal form

In this chapter we will construct the second order Birkhoff normal form of the quantum FPU Hamiltonian, using equations (4.11), (4.12) and (4.13) (remembering that in our unity of measure $\hbar = 1$), where

$$\hat{h} = \hat{H}_2, \qquad \hat{P}_1 = \hat{H}_3, \qquad \hat{P}_2 = \hat{H}_4$$

Remark 5.1. In the following, as the *order* of the normal form is defined to be the number of perturbative steps, we will call the *first* (or *second*) order normal form the corrections up to the cubic (or quartic) terms. So $\hat{P}_1$ and $\hat{G}_1$ are cubic in a, and $a^\dagger$, while $\hat{P}_2$ and $\hat{G}_2$ are quartic.

As we need to manage averages along the flow of $\hat{H}_2$ of operators containing a and $a^\dagger$, first of all we need to solve the Heisenberg equation (4.9) for a and $a^\dagger$, with $\hat{h} = \sum_{k=1}^{N-1} \omega_k a_k^\dagger a_k$. Heisenberg equation for the annihilation operators reads

$$\dot{a}_k(t) = -i[a_k(t), \hat{h}(a, a^\dagger)] = -i \sum_{q=1}^{N-1} \omega_q [a_k(t), a_q^\dagger(t) a_q(t)] = -i\omega_k a_k(t),$$

and so

$$a_k(t) = a_k e^{-i\omega_k t} \qquad \forall k = 1, \dots, N-1. \tag{5.1}$$

The creation operator is its hermitian conjugate, so

$$a_k^\dagger(t) = a_k^\dagger e^{i\omega_k t} \qquad \forall k = 1, \dots, N-1. \tag{5.2}$$

In order to calculate averages, we will proceed in the following way. $\hat{H}_3$ and $\hat{H}_4$ contain linear combinations of products of a and $a^\dagger$. When the time evolution operators at a time $s \in \mathbb{R}$ are applied, each a_k brings a factor $e^{-i\omega_k s}$, while each $a_k^\dagger$ brings a factor $e^{i\omega_k s}$. Overall, a phase will be added containing combinations of frequencies with relative signs according to (5.1) and (5.2). For example, the time evolution acts on $a_k^\dagger a_l a_m$ giving

$$a_k^\dagger a_l a_m e^{i(\omega_k - \omega_l - \omega_m)s}.$$

It is clear now that to perform averages we need to calculate, for some $\Omega \in \mathbb{R}$, quantities like

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T e^{-is\Omega} ds.$$

If $\Omega = 0$ then the limit is trivially 1. If $\Omega \neq 0$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T e^{-is\Omega} ds = \lim_{T\to\infty} \frac{1}{T} \frac{1}{-i\Omega} (e^{-iT\Omega} - 1) = 0.$$

Finally on has

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T e^{-is\Omega} ds = \delta_{\Omega,0}. \tag{5.3}$$

Reprising the last example,

$$\overline{a_k^\dagger a_l a_m} = a_k^\dagger a_l a_m \, \delta_{\omega_k - \omega_l - \omega_m, 0}.$$

Thus, for each term of the perturbation we will see if the relative combination of the frequencies, according to the conservation laws given by the selectors, vanishes. If such a combination can be null, the term will be added to $\hat{S}_1$, otherwise it averages to zero.
Let us introduce now the idea of resonances, which has the uttermost importance in Hamiltonian perturbation theory.

Definition 5.1 (Resonance)**.** Let $\Omega = (\omega_1, \dots, \omega_{N-1}) \in \mathbb{R}^{N-1}$. A *resonance* of order $r \in \mathbb{N}$ for Ω is a vector $\nu \in \mathbb{Z}^{N-1}$ such that

$$\sum_{i=1}^{N-1} \nu_i \Omega_i = 0, \qquad \sum_{i=1}^{N-1} |\nu_i| = r.$$

Thus, we can state that the only terms with a non-vanishing average are the *resonant* ones, while the non-resonant averages to zero. More precisely, let $\hat{f}$ be a normal ordered polynomial of annihilation and creation operators $(a_1, \dots, a_{N-1}, a_1^\dagger, \dots, a_{N-1}^\dagger)$, thus f can be written in a multi-index notation

$$\hat{f} = \sum_{\alpha,\beta \in \mathbb{N}^{N-1}} f_{\alpha\beta} (a^\dagger)^\alpha (a)^\beta$$

where we denote $(a^\dagger)^\alpha = \prod_i (a_i^\dagger)^{\alpha_i}$ and equivalently for $(a)^\beta$. We will call such an operator a *second quantization operator* (or simply *operator*).

Definition 5.2 (Harmonic, spectrum)**.** Given $\hat{f}$, we define its ν-th *harmonic* the quantity

$$\langle \hat{f} \rangle_\nu = \sum_{\substack{\alpha,\beta \in \mathbb{N}^{N-1} \\ \alpha - \beta = \nu}} f_{\alpha\beta} (a^\dagger)^\alpha (a)^\beta$$

and the *spectrum* of $\hat{f}$ the set

$$\mathrm{Sp}(\hat{f}) = \{ \nu \in \mathbb{Z}^{N-1} \colon \langle \hat{f} \rangle_\nu \neq 0 \}.$$

The integer

$$D(\hat{f}) = \max_{\alpha - \beta \in \mathrm{Sp}(\hat{f})} \{ \sum_i |\alpha_i| + \sum_i |\beta_i| \}$$

is called the *degree* of $\hat{f}$. It is easy to check that if $\hat{f}$ has degree d, its spectrum contains only vectors ν such that $\sum_i |\nu_i| \leq d$. We can also define the so-called *resonant lattice* relative to the frequency vector $\Omega \in \mathbb{R}^{N-1}$

Definition 5.3 (Resonant lattice)**.** We define the *resonant lattice* relative to the frequency vector $\Omega \in \mathbb{R}^{N-1}$ the set

$$\mathscr{R}_\Omega = \{ \nu \in \mathbb{Z}^{N-1} \colon \Omega \cdot \nu = 0 \},$$

i.e. the set containing all the resonances (of any order) for Ω.

From the statements above we can give the following proposition, which formalize the relations between averages and resonances.

Proposition 5.1. *The average along the flow of $\sum_k \omega_k a_k^\dagger a_k$ of an operator $\hat{f}$ is*

$$\overline{\hat{f}} = \sum_{\substack{\alpha,\beta \in \mathbb{N}^{N-1} \\ \alpha - \beta \in \mathscr{R}_\Omega \cap Sp(\hat{f})}} f_{\alpha\beta} (a^\dagger)^\alpha (a)^\beta.$$

For example, if $\hat{f}$ is cubic or quartic, one must check the resonances up to the third or fourth order and so on.

5.1.1 First order normal form

Here we will show the construction of the first order Birkhoff normal form, i.e. the computation of

$$\hat{S}_1 = \lim_{T \to \infty} \frac{1}{T} \int_0^T \hat{U}_h^\dagger(s) \hat{H}_3 \hat{U}_h(s) ds,$$

where $\hat{H}_3 = \hat{H}_3^{(3)} + \hat{H}_3^{(1)}$,

$$\hat{H}_3^{(3)} = \frac{\alpha}{12\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \prod_{s=1}^{3} \sqrt{\omega_{k_s}} \Delta_3(k_1,k_2,k_3) \\ (a_{k_1} a_{k_2} a_{k_3} + 3 a_{k_1}^\dagger a_{k_2} a_{k_3} + 3 a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} + a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger)$$

$$\hat{H}_3^{(1)} = \frac{\alpha}{4\sqrt{N}} \sum_{k=1}^{B(N)} \sqrt{\omega_{2k}}(\omega_k - \omega_{N-k})(a_{2k} + a_{2k}^\dagger), \qquad B(N) = \begin{cases} \frac{N-1}{2} & \text{if } N \text{ is odd} \\ \frac{N-2}{2} & \text{if } N \text{ is even} \end{cases}.$$

where $\Delta_3(k_1, k_2, k_3) = \delta_{k_1+k_2,k_3} + \delta_{k_3+k_1,k_2} + \delta_{k_2+k_3,k_1} - \delta_{k_1+k_2+k_3,2N}$. Being $\omega_k > 0$ $\forall k$ one can easily notice that $\overline{\hat{H}_3^{(1)}} = 0$, while the terms of $\hat{H}_3^{(3)}$ containing all creation or annihilation operators do not contribute. The terms that might contribute to the average are

$$\frac{\alpha}{4\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \prod_{s=1}^{3} \sqrt{\omega_{k_s}} \Delta_3(k_1, k_2, k_3)(a_{k_1}^\dagger a_{k_2} a_{k_3} + a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}).$$

At this point all we have to do is find the solutions of the equation $\omega_{k_1} - \omega_{k_2} - \omega_{k_3} = 0$, according to the relations between k_1, k_2, k_3 given by Δ_3, i.e.

$$\begin{aligned} \omega_{k_1} - \omega_{k_2} - \omega_{k_1+k_2} &= 0 \\ \omega_{k_1} - \omega_{k_1+k_3} - \omega_{k_3} &= 0 \\ \omega_{k_2+k_3} - \omega_{k_2} - \omega_{k_3} &= 0 \\ \omega_{k_1} - \omega_{k_2} - \omega_{2N-k_1-k_2} &= 0. \end{aligned}$$

Being $\omega_{2N-k} = \omega_k$, we only need to find solutions of the equations

$$\begin{aligned} \omega_{k+q} - \omega_k - \omega_q &= 0 \\ \omega_k - \omega_q - \omega_{k+q} &= 0. \end{aligned}$$

We will solve this type of equations with a simple trick. Being $\omega_k = 2\sin\frac{\pi k}{2N} = \frac{e^{i\frac{\pi k}{2N}} - e^{-i\frac{\pi k}{2N}}}{i}$, by setting $x = e^{i\frac{\pi k}{2N}}$ and $y = e^{i\frac{\pi q}{2N}}$, we have

$$\begin{aligned} \omega_{k+q} - \omega_k - \omega_q = 0 \quad &\leftrightarrow \quad (xy - \frac{1}{xy}) - (x - \frac{1}{x}) - (y - \frac{1}{y}) = 0 \\ \omega_k - \omega_q - \omega_{k+q} = 0. \quad &\leftrightarrow \quad (xy - \frac{1}{xy}) - (x - \frac{1}{x}) + (y - \frac{1}{y}) = 0 \end{aligned}$$

Consider the first equation, which can be written in the form

$$\frac{(x-1)(y-1)(xy-1)}{xy} = 0, \quad \leftrightarrow \quad x = 1,\ y = 1,\ xy = 1 \quad \leftrightarrow \quad k = 0,\ q = 0,\ k+q = 0,$$

which is impossible, being $1 \leq k, q \leq N-1$. The second equation can be written in the form

$$\frac{(x+1)(y-1)(xy+1)}{xy} = 0 \quad \leftrightarrow \quad x = -1,\ y = 1,\ xy = -1 \quad \leftrightarrow \quad k = 2N,\ q = 0,\ k = -q,$$

which is also impossible. In this way we have seen that the equation $\omega_{k_1} - \omega_{k_2} - \omega_{k_3} = 0$ has no solution, and so $\hat{H}_3$ averages to zero:

$$\hat{S}_1 = 0.$$

The first generatrix $\hat{G}_1$ can be calculated using the equation (4.12). Being $\overline{\hat{H}_3} = 0$, we need to compute the quantity

$$\hat{G}_1 = \lim_{T\to\infty} \frac{1}{T} \int_0^T (s-T)\hat{U}_h^\dagger(s)\hat{H}_3\hat{U}_h(s)ds.$$

Repeating the same argument as in the previous section, it is clear that we must learn to compute expressions of the form

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T (s-T)e^{i\Omega s}ds.$$

A direct computations shows that, if $\Omega \neq 0$ this limit is $\frac{1}{i\Omega}$. On the other hand, if $\Omega = 0$, it diverges to infinity, while this fact does not worry us, because as we have seen in the previous section, every combination of the frequencies is non-zero.
With this is mind one can find that the expression of the generatrix is $\hat{G}_1 = \hat{G}_1^{(3)} + \hat{G}_1^{(1)}$, where

$$\hat{G}_1^{(3)} = \frac{\alpha}{12\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \prod_{s=1}^{3} \sqrt{\omega_{k_s}}\Delta_3(k_1,k_2,k_3)\left[\frac{a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger}{i(\omega_{k_1}+\omega_{k_2}+\omega_{k_3})} + \right.$$
$$\left. + 3\frac{a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}}{i(\omega_{k_1}+\omega_{k_2}-\omega_{k_3})} + 3\frac{a_{k_1}^\dagger a_{k_2} a_{k_3}}{i(\omega_{k_1}-\omega_{k_2}-\omega_{k_3})} - \frac{a_{k_1} a_{k_2} a_{k_3}}{i(\omega_{k_1}+\omega_{k_2}+\omega_{k_3})}\right] \quad (5.4)$$

and

$$\hat{G}_1^{(1)} = \frac{\alpha}{4\sqrt{N}} \sum_{k=1}^{B(N)} (\omega_k - \omega_{N-k}) \left[\frac{a_{2k}^\dagger}{i\sqrt{\omega_{2k}}} - \frac{a_{2k}}{i\sqrt{\omega_{2k}}}\right] \quad (5.5)$$

5.1.2 Second order normal form

We now proceed in the computation of the second order Birkhoff normal form, using equation (4.13). Now we show the computation of $\overline{\hat{H}_4}$, with $\hat{H}_4 = \hat{H}_4^{(4)} + \hat{H}_4^{(2)} + \hat{H}_4^{(0)}$ with the procedure used in the previous section. Trivially, $\overline{\hat{H}_4^{(0)}} = \hat{H}_4^{(0)}$. The quadratic term is

$$\hat{H}_4^{(2)}(a,a^\dagger) = \frac{3\beta}{16N} \sum_{k_1,k_3,k_4=1}^{N-1} \omega_{k_1}\sqrt{\omega_{k_3}\omega_{k_4}}$$
$$(2\delta_{2k_1+k_3,k_4} + \delta_{2k_1,k_3+k_4} - 2\delta_{2k_1+k_3,k_4+2N} - \delta_{2k_1+k_3+k_4,2N})$$
$$(a_{k_3}a_{k_4} + 2a_{k_3}^\dagger a_{k_4} + a_{k_3}^\dagger a_{k_4}^\dagger).$$

The terms proportional to $a_{k_3}a_{k_4}$ and to $a_{k_3}^\dagger a_{k_4}^\dagger$ do not contribute, while $a_{k_3}^\dagger a_{k_4}$ has a non-zero average only if $k_3 = k_4$. Evaluating the sum one obtains

$$\overline{\hat{H}_4^{(2)}} = \frac{3\beta}{8N} \sum_{k=1}^{N-1} (\omega_k^2 - \omega_k\omega_{N-k}) a_k^\dagger a_k.$$

We now show the average of the quartic term

$$\hat{H}_4^{(4)} = \frac{\beta}{32N} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \prod_{s=1}^{4} \sqrt{\omega_{k_s}} \Delta_4(k_1,k_2,k_3,k_4)(a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger a_{k_4}^\dagger + \\ + 4a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger a_{k_4} + 6a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} + 4a_{k_1}^\dagger a_{k_2} a_{k_3} a_{k_4} + a_{k_1} a_{k_2} a_{k_3} a_{k_4})$$

where $\Delta_4(k_1,k_2,k_3,k_4)$ is the selector (3.14), that is

$$\overline{\hat{H}_4^{(4)}} = \frac{3\beta}{4N} \sum_{k_1,k_2=1}^{N-1} \omega_{k_1}\omega_{k_2} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2} a_{k_1}.$$

In fact, surely the terms containing all annihilation or creation operators averages to zero. Let us consider the term proportional to $a_{k_1}^\dagger a_{k_2} a_{k_3} a_{k_4}$, which lead to the equation

$$\omega_{k_1} - \omega_{k_2} - \omega_{k_3} - \omega_{k_4} = 0$$

where k_1, k_2, k_3 and k_4 are linked together by Δ_4. The term proportional to $a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger a_{k_4}$ lead to the same equation. Considering all the relations given by the selector, one finds that the equations that must be solved are four

$$\omega_{k+l+m} + \omega_k + \omega_l - \omega_m = 0$$
$$\omega_{k+l+m} + \omega_k - \omega_l - \omega_m = 0$$
$$\omega_{k+l+m} - \omega_k - \omega_l - \omega_m = 0$$
$$\omega_{k+l-m} - \omega_k - \omega_l - \omega_m = 0$$

which, for $k,l,m = 1,\dots,N-1$, have no solution. The term proportional to $a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}$ instead lead to the equation

$$\omega_{k_1} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4} = 0$$

where k_1, k_2, k_3 and k_4 are linked together by Δ_4. The only terms that lead to a contribute in the average are

$$\delta_{k_1+k_2,k_3+k_4} \quad \Longrightarrow \quad \omega_{k_3+k_4-k_2} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4} = 0$$

which has the solutions $k_2 = k_3$ and $k_2 = k_4$, and thus gives a contribute $\delta_{k_2,k_3}\delta_{k_1,k_4} + \delta_{k_1,k_3}\delta_{k_2,k_4}$; the other terms are

$$\delta_{k_1+k_3,k_2+k_4} \quad \Longrightarrow \quad \omega_{k_2+k_4-k_3} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4} = 0 \quad \Longrightarrow \quad \delta_{k_2,k_3}\delta_{k_1,k_4}$$
$$\delta_{k_1+k_4,k_2+k_3} \quad \Longrightarrow \quad \omega_{k_2+k_3-k_4} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4} = 0 \quad \Longrightarrow \quad \delta_{k_2,k_4}\delta_{k_1,k_3}$$

so finally one has

$$\begin{aligned}
\overline{\hat{H}_4^{(4)}} &= \frac{6\beta}{32N} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \prod_{s=1}^{4} \sqrt{\omega_{k_s}} (2\delta_{k_2,k_4}\delta_{k_1,k_3} + 2\delta_{k_2,k_3}\delta_{k_1,k_4}) a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \\
&= \frac{3\beta}{8N} \sum_{k_1,k_2=1}^{N-1} \omega_{k_1}\omega_{k_2} (a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2} a_{k_1} + a_{k_1}^\dagger a_{k_2}^\dagger a_{k_1} a_{k_2}) \\
&= \frac{3\beta}{4N} \sum_{k_1,k_2=1}^{N-1} \omega_{k_1}\omega_{k_2} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2} a_{k_1}.
\end{aligned}$$

The computation of the quantity

$$\frac{1}{2i}\overline{[\hat{H}_3, \hat{G}_1]}.$$

must be done as follows. First one must compute the sixteen commutators between cubic terms (which lead to quartic terms), the sixteen commutators between cubic and linear terms (which lead to quadratic terms), and the four commutators between linear terms (which give a constant term)

$$\frac{1}{2i}[\hat{H}_3^{(3)}+\hat{H}_3^{(1)}, \hat{G}_1^{(3)}+\hat{G}_1^{(1)}] = \frac{1}{2i}([\hat{H}_3^{(3)}, \hat{G}_1^{(3)}]+[\hat{H}_3^{(3)}, \hat{G}_1^{(1)}]+[\hat{H}_3^{(1)}, \hat{G}_1^{(1)}]+[\hat{H}_3^{(1)}, \hat{G}_1^{(3)}])$$

then, for each contribution, compute the normal ordering (so quartic terms give quartic, quadratic and constant normal ordered terms, and quadratic terms give quadratic and constant normal ordered terms) and the average as done previously. We report the computation in the appendices. The result is

– from $\frac{1}{2i}[\hat{H}_3^{(3)}, \hat{G}_1^{(3)}]$ (excluding constant terms)

$$\frac{\alpha^2}{4N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2}a_{k_1}$$
$$\left(2\frac{1}{\omega_{k_2}-\omega_{k_3}-\omega_{k_1}}-\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}-\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right)$$
$$+\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)a_{k_3}^\dagger a_{k_3}$$
$$\left(\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}-2\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right)$$

– from $\frac{1}{2i}[\hat{H}_3^{(3)}, \hat{G}_1^{(1)}]$ (excluding constant terms)

$$-\frac{\alpha^2}{8N}\sum_{q=1}^{B(N)}\sum_{k=1}^{N-1}(\delta_{k,q}-\delta_{k+q,N})(\omega_q-\omega_{N-q})\omega_k a_k^\dagger a_k;$$

– from $\frac{1}{2i}[\hat{H}_3^{(1)}, \hat{G}_1^{(3)}]$ (excluding constant terms)

$$-\frac{\alpha^2}{8N}\sum_{k=1}^{N-1}\sum_{q=1}^{B(N)}(\delta_{k,q}-\delta_{k+q,N})(\omega_q-\omega_{N-q})\omega_k a_k^\dagger a_k;$$

– $\frac{1}{2i}[\hat{H}_3^{(1)}, \hat{G}_1^{(1)}]$ is a constant.

The second order Birkhoff normal form is then $\hat{h}+\hat{S}_1+\hat{S}_2$, where, removing the constant terms

$$\hat{h} = \sum_{k=1}^{N-1}\omega_k a_k^\dagger a_k,$$

$$\hat{S}_1 = 0,$$

and, denoting $\Omega_k^2 := \omega_k^2 - \omega_k\omega_{N-k}$,

$$\begin{aligned}\hat{S}_2(a^\dagger, a) = &\left(\frac{3\beta}{8N} - \frac{\alpha^2}{4N}\right)\sum_{k=1}^{N-1}\Omega_k^2 a_k^\dagger a_k + \frac{3\beta}{4N}\sum_{k_1,k_2=1}^{N-1}\omega_{k_1}\omega_{k_2}a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2}a_{k_1} \\ &\frac{\alpha^2}{4N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2}a_{k_1} \\ &\left(2\frac{1}{\omega_{k_2}-\omega_{k_3}-\omega_{k_1}} - \frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}} - \frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right) \\ &+\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)a_{k_3}^\dagger a_{k_3} \\ &\left(\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}} - 2\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right) \qquad (5.6)\end{aligned}$$

We don't need to compute $\hat{G}_2$.

5.2 Shift of the energy levels

It is now interesting to calculate the shift in the energy levels of the harmonic Hamiltonian due to the anharmonic interaction. All the calculation will be done neglecting the constant terms. The harmonic Hamiltonian is given by the unperturbed part

$$\hat{h} = \sum_{k=1}^{N-1}\omega_k a_k^\dagger a_k, \qquad \omega_k = 2\sin\frac{\pi k}{2N}.$$

As it is known from elementary quantum mechanics, the quantum harmonic oscillator can be written in function of the *number operator* $\hat{n}_k := a_k^\dagger a_k$, as $\hat{h} = \sum_k \omega_k \hat{n}_k$, which admits a basis of eigenstates $|n\rangle := |n_1, n_2, \ldots, n_{N-1}\rangle$,

$$\hat{n}_k |n\rangle = n_k |n\rangle \qquad \forall k = 1, \ldots, N-1,$$

so that the energy levels of the unperturbed Hamiltonian in the eigenstate $|n\rangle$ are

$$E_{\{n_k\}} = \frac{\langle n|\,\hat{h}\,|n\rangle}{\langle n\,|\,n\rangle} = \sum_{k=1}^{N-1}\omega_k n_k.$$

The new terms of the perturbation $\hat{S}_2$ introduced with the second step of perturbation theory admit the same eigenstates, thanks to $[\hat{h}, \hat{S}_2] = 0$. The difference between the energy levels of the harmonic system and the energy levels of the perturbed system will be

$$\Delta E_{\{n_k\}} = \frac{\langle n|\,\hat{S}_2\,|n\rangle}{\langle n\,|\,n\rangle}.$$

$\hat{S}_2$ contains quadratic terms and quartic terms. These terms contain $a_j^\dagger a_k^\dagger a_k a_j = \hat{n}_k\hat{n}_j - \delta_{jk}\hat{n}_k$ so will bring quartic and quadratic corrections. The quartic corrections are

$$\Delta E^{(4)}_{\{n_k\}} = \frac{3\beta}{4N}\sum_{k_1,k_2=1}^{N-1}\omega_{k_1}\omega_{k_2}n_{k_1}n_{k_2} + \frac{\alpha^2}{4N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)n_{k_1}n_{k_2}\left(2\frac{1}{\omega_{k_2}-\omega_{k_3}-\omega_{k_1}} - \frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}} - \frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right)$$

while the quadratic corrections (caused by the quadratic and quartic terms of $\hat{S}_2$) are

$$\Delta E^{(2)}_{\{n_k\}} = \left(\frac{3\beta}{8N} - \frac{\alpha^2}{4N}\right)\sum_{k=1}^{N-1}\Omega_k^2 n_k - \frac{3\beta}{4N}\sum_{k=1}^{N-1}\omega_k^2 n_k + \frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)n_{k_3}\left(\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}} - 2\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right) + \frac{\alpha^2}{2N}\sum_{k=1}^{B(N)}\omega_k^2\omega_{2k}n_k\left(\frac{1}{\omega_{2k}} + \frac{1}{2\omega_k+\omega_{2k}} + \frac{1}{\omega_{2k}-2\omega_k}\right)$$

5.3 Classical non-resonant normal form

In this section we will calculate the second order Birkhoff normal form of the previous section for the classical case, using the complex variables z_k and z_k^* with the Poisson structure $\{z_k, z_q^*\} = -i\delta_{k,q}$, starting from the Hamiltonian (3.17). The Hamilton equations for the unperturbed part $h = \sum_k \omega_k |z_k|^2$

$$\dot{z}_k = \{z_k, h\} = -i\omega_k z_k \quad \Longrightarrow \quad z_k(t) = e^{-i\omega_k t}z_0$$

are easily solved: the complex coordinates have the same evolution law under the unperturbed Hamiltonian as the creation and annihilation operators. The only (and crucial) difference is that $z_k \in \mathbb{C}$ are commuting numbers, while a_k is a non-commuting operator in an Hilbert space. This fact cause the normal ordering in complex variables to be trivial: while in the quantum case $N[\hat{H}_3](a,a^\dagger) = \hat{H}_3^{(3)}(a,a^\dagger) + \hat{H}_3^{(1)}(a,a^\dagger)$, the normal ordering of $\hat{H}_3(z,z^*)$ brings only cubic terms, corresponding to $\hat{H}_3^{(3)}$ where the z, z^* are in place of $a, a^\dagger$. The same fact is obviously true also for H_4 and G_1. Beside this difference, the calculation of the normal form is, algebraically speaking, exactly the same.
One finds that the second order non-resonant Birkhoff normal form for (3.17) is,

neglecting the remainder,

$$\sum_{k=1}^{N-1}\omega_k|z_k|^2+\frac{3\beta}{4N}\sum_{k_1,k_2=1}^{N-1}\omega_{k_1}\omega_{k_2}|z_{k_1}|^2|z_{k_2}|^2+ \\ +\frac{\alpha^2}{4N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)|z_{k_1}|^2|z_{k_2}|^2 \\ \left(2\frac{1}{\omega_{k_2}-\omega_{k_3}-\omega_{k_1}}-\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}-\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right) \tag{5.7}$$

The difference between the classical and the quantum normal form thus is only in the normal ordering, although this creates several terms which are *purely quantum contributions* to the energy of the system. It is interesting to notice that these purely quantum contributions are visible only in the second order normal form.

CHAPTER 6

Acoustic modes and quantum Korteweg-de Vries equation

6.1 The small divisors problem for the acoustic modes

The above construction works fine, at least symbolically, for $N > 0$. Let us recall the expression for the frequency

$$\omega_k = 2 \sin \frac{\pi k}{2N} \approx \frac{\pi k}{N} + O(\frac{k^3}{N^3})$$

for k/N small enough. Since the frequencies for such momenta are linear in k, we will denote *acoustic modes* the normal modes of oscillation for $k \ll N$. This simple fact causes quasi-resonance of the form

$$\omega_1 \approx \omega_2/2 \approx \omega_3/3 \approx \dots$$

with a decreasing level of approximation, which leads to the well known (at least classically) problem of *small divisors* in the second order Birkhoff normal form. To understand the entity of the problem, let us consider the contribution to the Birkhoff normal form constructed in the previous chapter given by

$$\frac{\alpha}{4\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \prod_{s=1}^{3} \sqrt{\omega_{k_s}} \delta_{k_1+k_2,k_3} a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3}$$

which is of course contained in $\hat{H}^{(3)}_3$. Its average under the time evolution of $\hat{h} = \sum_k \omega_k a^\dagger_k a_k$, as we have seen, is zero because

$$\omega_{k_1} + \omega_{k_2} - \omega_{k_1+k_2} \neq 0 \qquad \forall k_1, k_2 = 1, \dots, N-1.$$

For the acoustic modes this quantity, although non-zero, is small $O(N^{-3/2})$: it is a *quasi-resonance*. In the computation of the first generatrix (and so in $\hat{S}_2$), this small quantity goes in the denominator, so becomes "big", also comparable with the

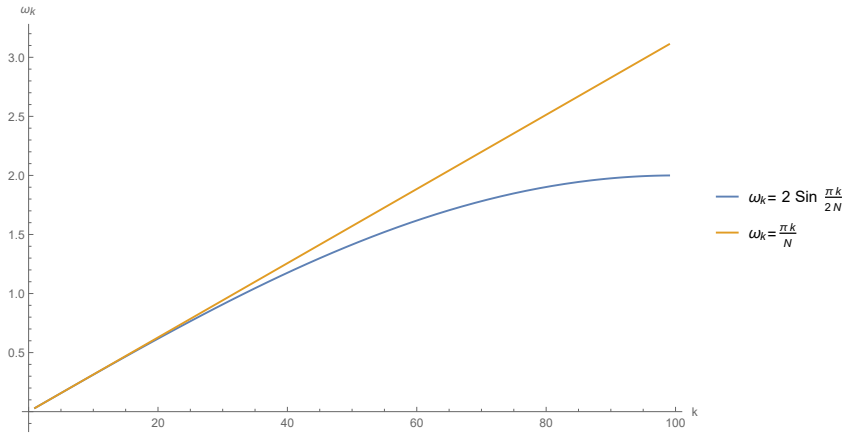

Figure 6.1: The approximation $\omega_k \approx \pi k/N$ for the acoustic modes. In this picture we put $N = 100$.

unperturbed part $\hat{h}$, which is precisely the problem of small divisors. For acoustic modes, then, the time evolution operator $\hat{U}_1$ yields a unitary transformation which is no more close to the identity, and $\hat{S}_2$ is no more a small perturbation, which makes the whole perturbation theory collapse. The normal form computed in the last chapter is then useless to describe the lattice acoustic vibrations for our system: we need to construct a new normal form, approximating the dispersion law to be a linear one and thus treating the quasi-resonances in the old normal form like exact ones.

Remark 6.1. This problem is well known in classical Hamiltonian perturbation theory, and date back to studies of celestial mechanics by Charles-Eugène Delaunay, who lived in the 19th century.

Of course this is also true for the classical case, but it is interesting to notice that while in the classical case the choice of acoustic modes as initial data may sound exotic (at least in a thermodynamic sense) in the quantum environment such a choice is way more plausible. Let us recall the numerical density for the mode k in a boson gas at temperature $T = \beta^{-1}$

$$n(k) = \frac{1}{e^{\beta\varepsilon(k)} - 1}$$

where $\varepsilon(k)$ is the energy related to the mode k. If T is small enough we have

$$n(k) \simeq e^{-\beta\varepsilon(k)},$$

so, being $\varepsilon(k)$ an increasing function of k, at low temperature the optical modes (short wavelength) are suppressed and the acoustic modes (long wavelength) are the only modes excited.

In the following we will construct a Birkhoff normal form adapted to the acoustic modes, known as quantum *resonant normal form*. As pointed out by [11], where the

classical problem is studied, a suitable rescaling transforms the Hamilton equations for this type of normal form (of the classical FPU problem) into the so-called Fourier-Galerkin truncation to $N-1$ modes of the $2N$ periodic *Korteweg-de Vries* equation (in the following denoted by KdV)

$$U_t = \frac{1}{24}U_{xxx} + \frac{\alpha}{\sqrt{2}}UU_x \tag{6.1}$$

with periodic boundary conditions

$$U(x+L,t) = U(x,t), \qquad \forall x,t \in \mathbb{R}, \qquad L = 2N.$$

Our aim is to study the quantum problem and see the analogous of the KdV equation, which will be the equivalent of the Heisenberg equations for the creation operator.

6.2 Construction of the quantum resonant normal form

The core of the method resides in the expansion of the dispersion relation

$$\omega_k = \xi_k - \frac{1}{24}\xi_k^3 + O(\xi_k^5), \qquad \xi_k = \frac{\pi k}{N}$$

clearly adapted to the acoustic modes. The quadratic part $\hat{h}$ of the qFPU Hamiltonian operator is now split

$$\sum_{k=1}^{N-1} \omega_k a_k^\dagger a_k = \sum_{k=1}^{N-1} \xi_k a_k^\dagger a_k + \sum_{k=1}^{N-1} (-\frac{\xi_k^3}{24} + \ldots) a_k^\dagger a_k.$$

For initial excitation of acoustic modes, the sum

$$\hat{J}(a,a^\dagger) := \sum_{k=1}^{N-1} \xi_k a_k^\dagger a_k$$

is regarded as the unperturbed part of the Hamiltonian operator, while the perturbation is given by

$$\begin{aligned} -\frac{1}{24}\sum_{k=1}^{N-1} \xi_k^3 a_k^\dagger a_k + \frac{\alpha}{4\sqrt{N}} \sum_{k=1}^{B(N)} \sqrt{\xi_{2k}}\xi_{2k-N}(a_{2k} + a_{2k}^\dagger) + \\ + \frac{\alpha}{12\sqrt{N}} \sum_{k_1,k_2,k_3=1}^{N-1} \sqrt{\xi_{k_1}\xi_{k_2}\xi_{k_3}}\Delta_3(k_1,k_2,k_3)[a_{k_1}a_{k_2}a_{k_3} + \\ + 3a_{k_1}^\dagger a_{k_2}a_{k_3} + 3a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} + a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger]. \end{aligned}$$

A step of normalization (in the sense of perturbation theory) will be performed, with the flow of the unperturbed part given by

$$a_k(t) = e^{-i\xi_k t}a_k, \qquad a_k^\dagger(t) = e^{i\xi_k t}a_k^\dagger, \qquad \forall k = 1,\ldots,N-1.$$

While the quadratic term coincides with its average, and the linear term averages to zero, the new first order perturbation is no longer zero because of the acoustic dispersion law. In fact the average along the flow of $\hat{J}$ is obtained with the same method above and is given by

$$\hat{S}_{1,\mathrm{res}} = -\frac{1}{24}\sum_{k=1}^{N-1}\xi_k^3 a_k^\dagger a_k + \frac{\alpha}{4\sqrt{N}}\sum_{j,l,m=1}^{N-1}\sqrt{\xi_j\xi_l\xi_m}(a_j^\dagger a_l a_m\delta_{j,l+m} + a_j^\dagger a_l^\dagger a_m\delta_{j+l,m})$$

Proposition 6.1. *The first order resonant Birkhoff normal form for the qFPU Hamiltonian operator is, neglecting the remainder,*

$$\hat{R}(a,a^\dagger) = \sum_{k=1}^{N-1}\xi_k a_k^\dagger a_k - \frac{1}{24}\sum_{k=1}^{N-1}\xi_k^3 a_k^\dagger a_k + \frac{\alpha}{4\sqrt{N}}\sum_{j,l,m=1}^{N-1}\sqrt{\xi_j\xi_l\xi_m}(a_j^\dagger a_l a_m\delta_{j,l+m} + a_j^\dagger a_l^\dagger a_m\delta_{j+l,m}) \quad (6.2)$$

It is interesting to explicitly verify that $[\hat{h},\hat{S}_{1,\mathrm{res}}]=0$. Clearly $[\hat{h},\frac{1}{24}\sum_{k=1}^{N-1}\xi_k^3 a_k^\dagger a_k]=0$, so we only have to compute $[\hat{h},\frac{\alpha}{4\sqrt{N}}\sum_{jlm}\sqrt{\xi_j\xi_l\xi_m}(a_j^\dagger a_l a_m\delta_{j,l+m}+a_j^\dagger a_l^\dagger a_m\delta_{j+l,m}]$. Being $[\hat{n}_k,a_q]=-\delta_{k,q}a_k$ and $[\hat{n}_k,a_q^\dagger]=\delta_{k,q}a_k^\dagger$ one has

$$[\hat{n}_k,a_j^\dagger a_l a_m] = [\hat{n}_k,a_j^\dagger]a_l a_m + a_j^\dagger[\hat{n}_k,a_l a_m] = \delta_{k,j}a_k^\dagger a_l a_m - \delta_{k,m}a_j^\dagger a_l a_m - \delta_{k,l}a_j^\dagger a_l a_m$$
$$[\hat{n}_k,a_j^\dagger a_l^\dagger a_m] = [\hat{n}_k,a_j^\dagger a_l^\dagger]a_m + a_j^\dagger a_l^\dagger[\hat{n}_k,a_m] = \delta_{k,l}a_j^\dagger a_l^\dagger a_m + \delta_{k,j}a_j^\dagger a_l^\dagger a_m - \delta_{k,m}a_j^\dagger a_l^\dagger a_m.$$

So we have

$$\begin{aligned}
&\frac{\alpha}{4\sqrt{N}}\sum_{kjlm}\xi_k\sqrt{\xi_j\xi_l\xi_m}[a_k^\dagger a_l a_m\delta_{j,l+m}(\delta_{k,j}\delta_{k,m}-\delta_{k,l}) + a_j^\dagger a_l^\dagger a_m\delta_{j+l,m}(\delta_{k,l}+\delta_{k,j}-\delta_{k,m})]\\
=&\frac{\alpha}{4\sqrt{N}}\sum_{jlm}\Big[a_j^\dagger a_l a_m\delta_{j,l+m}\big(\xi_j^{3/2}\sqrt{\xi_l\xi_m}-\xi_m^{3/2}\sqrt{\xi_j\xi_l}-\xi_l^{3/2}\sqrt{\xi_j\xi_m}\big)\\
&\quad + a_j^\dagger a_l^\dagger a_m\delta_{j+l,m}\big(\xi_l^{3/2}\sqrt{\xi_j\xi_m}+\xi_j^{3/2}\sqrt{\xi_l\xi_m}-\xi_m^{3/2}\sqrt{\xi_j\xi_l}\big)\Big]\\
=&\frac{\alpha}{4\sqrt{N}}\sum_{jlm}\Big[a_{l+m}^\dagger a_l a_m\big(\xi_{l+m}^{3/2}\sqrt{\xi_l\xi_m}-\xi_m^{3/2}\sqrt{\xi_{l+m}\xi_l}-\xi_l^{3/2}\sqrt{\xi_{l+m}\xi_m}\big)\\
&\quad + a_j^\dagger a_l^\dagger a_{j+l}\big(\xi_l^{3/2}\sqrt{\xi_j\xi_{j+l}}+\xi_j^{3/2}\sqrt{\xi_l\xi_{j+l}}-\xi_{j+l}^{3/2}\sqrt{\xi_j\xi_l}\big)\Big].
\end{aligned}$$

Now, being $\xi_{l+m}=\xi_l+\xi_m$, it is easy to verify that

$$\xi_{l+m}^{3/2}\sqrt{\xi_l\xi_m} = \xi_m^{3/2}\sqrt{\xi_{l+m}\xi_l} + \xi_l^{3/2}\sqrt{\xi_{l+m}\xi_m} \qquad \forall l,m=1,\dots,N-1$$

so that $[\hat{h},\hat{S}_{1,\mathrm{res}}]=0$.

6.3 Towards the quantum KdV equation

The Heisenberg equation for the creation operator a_k, $k = 1, \dots, N-1$, evolving in time with the dynamics given by $\hat{R}$ is

$$\begin{aligned}
\dot{a}_k &= -i[a_k, \hat{R}] \\
&= -i\xi_k a_k + \frac{i}{24}\xi_k^3 a_k - \frac{i\alpha}{4\sqrt{N}} \sum_{j,l,m=1}^{N-1} \sqrt{\xi_j \xi_l \xi_m}([a_k, a_j^\dagger a_l a_m]\delta_{j,l+m} + [a_k, a_j^\dagger a_l^\dagger a_m]\delta_{j+l,m}) \\
&= -i\xi_k a_k + \frac{i}{24}\xi_k^3 a_k + \\
&\quad - \frac{i\alpha}{4\sqrt{N}} \sum_{j,l,m=1}^{N-1} \sqrt{\xi_j \xi_l \xi_m}(a_l a_m \delta_{k,j}\delta_{j,l+m} + a_l^\dagger a_m \delta_{k,j}\delta_{j+l,m} + a_j^\dagger a_m \delta_{k,l}\delta_{j+l,m})
\end{aligned}$$

so finally one has

$$\dot{a}_k = -i\xi_k a_k + \frac{i}{24}\xi_k^3 a_k - \frac{i\alpha\sqrt{\xi_k}}{4\sqrt{N}} \sum_{l,m=1}^{N-1} \sqrt{\xi_l \xi_m}(a_l a_m \delta_{k,l+m} + 2a_l^\dagger a_m \delta_{k+l,m}).$$

The Heisenberg equations for the creation operators are

$$\dot{a}_k^\dagger = i\xi_k a_k^\dagger - \frac{i}{24}\xi_k^3 a_k^\dagger + \frac{i\alpha\sqrt{\xi_k}}{4\sqrt{N}} \sum_{l,m=1}^{N-1} \sqrt{\xi_l \xi_m}(a_l^\dagger a_m^\dagger \delta_{k,l+m} + 2a_l^\dagger a_m \delta_{k+l,m}).$$

We wish now to polish this equation up and put it in a suitable form. Our first step is to introduce the so-called *co-rotating coordinates*, which are

$$a_k = e^{-i\xi_k t} z_k, \quad a_k^\dagger = e^{i\xi_k t} z_k^\dagger, \qquad \forall k = 1, \dots, N-1.$$

The new coordinates z_k and $z_k^\dagger$ do not commute, in fact

$$[z_k, z_{k'}^\dagger] = [e^{i\xi_k t} a_k, e^{-i\xi_{k'} t} a_{k'}^\dagger] = e^{i(\xi_k - \xi_{k'})t}[a_k, a_k^\dagger] = \delta_{k,k'}$$

which makes the transformation canonical. Being $\dot{a}_k = -i\xi_k a_k + e^{-i\xi_k t}\dot{z}_k$ the Heisenberg equations for a_k and $a_k^\dagger$ become

$$\begin{aligned}
\dot{z}_k &= \frac{i}{24}\xi_k^3 z_k - \frac{i\alpha\sqrt{\xi_k}}{4\sqrt{N}} \sum_{l,m=1}^{N-1} \sqrt{\xi_l \xi_m}(z_l z_m \delta_{k,l+m} + 2z_l^\dagger z_m \delta_{k+l,m}) \\
\dot{z}_k^\dagger &= -\frac{i}{24}\xi_k^3 z_k^\dagger + \frac{i\alpha\sqrt{\xi_k}}{4\sqrt{N}} \sum_{l,m=1}^{N-1} \sqrt{\xi_l \xi_m}(z_l^\dagger z_m^\dagger \delta_{k,l+m} + 2z_l^\dagger z_m \delta_{k+l,m}).
\end{aligned}$$

The second and final step is a non-canonical rescaling together with an exchange of the creation and annihilation operators

$$u_k = \sqrt{\xi_k} z_k^\dagger, \quad \forall k = 1, \dots, N-1, \qquad [u_k, u_{k'}^\dagger] = -\xi_k \delta_{kk'}$$

which leads us to the following result.

Proposition 6.2. *The Heisenberg equation for the creation operator $a_k^\dagger$ for the acoustic modes of the qFPU problem is equivalent to*

$$\dot{u}_k = -\frac{i}{24}\xi_k^3 u_k + \frac{i\alpha\xi_k}{4\sqrt{N}} \sum_{l,m=1}^{N-1} (u_l u_m \delta_{k,l+m} + 2u_l^\dagger u_m \delta_{k+l,m}) \tag{6.3}$$

with $[u_k, u_{k'}^\dagger] = -\xi_k \delta_{k,k'}$.

Remark 6.2. This equation is the one obtained in [11], where instead of commuting coordinates $u_k, u_k^* \in \mathbb{C}$ we have non-commuting operators $u_k, u_k^\dagger$.

There is a strong connection between this last equation and the so called *quantum KdV* equation (in the following qKdV)

$$\psi_t = \frac{1}{24}\psi_{xxx} + \frac{\alpha}{2\sqrt{2}}(\psi\psi_x + \psi_x\psi) \tag{6.4}$$

where $\psi(x,t)$ is a L-periodic hermitian field operator such that $[\psi(x,t), \psi(x',t)] = i\delta_x(x-x')$ where δ_x is the weak derivative of the delta distributions with respect to the x variable.

Definition 6.1 (Fourier-Galerkin truncation)**.** The *Fourier-Galerkin truncation* to the first N modes of a L-periodic field operator $U(x,t)$ is

$$\frac{1}{\sqrt{L}} \sum_{k=-N}^{N} \widetilde{U}_k(t) e^{\frac{2\pi i k x}{L}},$$

where $\widetilde{U}_k(t) = L^{-1/2} \int_0^L U(x,t) e^{-\frac{2\pi i k x}{L}}\, dx$.

Theorem 6.1. *The normal form* (6.3) *coincide with the Fourier-Galerkin truncation to the first $N-1$ modes of the qKdV equation* (6.4)

$$\psi_t = \frac{1}{24}\psi_{xxx} + \frac{\alpha}{2\sqrt{2}}(\psi\psi_x + \psi_x\psi),$$

with periodic zero-average initial datum, namely

$$\psi(x+L,0) = \psi(x,0), \qquad \int_0^L \psi(x,0)\, dx = 0,$$

where $L = 2N$.

Proof. Consider the qKdV equation (6.4). The field $\psi(x,t)$ admits the Fourier expansion

$$\psi(x,t) = \frac{1}{\sqrt{L}} \sum_{k \in \mathbb{Z}\setminus\{0\}} U_k(t) e^{\frac{2\pi i k x}{L}},$$

with $U_k(t) = \frac{1}{\sqrt{L}} \int_0^L \psi(x,t) e^{-\frac{2\pi i k x}{L}}$ and $U_{-k}(t) = U_k^\dagger(t)$, where we impose the commutation rule

$$[U_k(t), U_q^\dagger(t)] = -\xi_k \delta_{k,q}.$$

One immediately finds

$$\psi_t = \frac{1}{\sqrt{L}} \sum_k \frac{dU_k}{dt} e^{\frac{2\pi i k x}{L}}, \qquad \psi_{xxx} = \frac{1}{\sqrt{L}} \sum_k \left[\left(\frac{2\pi i k}{L} \right)^3 U_k \right] e^{\frac{2\pi i k x}{L}},$$

as well as

$$\begin{aligned} \frac{1}{2}(\psi_x \psi + \psi \psi_x) = \frac{1}{2} \frac{\partial}{\partial x} \psi^2 &= \frac{\partial}{\partial x} \frac{1}{2L} \sum_{q,p} U_p U_q e^{\frac{2\pi i (q+p) x}{L}} \\ &= \frac{1}{\sqrt{L}} \sum_k \left[\frac{2\pi i k}{L} \frac{1}{2\sqrt{L}} \sum_{q,p} U_p U_q \delta_{k,q+p} \right] e^{\frac{2\pi i k x}{L}}. \end{aligned}$$

Thus, the generic Fourier coefficient U_k evolves according to

$$\frac{dU_k}{dt} = -\frac{i}{24} \left(\frac{2\pi k}{L} \right)^3 U_k + \frac{2\pi k}{L} \frac{i\alpha}{2\sqrt{2L}} \sum_{q,p \in \mathbb{Z} \setminus \{0\}} U_p U_q \delta_{k,q+p}. \tag{6.5}$$

Let us rewrite in a suitable way the convolution at the right hand side of the last equation.

$$\begin{aligned} \sum_{q \in \mathbb{Z} \setminus \{0\}} U_{k-q} U_q &= \sum_{q=1}^{+\infty} U_{k-q} U_q + \sum_{q=-\infty}^{-1} U_{k-q} U_q \\ &= \sum_{q=1}^{k-1} U_{k-q} U_q + \sum_{q=k+1}^{+\infty} U_{-(q-k)} U_q + \sum_{q=1}^{+\infty} U_{k+q} U_{-q} \\ &= \sum_{q=1}^{k-1} U_{k-q} U_q + \sum_{q=1}^{+\infty} U_q^\dagger U_{k+q} + \sum_{q=1}^{+\infty} U_{k+q} U_q^\dagger \end{aligned}$$

Being $q \neq 0$ $U_q^\dagger U_{k+q} = U_{k+q} U_q^\dagger$, so the latter becomes

$$\begin{aligned} \sum_{q \in \mathbb{Z} \setminus \{0\}} U_{k-q} U_q &= \sum_{q=1}^{k-1} U_{k-q} U_q + 2 \sum_{q=1}^{+\infty} U_q^\dagger U_{k+q} \\ &= \sum_{q=1}^{k-1} U_{k-q} U_q + 2 \sum_{q=1}^{N-k-1} U_q^\dagger U_{k+q} + \left(2 \sum_{q=N-k}^{+\infty} U_q^\dagger U_{k+q} \right) \end{aligned}$$

The Fourier-Galerkin truncation to the first $N-1$ modes consists exactly in neglecting the contribution of the last quantity in the convolution above. Recalling that $2L = N$ and $2\pi k/L = \xi_k$, and renaming $U_k(t) = u_k(t)$, we have exactly (6.3). The commutation rule $[\psi(x,t), \psi(x',t)] = i\delta_x(x - x')$ derives directly from the one of

$[u_k(t), u^\dagger_{k'}(t)] = -\xi_k \delta_{k,k'}$ with $u_{-k} = u^\dagger_k$. In fact

$$\begin{aligned}
[\psi(x,t), \psi(x',t)] &= \frac{1}{L}\sum_k u_k(t) e^{i\xi_k x}, \sum_{k'} u_{k'} e^{i\xi_{k'} x}] \\
&= \frac{1}{L}\sum_{k,k'} [u_k, u_{k'}] e^{i(\xi_k x + \xi_{k'} x')} \\
&= -\frac{1}{L}\sum_{k,k'} \xi_k \delta_{k,-k'} e^{i(\xi_k x + \xi_{k'} x')} \\
&= -\frac{1}{L}\sum_k \xi_k e^{i\xi_k (x-x')} = i\delta_x(x-x')
\end{aligned}$$

where we used $\delta(x) = \frac{1}{L}\sum_k e^{i\xi_k x}$. □

Remark 6.3. The classical construction is almost equivalent, with the usual difference that in this work we are dealing with non-commuting operators instead of commuting complex coordinates. In the end, one finds that the acoustic modes, after an appropriate rescaling, obey to the Hamilton equations

$$\dot{u}_k = -\frac{i}{24}\xi_k^3 u_k + \frac{i\alpha\xi_k}{4\sqrt{N}} \sum_{l,m=1}^{N-1} (u_l u_m \delta_{k,l+m} + 2u_l^* u_m \delta_{k+l,m})$$

where $\{u_k, u^*_{k'}\} = i\xi_k \delta_{k,k'}$. In [11] it was found that these equation are the Fourier-Galerkin truncation of the Korteweg-de Vries equation (6.1), with $\{U(x), U(y)\} = \delta_x(x-y)$.

6.4 Integrability of the quantum KdV equation

Thanks to theorem 6.1, we can state that, in first approximation, systems like the one studied in [3] have dynamics close to the one described by the qKdV equation (6.4). In order to understand why such systems do not show thermalisation, studying the integrability property of this equation seems of the uttermost importance. We must remark, however, that we actually don't know neither *what* quantum thermalisation is, nor *how* integrability affects the thermalisation properties of our physical system. On the other hand, we think (guided by semi-classic arguments) that there is some kind of connection between the presence of an infinite number of conserved quantities for a quantum system, and thus its integrability, and its lack of thermalisation. The equation (6.4) is already present in literature, for example in [6], where it is obtained from the quantization of the classical KdV, and its integrability is studied using the so called *theory of hereditary operators*. In the following we will show how integrability is obtained, but we will not enter in such a vast world as the one of the nonlinear evolution equations for quantum operators.

In order to provide the quantum KdV equation (6.4) an Hamiltonian formulation, we must put it in an algebraic environment which is the one of almost-bounded distributions.

Definition 6.2 (Almost-bounded distribution)**.** A distribution $\phi(x)$ is said to be *almost-bounded* if, for every $n \in \mathbb{N}$, its n-th derivative is of the form

$$\phi^{(n)}(x) = b(x) + \Delta(x)$$

where b is locally bounded and where Δ is a distribution with discrete support such that the support has no accumulation point.

Consider the algebra fulfilling the commutation rule

$$[u(x), u(\widetilde{x})] = i\delta_x(x - \widetilde{x})$$

by taking suitable congruence classes in the algebra of the almost-bounded distributions of degree 3. We will call this algebra QF.

Since elements of QF may be considered as operators (by multiplication) on QF itself, we have found the required operator representation of the Poisson structure of the quantum KdV. Now, we have the prerequisites to define the time evolution for quantum systems by taking suitable Hamiltonian operators. For example, taking

$$H = \int (u(\xi)u(\xi)u(\xi) - \frac{1}{2}u_\xi(\xi)u_\xi(\xi))\, d\xi$$

and defining the action of a commutator on an integral, as integral in the convolution sense over the commutator with its integrand, we find

$$u(x)_t = -i[u(x), H] = u_{xxx}(x) + 3u_x(x)u(x) + 3u(x)u_x(x) \tag{6.6}$$

which is, up to multiplicative constants, the equation we found in the previous chapter. This equation is considered in [6] as the quantum version of KdV. The main problem is to prove that this equation is completely integrable in the usual sense, i.e. that it has infinitely many commuting symmetry groups (or conserved quantities in involution). In order to give a recursive description of the symmetries and the conserved quantities of the quantum KdV (6.6), an alternative representation of its dynamics is introduced. Define the space of *densities* to be QF where integrals over total derivatives are ignored (see [6]). This is exactly our case, since we are dealing with the quantum Korteweg de Vries equation with periodic boundary conditions, and $u(x + L) = u(x)\ \forall x$.

Let A and B two elements in QF. Define for all $A, B \in QF$ an *inner product* in QF by

$$\langle A, B\rangle := \int_{\mathbb{T}_L} A(x)B(x)\, dx$$

where the integration is performed in $\mathbb{T}_L$, since we have imposed periodic boundary conditions.

Remark 6.4. The differential operator D is antisymmetric with respect to that density-valued inner product.

Let $F = F(u)$ a density depending in some way on the field variable u. Then define its directional derivative of F in the direction of an element B of QF by

$$F'[B] = \frac{\partial}{\partial\varepsilon}F(u + \varepsilon B)|_{\varepsilon=0}.$$

These definitions, and the notion of density, provide as simple result that there is a unique operator ∇, mapping densities into density-valued linear functionals on QF such that

$$F'[B] = \langle \nabla F, B \rangle \qquad \text{for all} \qquad B \in QF.$$

The quantity ∇F is said to be the *gradient* of F. For example, one obtains the gradient of

$$H_1 = \int_{\mathbb{T}_L} (u(\xi)u(\xi)u(\xi) - \frac{1}{2}u_\xi(\xi)u_\xi(\xi))\, d\xi \tag{6.7}$$

as $u_{xx}(x) + 3u(x)u(x)$. The quantum KdV equation (6.6) can now be rewritten as

$$u_t = D\nabla H_1$$

where H_1 is given above in (6.7), and D denotes the operator of taking the derivative with respect to x which is an implectic operator (the equivalent of a Poisson tensor, in this notation). This equation has a very special property, like the classical case, which is that it can be endowed with two different Hamiltonian structure, i.e. two different Poisson tensors J_1 and J_2 and two different Hamiltonians H_1 and H_2 such that the equation can be read as $u_t = J_1\nabla H_1 = J_2\nabla H_2$. We have just seen the first Hamiltonian formulation, that is

$$J_1 = D \qquad H_1 = \int_{\mathbb{T}_L} (u(\xi)u(\xi)u(\xi) - \frac{1}{2}u_\xi(\xi)u_\xi(\xi))\, d\xi$$

which is the equivalent of the first Hamiltonian formulation of the classical KdV equation (see [20] for details).

We are now ready to derive the second Hamiltonian formulation of the quantum KdV (6.6). Denote by u the field variable and introduce

$$L(u)A := uA, \qquad R(u)A := Au$$

where $A \in QF$. These are operators of multiplication with u from the left and from the right. Then set

$$\Theta = D^3 + DL(u) + DR(u) + R(u)D + L(u)D + [L(u) - R(u)]D^{-1}[L(u) - R(u)]$$

which gives an operator being antisymmetric with respect to the inner product defined above. It is possible (but arduous) to verify that Θ is an implectic operator (i.e. a Poisson tensor), and thus provides the second Hamiltonian formulation of (6.6), with Hamiltonian

$$H_2 = \frac{1}{2}\int_{\mathbb{T}_L} u(\xi)u(\xi)\, d\xi \tag{6.8}$$

then we have $\nabla H_2 = u$ whence

$$u_t = \Theta\nabla H_2$$

is again the quantum KdV flow. It's easy to verify that in the commutative case, where $R(u) = L(u)$, this second implectic operator of the quantum KdV is equivalent to the second Poisson tensor of the KdV.

Now [6] apply the theory of hereditary operators of [7] and [8] in order to have a recursive generation of conserved densities and vector fields. It is proven, using

Bäcklund transformations, that the two implectic operators are compatible (i.e. their sum is again an implectic operator), so

$$\Phi = \Theta D^{-1}$$

is an hereditary and a strong symmetry. Qualitatively, if $K(u)$ is the quantum KdV vector field, then

- a *symmetry* is a vector field $S(u)$ such that $[K, S] = K'[S] - S'[K] = 0$;
- a *strong symmetry* is an operator-valued function Φ which maps symmetries of $u_t = K(u)$ into symmetries of that equation;
- an *hereditary symmetry* is an operator-valued function Φ such that if it is a strong symmetry of any equation $u_t = K(u)$, then it is a strong symmetry also for $u_t = \Phi(u)K(u)$.

and generates out of the vector field of the quantum KdV a hierarchy of commuting flows $\Phi^n(u)K(u)$, $n \in \mathbb{Z}$, which constitute the symmetry group generators for the quantum KdV since it is among the members of the hierarchy. For the equivalent of Noether's theorem, these commuting symmetries produce an infinite number of conserved quantities in involution, which cause the integrability of the quantum Korteweg-de Vries equation in the same way as the classical case.

We want to remark that, although this fact is surely of mathematical and formal interest, we don't actually know the physical effects and consequences on the quantum Fermi-Pasta-Ulam system and its thermalisation. If this was a classical system, then its integrability should prevent ergodicity and then thermalisation, at least for a long period of time. However, this is a quantum system, and as we already pointed out, there isn't a real and solid theory of quantum thermalisation yet. The fact that the theory of nonlinear quantum evolution equations is a wide and complex field, and that there is not a real physical application of it, are the reasons why we didn't dedicate much space in this work on the study of this equation's integrability. The aim of this section was only to pointing out that the quantum Korteweg-de Vries equation, which describes the quantum FPU system for a long period of time, was already studied from a mathematical point of view and its integrability was proven.

APPENDIX A

Computation of $\frac{1}{2i}\overline{[\hat{H}_3, \hat{G}_1]}$

In this appendix we report the calculation of the average of the commutator $\frac{1}{2i}\overline{[\hat{H}_3, \hat{G}_1]}$, where $\hat{H}_3$ and $\hat{G}_1$ are reported above. As pointed before, there are four main contributions. The first one is given by the average of commutator between cubic terms $\frac{1}{2i}\overline{[\hat{H}_3^{(3)}, \hat{G}_1^{(3)}]}$ where

$$\frac{1}{2i}[\hat{H}_3^{(3)}, \hat{G}_1^{(3)}] = \frac{1}{2}\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3} \sum_{q_1,q_2,q_3} \prod_{s=1}^{3} \sqrt{\omega_{k_s}\omega_{q_s}}$$

$$\Delta_3(k_1,k_2,k_3)\Delta_3(q_1,q_2,q_3)\Bigg[a_{k_1}a_{k_2}a_{k_3} + 3a^\dagger_{k_1}a_{k_2}a_{k_3} + 3a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3} + a^\dagger_{k_1}a^\dagger_{k_2}a^\dagger_{k_3},$$

$$\frac{a_{q_1}a_{q_2}a_{q_3}}{\omega_{q_1}+\omega_{q_2}+\omega_{q_3}} + 3\frac{a^\dagger_{q_1}a_{q_2}a_{q_3}}{\omega_{q_3}+\omega_{q_2}-\omega_{q_1}} + 3\frac{a^\dagger_{q_1}a^\dagger_{q_2}a_{q_3}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}} - \frac{a^\dagger_{q_1}a^\dagger_{q_2}a^\dagger_{q_3}}{\omega_{q_1}+\omega_{q_2}+\omega_{q_3}}\Bigg]. \quad \text{(A.1)}$$

There are sixteen commutators to average, which we report below taking into account the symmetry properties of the exchange of the indices k_s and q_s. The commutators were also normal ordered.

1. $[a_{k_1}a_{k_2}a_{k_3}, a_{q_1}a_{q_2}a_{q_3}] = 0$.
2. $[a_{k_1}a_{k_2}a_{k_3}, a^\dagger_{q_1}a_{q_2}a_{q_3}]$ surely contains no creation operators, so its average vanishes.
3. $[a_{k_1}a_{k_2}a_{k_3}, a^\dagger_{q_1}a^\dagger_{q_2}a_{q_3}] \simeq 6a^\dagger_{q_1}a_{k_1}a_{k_3}a_{q_3}\delta_{k_2,q_2} + 6a_{k_3}a_{q_3}\delta_{k_1,q_1}\delta_{k_2,q_2}$. While the quadratic term surely vanishes to zero, the average of the quartic term

$$9\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3} \sum_{q_1,q_2,q_3} \delta_{k_2,q_2} \frac{\omega_{k_2}\prod_{s=1,3}\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}}$$
$$\Delta_3(k_1,k_2,k_3)\Delta_3(q_1,k_2,q_3)\ 6\ a^\dagger_{q_1}a_{k_1}a_{k_3}a_{q_3}$$

is more delicate. With the technique explained above one can verify that the average of this term is zero.

4. $[a_{k_1}a_{k_2}a_{k_3}, a^\dagger_{q_1}a^\dagger_{q_2}a^\dagger_{q_3}] \simeq 9a^\dagger_{q_2}a^\dagger_{q_3}a_{k_2}a_{k_3}\delta k_1, q_1 + 18a^\dagger_{q_1}a_{k_1}\delta_{k_2,q_2}\delta_{k_3,q_3} + 6\delta_{k_1,q_1}\delta_{k_2,q_2}\delta_{k_3,q_3}$. Dropping the constant term, one needs to average the quartic term

$$-9\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3}\sum_{q_1q_2,q_3} \delta_{k_1,q_1}\frac{\omega_{k_1}\prod_{s=2,3}\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_1}+\omega_{q_2}+\omega_{q_3}} \Delta_3(k_1,k_2,k_3)\Delta_3(k_1,q_2,q_3)\; a^\dagger_{q_2}a^\dagger_{q_3}a_{k_2}a_{k_3}$$

which gives

$$-9\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3}\sum_{q_1q_2,q_3} \delta_{k_1,q_1}\frac{\omega_{k_1}\prod_{s=2,3}\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_1}+\omega_{q_2}+\omega_{q_3}} a^\dagger_{q_2}a^\dagger_{q_3}a_{k_2}a_{k_3}$$
$$(\delta_{k_3,q_3}\delta_{k_1+k_2,k_3}\delta_{q_1+q_2,q_3} + \delta_{k_2,q_3}\delta_{k_1+k_2,k_3}\delta_{q_1+q_3,q_2} + \delta_{k_2,q_3}\delta_{k_1+k_3,k_2}\delta_{q_1+q_2,q_3}$$
$$+ \delta_{k_3,q_3}\delta_{k_1+k_3,k_2}\delta_{q_1+q_3,q_2} + (\delta_{k_2,q_3}+\delta_{k_3,q_3})\delta_{k_2+k_3,k_1}\delta_{q_2+q_3,q_1}$$
$$+ (\delta_{q_3,k_2}+\delta_{q_3,k_3})\delta_{k_1+k_2+k_3,2N}\delta_{q_1+1_2+1_3,2N})$$

Due to the symmetry property in the exchange of the k_2 and k_3 indices, this sum of Kronocker deltas reduces to

$$-18\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3}\sum_{q_1q_2,q_3} \delta_{k_1,q_1}\delta_{k_3,q_3}\frac{\omega_{k_1}\prod_{s=2,3}\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_1}+\omega_{q_2}+\omega_{q_3}} a^\dagger_{q_2}a^\dagger_{q_3}a_{k_2}a_{k_3}$$
$$(\delta_{k_1+k_2,k_3}\delta_{q_1+q_2,q_3} + \delta_{k_1+k_3,k_2}\delta_{q_1+q_3,q_2}$$
$$+ \delta_{k_2+k_3,k_1}\delta_{q_2+q_3,q_1} + \delta_{k_1+k_2+k_3,2N}\delta_{q_1+1_2+1_3,2N})$$

which is equal to

$$-18\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_2}\sum_{q_1q_2,q_3} \frac{\omega_{q_1}\omega_{q_3}\sqrt{\omega_{k_2}\omega_{q_2}}}{\omega_{q_1}+\omega_{q_2}+\omega_{q_3}} a^\dagger_{q_2}a^\dagger_{q_3}a_{k_2}a_{k_3}$$
$$(\delta_{q_1+k_2,q_3}\delta_{q_1+q_2,q_3} + \delta_{q_1+q_3,k_2}\delta_{q_1+q_3,q_2}$$
$$+ \delta_{k_2+q_3,q_1}\delta_{q_2+q_3,q_1} + \delta_{q_1+k_2+q_3,2N}\delta_{q_1+1_2+1_3,2N})$$

thus, in the sum one can extract δ_{k_2,q_2}, while the remaining deltas together reform $\Delta_3(q_1,q_2,q_3)$. So finally, renaming $q \mapsto k$ one has

$$-\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}\Delta_3(k_1,k_2,k_3)a^\dagger_{k_1}a^\dagger_{k_2}a_{k_2}a_{k_1}.$$

The quadratic term instead gives

$$-\frac{\alpha^2}{16N}\sum_{k_1,k_2,k_3}\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}\Delta_3(k_1,k_2,k_3)a^\dagger_{k_3}a_{k_3}.$$

5. $[a^\dagger_{k_1}a_{k_2}a_{k_3}, a_{q_1}a_{q_2}a_{q_3}]$ surely contains no creation operators, so its average vanishes.

6. $[a^\dagger_{k_1}a_{k_2}a_{k_3}, a^\dagger_{q_1}a_{q_2}a_{q_3}] \simeq 2a^\dagger_{k_1}a_{k_2}a_{q_2}a_{q_3}\delta_{k_3,q_1} - 2a^\dagger_{q_1}a_{q_2}a_{k_2}a_{k_3}\delta_{k_1,q_3}$ averages to zero.

7. $[a^\dagger_{k_1}a_{k_2}a_{k_3}, a^\dagger_{q_1}a^\dagger_{q_2}a_{q_3}] \simeq 4a^\dagger_{k_1}a^\dagger_{q_1}a_{k_3}a_{q_3}\delta_{k_2,q_2} - a^\dagger_{q_1}a^\dagger_{q_2}a_{k_2}a_{k_3}\delta_{k_1,q_3} + 2a^\dagger_{k_3}a_{q_3}\delta_{k_1,q_1}\delta_{k_2,q_2}$.
The average of the first quartic term

$$36\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3}\sum_{q_1,q_2,q_3} \delta_{k_2,q_2}\frac{\prod_{s=1}^3\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}}a^\dagger_{k_1}a^\dagger_{q_1}a_{k_3}a_{q_3}$$

is obtained in the usual way and is

$$\begin{aligned}36\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 &\sum_{k_1,k_2,k_3}\sum_{q_1,q_2,q_3} \delta_{k_2,q_2}\frac{\prod_{s=1}^3\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}}a^\dagger_{k_1}a^\dagger_{q_1}a_{k_3}a_{q_3}\\ &(\delta_{k_3,q_1}\delta_{q_1+q_2,q_3}\delta_{k_2+k_3,k_1} + \delta_{k_3,q_1}\delta_{q_1+q_3,q_2}\delta_{k_1+k_3,k_2}\\ &\quad + \delta_{k_3,q_1}\delta_{q_2+q_3,q_1}\delta_{k_1+k_2,k_3} + \delta_{k_3,q_1}\delta_{q_1+q_2+q_3,2N}\delta_{k_1+k_2+k_3,2N}).\end{aligned}$$

This is equal to

$$\frac{\alpha^2}{4N}\sum_{k_1,k_2,k_3}\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\Delta_3(k_1,k_2,k_3)a^\dagger_{k_1}a^\dagger_{k_3}a_{k_3}a_{k_1}.$$

The average of the second quartic term

$$-9\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 \sum_{k_1,k_2,k_3}\sum_{q_1,q_2,q_3} \delta_{k_1,q_3}\frac{\prod_{s=1}^3\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}}a^\dagger_{q_1}a^\dagger_{q_2}a_{k_2}a_{k_3}$$

is

$$\begin{aligned}-9\Big(\frac{\alpha}{12\sqrt{N}}\Big)^2 &\sum_{k_1,k_2,k_3}\sum_{q_1,q_2,q_3} \delta_{k_1,q_3}\frac{\prod_{s=1}^3\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}}a^\dagger_{q_1}a^\dagger_{q_2}a_{k_2}a_{k_3}\\ &(\delta_{k_2,q_2}\delta_{k_2+k_3,k_1}\delta_{q_1+q_2,q_3} + \delta_{k_3,q_2}\delta_{k_2+k_3,k_1}\delta_{q_1+q_2,q_3} + \delta_{k_3,q_2}\delta_{k_1+k_2,k_3}\delta_{q_1+q_3,q_2}\\ &+ \delta_{k_2,q_2}\delta_{k_1+k_3,k_2}\delta_{q_1+q_3,q_2} + \delta_{k_2,1_2}\delta_{k_1+k_2,k_3}\delta_{q_2+q_3,q_1} + \delta_{k_3,q_2}\delta_{k_1+k_3,k_2}\delta_{q_2+q_3,q_1}\\ &\quad + \delta_{k_2,q_2}\delta_{k_1+k_2+k_3,2N}\delta_{q_1+q_2+q_3,2N} + \delta_{k_3,q_2}\delta_{k_1+k_2+k_3,2N}\delta_{q_1+q_2+q_3,2N})\end{aligned}$$

exchanging where needed k_2 and k_3 one gets

$$-\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\sum_{q_1,q_2,q_3}\delta_{k_1,q_3}\delta_{k_2,q_2}\delta_{k_3,q_1}\frac{\prod_{s=1}^3\sqrt{\omega_{k_s}\omega_{q_s}}}{\omega_{q_3}-\omega_{q_2}-\omega_{q_1}}\Delta_3(q_1,q_2,q_3)a^\dagger_{q_1}a^\dagger_{q_2}a_{k_2}a_{k_3}$$

which is

$$-\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\Delta_3(k_1,k_2,k_3)a^\dagger_{k_1}a^\dagger_{k_2}a_{k_2}a_{k_1}.$$

The quadratic term instead averages to

$$\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\Delta_3(k_1,k_2,k_3)a^\dagger_{k_3}a_{k_3}.$$

8. $[a^\dagger_{k_1} a_{k_2} a_{k_3}, a^\dagger_{q_1} a^\dagger_{q_2} a^\dagger_{q_3}] \simeq 6a^\dagger_{k_1} a^\dagger_{q_1} a^\dagger_{q_2} a_{k_2} \delta_{k_3,q_3} + 6a^\dagger_{k_1} a^\dagger_{q_1} \delta_{k_3,q_3} \delta_{k_2,q_2}$ averages to zero.

9. $[a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3}, a_{q_1} a_{q_2} a_{q_3}] \simeq -6a^\dagger_{k_2} a_{q_2} a_{q_3} a_{k_3} \delta_{k_1,q_1} - 6a_{q_3} a_{k_3} \delta_{k_1,q_1} \delta_{k_2,q_2}$ as the third contribution averages to zero.

10. $[a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3}, a^\dagger_{q_1} a_{q_2} a_{q_3}] \simeq a^\dagger_{k_1} a^\dagger_{k_2} a_{q_2} a_{q_3} \delta_{k_3,q_1} - 4a\dagger_{q_1} a^\dagger_{k_1} a_{q_3} a_{k_3} \delta_{k_2,q_2} - 2a^\dagger_{q_1} a_{k_3} \delta_{q_2,k_2} \delta_{k_1,q_3}$. Its average can be computed in the same way of the seventh contribution, and gives the exact same contribution

11. $[a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3}, a^\dagger_{q_1} a^\dagger_{q_2} a_{q_3}] \simeq 2a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{q_2} a_{q_3} \delta_{k_3,q_1} - 2a^\dagger_{q_1} a^\dagger_{q_2} a^\dagger_{k_2} a_{k_3} \delta_{k_1,q_3}$ averages to zero.

12. $[a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3}, a^\dagger_{q_1} a^\dagger_{q_2} a^\dagger_{q_3}]$ surely contains no annihilation operators, so its average vanishes.

13. $[a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{k_3}, a_{q_1} a_{q_2} a_{q_3}] \simeq -9a^\dagger_{k_1} a^\dagger_{k_2} a_{q_1} a_{q_2} \delta_{k_3,q_3} - 18a^\dagger_{k_1} a_{q_1} \delta_{k_2,q_2} \delta k_1, q_1 - 6\delta_{k_1,q_1} \delta k_2, q_2 \delta_{k_3,q_3}$. Its average can be computed in the same way of the fourth contribution and gives the exact same contribution.

14. $[a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{k_3}, a^\dagger_{q_1} a_{q_2} a_{q_3}] \simeq -6a^\dagger_{q_1} a^\dagger_{k_1} a^\dagger_{k_2} a_{q_2} \delta_{k_3,q_3} - 6a^\dagger_{q_1} a^\dagger_{k_1} \delta_{q_2,k_2} | delta a_{q_3,k_3}$ as the eighth contribution averages to zero.

15. $[a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{k_3}, a^\dagger_{q_1} a^\dagger_{q_2} a_{q_3}]$ surely contains no annihilation operators, so its average vanishes.

16. $[a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{k_3}, a^\dagger_{q_1} a^\dagger_{q_2} a^\dagger_{q_3}] = 0$.

Finally we get

$$\begin{aligned}
\frac{1}{2i}\overline{[\hat{H}_3^{(3)}, \hat{G}_1^{(3)}]} = &-\frac{\alpha^2}{4N} \sum_{k_1,k_2,k_3} \frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}} \Delta_3(k_1,k_2,k_3) a^\dagger_{k_1} a^\dagger_{k_2} a_{k_2} a_{k_1} \\
&\frac{\alpha^2}{2N} \sum_{k_1,k_2,k_3} \frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}} \Delta_3(k_1,k_2,k_3) a^\dagger_{k_1} a^\dagger_{k_3} a_{k_3} a_{k_1} \\
&- \frac{\alpha^2}{4N} \sum_{k_1,k_2,k_3} \frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}} \Delta_3(k_1,k_2,k_3) a^\dagger_{k_1} a^\dagger_{k_2} a_{k_2} a_{k_1} \\
&+ \frac{\alpha^2}{8N} \sum_{k_1,k_2,k_3} \frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}} \Delta_3(k_1,k_2,k_3) a^\dagger_{k_3} a_{k_3} \\
&- \frac{\alpha^2}{4N} \sum_{k_1,k_2,k_3} \frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}} \Delta_3(k_1,k_2,k_3) a^\dagger_{k_3} a_{k_3}.
\end{aligned}$$

Renaming properly the indices we get the result (modulo constant terms)

$$\begin{aligned}\frac{1}{2i}\overline{[\hat{H}_3^{(3)},\hat{G}_1^{(3)}]} = \frac{\alpha^2}{4N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)a_{k_1}^\dagger a_{k_2}^\dagger a_{k_2}a_{k_1}\\ \left(2\frac{1}{\omega_{k_2}-\omega_{k_3}-\omega_{k_1}}-\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}-\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right)\\ +\frac{\alpha^2}{8N}\sum_{k_1,k_2,k_3}\omega_{k_1}\omega_{k_2}\omega_{k_3}\Delta_3(k_1,k_2,k_3)a_{k_3}^\dagger a_{k_3}\\ \left(\frac{1}{\omega_{k_1}+\omega_{k_2}+\omega_{k_3}}-2\frac{1}{\omega_{k_3}-\omega_{k_2}-\omega_{k_1}}\right)\end{aligned}$$

Now we show how to compute the average of

$$\begin{aligned}\frac{1}{2i}[\hat{H}_3^{(3)},\hat{G}_1^{(1)}] = \frac{1}{2i}\Bigg[\frac{\alpha}{12\sqrt{N}}\sum_{k_1,k_2,k_3=1}^{N-1}\prod_{s=1}^{3}\sqrt{\omega_{k_s}}\Delta_3(k_1,k_2,k_3)\\ (a_{k_1}a_{k_2}a_{k_3}+3a_{k_1}^\dagger a_{k_2}a_{k_3}+3a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}+a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger),\\ \frac{\alpha}{4\sqrt{N}}\sum_{q=1}^{B(N)}(\omega_q-\omega_{N-q})\left[\frac{a_{2q}^\dagger}{i\sqrt{\omega_{2q}}}-\frac{a_{2q}}{i\sqrt{\omega_{2q}}}\right]\Bigg]\end{aligned}$$

starting from the commutators

1. $[a_{k_1}a_{k_2}a_{k_3},a_{2q}]=0$.
2. $[a_{k_1}^\dagger a_{k_2}a_{k_3},a_{2q}]$ surely contains no creation operators, so it averages to zero.
3. $[a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3},a_{2q}] = -\delta_{k_1,2q}a_{k_2}^\dagger a_{k_3}-\delta_{k_2,2q}a_{k_1}^\dagger a_{k_3}$.
4. $[a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger,a_{2q}]$ surely contains no annihilation operators, so it averages to zero.
5. $[a_{k_1}a_{k_2}a_{k_3},a_{2q}^\dagger]$ surely contains no creation operators, so it averages to zero.
6. $[a_{k_1}^\dagger a_{k_2}a_{k_3},a_{2q}^\dagger] = a_{k_1}^\dagger a_{k_2}\delta_{k_3,2q}+a_{k_1}^\dagger a_{k_3}\delta_{k_2,2q}$.
7. $[a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3},a_{2q}^\dagger]$ surely contains no annihilation operators, so it averages to zero.
8. $[a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger,a_{2q}^\dagger]=0$.

Remembering that $\overline{a_j^\dagger a_k} = a_j^\dagger a_k\delta_{j,k}$, putting all together and using the symmetry properties of exchange of the indices k one obtains the result

$$\frac{1}{2i}[\hat{H}_3^{(3)},\hat{G}_1^{(1)}] = -\frac{\alpha^2}{8N}\sum_{k=1}^{N-1}\sum_{q=1}^{B(N)}\omega_k(\omega_q-\omega_{N-q})(\delta_{k,q}+\delta_{k+q,N})a_k^\dagger a_k$$

The quantity $\frac{1}{2i}[\hat{H}_3^{(1)},\hat{G}_1^{(3)}]$ is obtained in a similar way and gives the exact same contribution. $\frac{1}{2i}[\hat{H}_3^{(1)},\hat{G}_1^{(1)}]$ instead gives only constant terms.

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