Università degli studi di Padova

Dipartimento di Matematica "Tullio Levi-Civita"

Master Degree in Mathematics
Final Dissertation

A conjecture on Fermi-Pasta-Ulam and Toda models

Thesis Supervisor:
Prof. Antonio Ponno

Candidate:
Luca Biasiolo, 1179914

June 22, 2020

Academic Year 2019-2020

"Okay. The answer to the ultimate question of life, the universe, and everything is... 42"
The Hitchhiker's Guide to the Galaxy

Abstract

In this thesis we will solve a conjecture on Fermi-Pasta-Ulam and Toda chains written in the continuum limit $N \to \infty$: this says that every first integral of the Toda chain admits an extension to the 4th order in the perturbative parameter h that is an approximated first integral of FPU.

Contents

1 Introduction

Mathematical physics has come a long way since its birth in the 19th century: there has been an enormous progress thanks to geniuses like Hamilton, Poincaré, Arnold, Kolmogorov and Nekhoroshev. They have opened entire new sub-fields and research branches with their results and their theorems. In recent years, KAM theory and integrable systems theory have been applied to new systems and problems and this has led to even more results and has also contributed to developments in other fields of mathematics and mathematical physics.
In this thesis, we will stick mainly with integrable systems theory and with hamiltonian perturbation theory. We will study, in particular, the connection between the Toda chain and the Fermi-Pasta-Ulam (FPU) chain, because both systems still present open questions nowadays and because there have been interesting developments in recent years. For example, Boris Dubrovin in [3] has proved that there is a small number of mass-spring models in which first integrals can be extended to successive perturbative orders and, fortunately, Toda chain is one of these. Moreover, in [7] the author has conjectured that first integrals of Toda chain can be extended, in a suitable sense, to approximated first integrals of FPU chain up to the fourth order of the perturbative parameter. This thesis will be a natural sequel of this work and its main goal will be solving the conjecture. This will be an interesting step forward for a better understanding of FPU chain.

Let's start with a brief historical and mathematical recap of the two systems.

FPU model The history of non-linear chains and integrable differential equations began in the summer of 1953. In that year, Fermi, Pasta and Ulam performed the first calculations on the "MANIAC I" machine of Los Alamos laboratories with the aim of studying the behaviour of one-dimensional chains of masses and springs with pairwise forces that contained quadratic and cubic terms. This experiment is well described in [4], where one can read that *"Fermi did some work on the ergodic problem when he was young, and when electronic computers were developed he came back to this as one of the problems computers might solve. He thought that if one added a nonlinear term to the force between particles in a one-dimensional lattice, energy would flow from mode to mode eventually leading the system to a statistical equilibrium state where the energy is shared equally among linear modes (equipartition of energy)".*
Following their calculations, if we call q_n the displacement of the n-th mass (with $m = 1 \quad \forall i = 1, \ldots, N$) and $F(r)$ the force when the displacement of the spring is r, we can write the equation of motion for the n-th mass as

$$\ddot{q}_n = F(q_{n+1} - q_n) - F(q_n - q_{n-1}) = F(r_n) - F(r_{n-1})$$

and the hamiltonian of the system as

$$H_{FPU}(q,p) = \sum_{n=1}^{N} \left(\frac{p_n^2}{2} + V_{FPU}(q_{n+1} - q_n) \right) \tag{1.1}$$

where $V_{FPU}(r)$ is the potential

$$V_{FPU}(r) = \frac{r^2}{2} + \alpha \frac{r^3}{3} + \beta \frac{r^4}{4} + \gamma \frac{r^5}{5} + \dots$$

with α, β, γ etc. constants. Fermi, Pasta and Ulam invented this ad-hoc problem with the aim of studying a system which was simple from the physical point of view but unmanageable with paper and pencil only. Their goal was also to begin the study of nonlinear systems physics and the mathematics beneath them. As mentioned above, they tried to observe the "mixing" process and the "thermalization" speed in the chain, that is how the energy propagates in the chain as the time increases and finally becomes the same for every particle. They started from an initial condition in which only the first harmonic mode $q_n(0) = Bsin(\frac{\pi n}{N+1})$ was excited and, surprisingly, they discovered that this does not happen: as the time increased, the energy was shared only between a few normal modes instead of being gradually distributed among all of them. Indeed, they found that only the first five harmonic modes were excited, while the others had negligible energies. Further studies on the problem showed how FPU system also presents a recurrence: *"After what would have been several hundred ordinary up and down vibrations, (the system) came back almost exactly to its original sinusoidal shape"* ([4]).

Toda model The Toda chain is a one-dimensional nonlinear chain of masses and springs with pairwise exponential potential. It was invented by Morikazu Toda in 1966. In [8] we can read that *"From the idea that the fundamentals of the mathematical methods for nonlinear lattices would be elucidated by rigorous results, I was led in 1966 to the lattice with exponential interaction"*. He looked for a *"potential which admits integration of the equations of motion [...]. It is also required that the potential must have some physical meaning, so that it really provides us with a mechanical system with wide applicability. Under these conditions, many functions were tried"*. These excerpts show how the model was invented simply by trying out different potentials and finding out which one of them most simplified the calculations.
The hamiltonian this time is

$$H_{Toda}(q,p) = \sum_{n=1}^{N} \left(\frac{p_n^2}{2} + V_{Toda}(q_{n+1} - q_n) \right)$$

with potential

$$V_{Toda}(r) = \frac{1}{\lambda^2} \left(e^{-\lambda r} - 1 - \lambda r \right)$$

where λ is a real number. In 1974 Flaschka and Henon independently proved that this Hamiltonian system is integrable and its constants of motion can be explicitly described (see [6] and [5]). In other articles it was shown how the Toda chain is an integrable version of the FPU chain. This strong connection is still present in the continuum limit $N \to \infty$ and will be used further on this thesis. For now, let's see it for N finite: we take $\lambda = 2\alpha$ in the Toda potential (α coming from V_{FPU}) and we expand it using Taylor series around $r = 0$ obtaining

$$V_{Toda}(r) = \frac{r^2}{2} + \alpha\frac{r^3}{3} + \beta_{Toda}\frac{r^4}{4} + \gamma_{Toda}\frac{r^5}{5} + \dots$$

with $\beta_{Toda} = \frac{2}{3}\alpha^2$, $\gamma_{Toda} = \frac{1}{3}\alpha^3$ etc.. We can thus write

$$V_{FPU}(r) - V_{Toda}(r) = \frac{(\beta - \beta_{Toda})r^4}{4} + \frac{(\gamma - \gamma_{Toda})r^5}{5} + \dots$$

that shows how FPU is tangent to Toda up to order three. It is therefore possible to study the first using the second, which offers a much more manageable model.

Let's now begin our study with some useful definitions coming from hamiltonian perturbation theory.

Definition 1.1 (Non-degenerate hamiltonian)**.** *An hamiltonian $H_0(I)$ which depends only on its action variables is said to be non-degenerate if* $\det(H_0''(I)) \neq 0 \quad \forall I \in D \subset \mathbb{R}^n$

Definition 1.2 (Generic perturbation)**.** *Consider a perturbed hamiltonian $H(I, \phi)$ written in action-angle variables of the form*

$$H(I, \phi) = H_0(I) + \epsilon H_1(I, \phi) + \dots \tag{1.2}$$

where $I \in D \subset \mathbb{R}^n$ and $\phi \in \mathbb{T}^n$. We say that $H_1(I, \phi)$ is a generic perturbation if its Fourier series

$$H_1(I, \phi) = \sum_{m \in \mathbb{Z}^n} H_{1m}(I) e^{im\cdot\phi}$$

has $H_{1m}(I) \neq 0 \quad \forall m \in \mathbb{Z}^n$.

The next theorem says that, under generic perturbations, non-degenerate integrable hamiltonians exhibit only trivial first integrals:

Theorem 1.1 (Poincaré's theorem)**.** *Consider the perturbed hamiltonian 1.2. Suppose that H_0 is non-degenerate in D and that $H_1(I, \phi)$ is a generic perturbation.*
Then the only first integrals which can be written as power series in ϵ are functions of H

$$F(H) = F(H_0 + \epsilon H_1 + \dots) = F(H_0) + \epsilon F'(H_0) H_1 + \dots$$

where $F \in \mathcal{C}^\infty(D \times \mathbb{T}^n)$, $F : D \times \mathbb{T}^n \to \mathbb{R}$ and we used Taylor expansion in the second passage.

Therefore, degenerate hamiltonian under non-generic perturbations might have extensions of their first integrals from the unperturbed case to the perturbed one. This is exactly the starting point of the theory developed by Dubrovin in [3] and in other articles, which regards hamiltonian systems in both cases of finite and infinite degrees of freedom. Luckily for us, Toda and FPU do not fulfil the hypothesis of Poincare's theorem, so we can hope to find extensions.

2 Dubrovin's theorem

Let's consider again a one-dimensional chain of N particles that interact pairwise with potential ϕ, function of the displacement between a particle and the next. If we agree to call $q_1, \ldots, q_N$ the positions of the particles and $p_1, \ldots, p_N$ their velocities, this system can be described by the hamiltonian

$$H(q,p) = \sum_{n=1}^{N} \left(\frac{p_n^2}{2} + \phi(q_{n+1} - q_n) \right) \tag{2.1}$$

that $\forall i = 1, \ldots, N$ yield the following equations of motion

$$\begin{cases} \dot{q_n} = \frac{\partial H(q_n,p_n)}{\partial p_n} = p_n \\ \dot{p_n} = -\frac{\partial H(q_n,p_n)}{\partial q_n} = \phi'(q_{n+1} - q_n) - \phi'(q_n - q_{n-1}) \end{cases}$$

We are interested in the case $N \to \infty$, for which we have the following

Proposition 2.1 (Extension to the continuum limit)**.** *The extension of 2.1 to the continuum limit $N \to \infty$ is given by*

$$\mathcal{H}(V,R) = \int \left[\frac{V^2}{2} + \phi(R) - \frac{h^2}{24} V_x^2 \right] dx + \mathcal{O}(h^4) \tag{2.2}$$

$$= \mathcal{H}_0(V,R) + h^2 \mathcal{H}_2(V,R) + \mathcal{O}(h^4) \tag{2.3}$$

where $h = 1/N$ is the perturbative parameter.

Proof. (sketch) The generating function

$$F(q,s) = \sum_{n=1}^{N} s_n (q_n - q_{n-1})$$

transforms 2.1 in

$$K(r,s) = \sum_{n=1}^{N} \left[\frac{(s_n - s_{n-1})^2}{2} + \phi(r_n) \right]$$

Being a canonical transformation, the Poisson tensor remains untouched and the new equations of motion are

$$\begin{cases} \dot{s_n} = \frac{\partial K(r,s)}{\partial r_n} = \phi'(r_n) \\ \dot{r_n} = -\frac{\partial K(r,s)}{\partial s_n} = (s_{n+1} - 2s_n + s_{n-1}) \end{cases}$$

Defining $h := \frac{1}{N}$, $x := hn$ and $\tau := ht$ we can interpolate s_n and r_n using two smooth functions R and S as follows:

$$\begin{cases} r_n(t) = R(x,\tau) \\ s_n(t) = \frac{S(x,\tau)}{h} \end{cases}$$

We are interested in the case of h small, so we can take advantage of Taylor expansion in order to change again the equations of motion. After some minor manipulations (see [3] or the appendix of [7] for further details) and after the last change of variables

$$\begin{cases} V(x,\tau) := S_x(x,\tau) \\ R(x,\tau) := R(x,\tau) \end{cases}$$

we finally obtain the hamiltonian we were looking for. □

We are now in the correct position to introduce the main theorem of this thesis, which concerns first integrals of $\mathcal{H}_0$ and their second-order extensions.

Theorem 2.1 (Dubrovin's Theorem)**.** *If in 2.2 the potential has the form*

$$\phi(R) = ke^{cR} + aR + b$$

where a, b, c, k are constants, one can find a second-order extension of the first integrals of $\mathcal{H}_0(V, R)$. These extensions are therefore approximated first integrals of $\mathcal{H}(V, R)$.

Proof. See Dubrovin's article [3]. □

This theorem immediately tells us that the first integrals of the Toda chain are extensible to the second order.

2.1 Extension

We have to introduce now some standard mathematical machinery used in the theory of hamiltonian PDEs.

Definition 2.1 (Poisson brackets)**.** *Given two functionals $F(V, R) = \int f dx$ and $G(V, R) = \int g dx$, their Poisson bracket is*

$$\{F, G\} = \int (\nabla_{L^2} F \mathbb{J}_2^* \nabla_{L^2} G) dx = \int \left[\frac{\delta F}{\delta R} \partial_x \frac{\delta G}{\delta V} + \frac{\delta F}{\delta V} \partial_x \frac{\delta G}{\delta R} \right]$$

where

$$\nabla_{L^2} f = \left(\frac{\delta f}{\delta V}, \frac{\delta f}{\delta R} \right) \qquad \mathbb{J}_2^* = \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix}$$

are respectively the L^2 gradient (a vector with functional derivatives as components) and the Poisson tensor in the coordinates (V, R).

Definition 2.2 (Euler-Lagrange operator)**.** *Given $f(u(x)) \in \mathcal{C}^\infty(D)$, where $D \subset \mathbb{R}$, the Euler-Lagrange operator is the operator that acts on f by the formula*

$$E_u f = \partial_u f - \partial_x \partial_{u_x} f + \partial_x^2 \partial_{u_{xx}} f + \dots$$

We want now to prove a simple result whose immediate corollary will be used throughout the thesis.

Proposition 2.2. *If $F[u] = \int f(u)dx$ is a functional, $F[u]$ is constant $\forall u$ iff $E_u f = 0$.*

Proof. $F[u] = \text{const}\ \forall u \iff \delta F[u] = 0\ \forall u$.
Now, we know that

$$\delta F[u] = \int E_u f(u) \delta u dx$$

so that

$$\delta F[u] = 0 \quad \forall u \iff \int E_u f(u) \delta u dx = 0 \quad \forall u \quad \forall \delta u$$

which means

$$\delta F[u] = 0 \iff E_u f = 0$$

□

Corollary 2.1. *Two local functionals $F = \int f dx$ and $G = \int g dx$ commute with respect to the Poisson bracket $\{F, G\}$ if and only if*

$$E_V \left(\frac{\delta F}{\delta R} \partial_x \frac{\delta G}{\delta V} + \frac{\delta F}{\delta V} \partial_x \frac{\delta G}{\delta R} \right) = 0$$
$$E_R \left(\frac{\delta F}{\delta R} \partial_x \frac{\delta G}{\delta V} + \frac{\delta F}{\delta V} \partial_x \frac{\delta G}{\delta R} \right) = 0$$

Let's consider now a modification of 2.2

$$\tilde{\mathcal{H}}(V,R) = \tilde{\mathcal{H}}_0(V,R) + h^2 \tilde{\mathcal{H}}_2(V,R) + \mathcal{O}(h^4) \tag{2.4}$$
$$= \int \left[\left(\frac{V^2}{2} + \phi(R) \right) + h^2 \left(\psi_1(R) - \frac{V_x^2}{24} \right) \right] dx + \mathcal{O}(h^4) \tag{2.5}$$

Notice that the only difference between this hamiltonian and 2.2 is the presence of $\psi_1(R)$ at the second order of perturbation. We take now into account a first integral $J_0(V,R) = \int j_0(V,R)dx$ of $\tilde{\mathcal{H}}_0(V,R)$ and we look for conditions on a functional

$$J_2(V,R) = \int j_2(R, V, R_x, V_x, R_{xx}, V_{xx}) dx$$

such that $J = J_0 + h^2 J_2 + \mathcal{O}(h^4)$ satisfies $\{J, \tilde{\mathcal{H}}\} = \mathcal{O}(h^4)$, i.e. it commutes with respect to $\tilde{\mathcal{H}}$ up to the second order. J is called the second-order extension of J_0. The density of J_2, up to a total x-derivative, can be written in the following form (see [3])

$$j_2 = \frac{1}{2}(a(V,R)R_x^2 + 2b(V,R)R_x V_x + c(V,R)V_x^2) + p(V,R)R_x + q(V,R)V_x + d(V,R) \tag{2.6}$$

At this point, we can state and prove the extension we were looking for.

Theorem 2.2 (Extended Dubrovin's theorem)**.** *If in 2.5 the potential has the form*

$$\phi(R) = ke^{cR} + aR + b$$

where a, b, c, k are constants, one can find a second-order extension of the first integrals of $\tilde{\mathcal{H}}_0(V, R)$. These extensions are therefore approximated first integrals of $\tilde{\mathcal{H}}(V, R)$. Moreover, if j_0 is the density of a first integral, the coefficients of 2.6 satisfy the following formulas

$$a(V, R) = -\frac{j_{0VVR}}{6}\frac{\phi''(R)^2}{\phi'''(R)} \qquad b(V, R) = -\frac{\phi''(R)^2 j_{03V}(V, R)}{6\phi'''(R)} \tag{2.7}$$

$$c(V, R) = -\frac{\phi''(R) j_{0VVR}(V, R)}{6\phi'''(R)} - \frac{1}{12} j_{0VV}(V, R) \tag{2.8}$$

$$p_V = q_R, \qquad d_{RR} = \phi''(R) d_{VV} + \psi_1''(R) j_{0VV} \tag{2.9}$$

Proof. (sketch) One starts by imposing that

$$\{J, \tilde{\mathcal{H}}\} = \{J_0, \tilde{\mathcal{H}}_0\} + h^2(\{J_2, \tilde{\mathcal{H}}_0\} + \{J_0, \tilde{\mathcal{H}}_2\}) = \mathcal{O}(h^4)$$

and recalling that $\{J_0, \tilde{\mathcal{H}}_0\} = 0$, one has to calculate the remaining terms. This can be done with the help of a computer software. We used Wolfram Mathematica and obtained the following functional

$$\begin{aligned}\{J, \tilde{\mathcal{H}}\} = h^2 \int \Big[&\frac{j_{0R}}{12} V_{xxx} + \frac{1}{2}(c_R - 2b_V)V_x^3 + \frac{\phi''(R)}{2}(a_V - 2b_R)R_x^3 - \frac{1}{2}(a_R + 2c_R\phi''(R))R_x^2 V_x \\ &- \frac{1}{2}(c_V\phi''(R) + 2a_V)R_x V_x^2 - aR_{xx}V_x - bV_{xx}V_x - b\phi''(R)R_{xx}R_x - c\phi''(R)V_{xx}R_x + \\ &+ (q_R - p_V)V_x^2 + \phi''(R)(p_V - q_R)R_x^2 + d_R V_x + (d_V\phi''(R) + j_{0V}\psi_1''(R))R_x \Big] dx + \mathcal{O}(h^4)\end{aligned}$$

Denoting I the integrand, we use Corollary 2.1 to transform the problem in the two equations

$$E_V I = 0 \qquad E_R I = 0$$

Checking term by term, one can find the equations that make the coefficients vanish, obtaining the formulas above. Finally, one recalls that j_0 is the density of a first integral, so it must satisfy

$$j_{0RR} = \phi''(R) j_{0VV}$$

and following the proof given by Dubrovin in [3], one arrives to the thesis. In [7] there are further details. □

Let us remark a few things:

- The equation $p_V = q_R$ tells us that p and q are linked together. Indeed, one can write

$$p(V,R) = \nu_R(V,R), \qquad q(V,R) = \nu_V(V,R) \Rightarrow \partial_x \nu(V,R) = pR_x + qV_x$$

  for some function $\nu(V,R)$, so that p and q are components of a gradient. This tells us that $pR_x + qV_x$ form a total x-derivative, which can be discarded from j_2 because its integral vanishes.

- Consider now equation 2.9 for d. This has two unknowns ($\psi_1(V,R)$ and $d(V,R)$), so one has to first fix $\psi_1(R)$ and then see if this equation admits a solution.

- We will use this theorem and the strong connection between Toda and FPU chains to extend first integrals of the former (which will be our unperturbed system) to approximated first integrals of the latter.

2.2 Harmonic oscillator case

Before moving towards FPU chain, we examine the special case of an harmonic oscillator to see what results we obtain. The potential this time reads

$$\phi(R) = \omega \frac{R^2}{2} \quad \Rightarrow \quad \phi'''(R) = 0 \tag{2.10}$$

Proposition 2.3. *The coefficients of 2.6 in this case satisfy the following formulas:*

$$a = \omega c + \frac{j_{0RR}}{12} \qquad b_V = c_R \qquad b_R = \omega c_V \qquad p_V = q_R \qquad d_{RR} = \omega d_{VV} + \frac{\gamma}{\omega}\psi_1''(R)$$

Proof. (sketch) We cannot immediately substitute 2.10 in the formulas we found when extending Dubrovin's theorem because, if we did, denominators would become zero. We have thus to recalculate the Poisson brackets:

$$\begin{aligned}\{J, \tilde{\mathcal{H}}\} = h^2(\{J_2, \tilde{\mathcal{H}}_0\} + \{J_0, \tilde{\mathcal{H}}_2\}) = h^2 \int \Bigg[& \frac{j_{0R}}{12} V_{3x} - bV_{xx}V_x - \omega b R_{xx}R_x - aR_{xx}V_x - \\ & - \omega c V_{xx} R_x - \frac{(\omega c_V + 2a_V)}{2} V_x^2 R_x - \frac{(a_R + 2\omega c_R)}{2} R_x^2 V_x + \frac{(c_R - 2b_V)}{2} V_x^3 + \\ & + \frac{\omega}{2}(a_V - 2b_R) R_x^3 + (q_R - p_V) V_x^2 + \omega(p_V - q_R) R_x^2 + d_R V_x + \\ & + (d_V \omega + j_{0V} \psi_1''(R)) R_x \Bigg] dx + \mathcal{O}(h^4)\end{aligned}$$

As before, we denote I the integrand and apply Corollary 2.1 to transform the problem in the two equations

$$E_R I = 0 \qquad E_V I = 0$$

from which one can obtain the formulas the coefficients must satisfy and also some constraints on j_0:

$$j_{03R} = j_{0RRV} = j_{02R2V} = 0$$

These yield (see [7]) that the unperturbed first integral must have the following form

$$J_0(R,V) = \int j_0(R,V)dx = \int \left[\frac{\gamma}{\omega}\left(\frac{V^2}{2} + \frac{\omega}{2}R^2\right) + \alpha VR + \beta R + \delta V + \lambda\right] dx$$

where α, β, γ, δ and λ are arbitrary constants. We can observe that this is simply a linear combination of first integrals: in fact, the first term is the unperturbed hamiltonian, whereas the other three are linked respectively to the translation symmetry, the total momentum and the length of the system. □

3 Fourth-order extension to FPU

In this section we want to see how the previous results can be applied to FPU chain in the continuum limit $N \to \infty$ and how we can build up a 4th-order extension of first integrals. We rely again on [7] to write the FPU hamiltonian in this case:

Proposition 3.1. *The FPU hamiltonian in the continuum case $N \to \infty$ is given by*

$$\begin{aligned}\mathcal{K}_{FPU}(V,R) = \int \Bigg[\left(\frac{V^2}{2} + \frac{1}{\epsilon}\phi_{Toda}(\sqrt{\epsilon}R) \right) + \left(\psi_1(R) - \frac{h^2}{24}V_x^2 \right) + \\ + \left(\psi_2(R) + \frac{h^4}{720}V_{xx}^2 \right) \Bigg] dx + \mathcal{O}(h^6) = \\ = \mathcal{K}_0(V,R) + \mathcal{K}_2(V,R) + \mathcal{K}_4(V,R) + \mathcal{O}(h^6)\end{aligned}$$

where $h = \frac{1}{N}$ and $\epsilon = \frac{E}{N}$ are respectively the perturbative coefficient and the specific energy of the chain and the potentials $\psi_i(R)$ are given by the formulas

$$\begin{cases} \psi_1(R) = 0 \\ \psi_2(R) = \epsilon\Delta\beta\frac{R^4}{4} \\ \psi_3(R) = \epsilon^{3/2}\Delta\gamma\frac{R^5}{5} \\ \qquad \dots \\ \psi_n(R) = \epsilon^{n/2}\Delta g_n\frac{R^{n+2}}{n+2} \end{cases}$$

where $\Delta\beta = (\beta - \beta_{Toda})$, $\Delta\gamma = (\gamma - \gamma_{Toda})$ etc..

Proof. (sketch) We start from the hamiltonian H_{FPU} seen in the introduction and we apply the same canonical transformation of proposition 2.1. Then we use the tangency between Toda and FPU chains to write

$$K_{FPU}(s,r) = K_{Toda}(s,r) + \sum_{n=1}^{N} \left(\Delta\beta\frac{r_n^4}{4} + \Delta\gamma\frac{r_n^5}{5} + \dots \right)$$

and, similarly as before, using h and ϵ we interpolate as follows:

$$\begin{cases} s_n(t) = \frac{\sqrt{\epsilon}}{h}S(\tau,x) \\ r_n(t) = \sqrt{\epsilon}R(\tau,x) \end{cases}$$

Now, the change of coordinates

$$\begin{cases} V(x,\tau) := S_x(x,\tau) \\ R(x,\tau) := R(x,\tau) \end{cases}$$

and minor manipulations (see [7]) lead to the hamiltonian $\mathcal{K}_{FPU}$, but we still need to find the potentials $\psi_n(R)$. To do this, first define $\Omega_\sigma = \{x \in \mathbb{C} | |Im(x)| \leq \sigma\}$ and for fixed τ^* call

$$v = \max_{\Omega_\sigma}\{|V(x,\tau^*)|, |R(x,\tau^*)|\}$$

then apply Cauchy estimates (see appendix A) to V, R and their derivatives:

$$|V| \leq v \qquad |V_x| \leq \frac{v}{\sigma} \qquad |V_{xx}| \leq C\frac{v}{\sigma^2} \qquad \dots \qquad |V^{(n)}| \leq C\frac{v}{\sigma^n}$$

For consistency, potentials must satisfy the following estimates

$$\psi_n(R) \leq C\frac{h^{2n}}{\sigma^{2n}}v^2$$

and we recall that from Korteweg de-Vries equation studied in [1] we must have

$$\sigma \leq \frac{h}{\epsilon^{1/4}}C$$

We conjecture now $\psi_i(R)$ are given by the formulas

$$\begin{cases} \psi_1(R) = 0 \\ \psi_2(R) = \epsilon\Delta\beta\frac{R^4}{4} \\ \psi_3(R) = \epsilon^{3/2}\Delta\gamma\frac{R^5}{5} \\ \qquad \dots \\ \psi_n(R) = \epsilon^{n/2}\Delta g_n\frac{R^{n+2}}{n+2} \end{cases}$$

This hypothesis is immediately proved correct because

$$\psi_n(R) = \epsilon^{n/2}\Delta g_n\frac{R^{n+2}}{n+2} \leq \frac{h^{2n}}{\sigma^{2n}}v^2C \quad \Rightarrow \quad \sigma \leq \frac{h}{\epsilon^{1/4}}C$$

and this concludes the proof. □

Let's now move on and let us truncate $\mathcal{K}_{FPU}$ to the second order

$$\mathcal{K}_{FPU}(V,R) = \int\left[\left(\frac{V^2}{2} + \frac{1}{\epsilon}\phi_{Toda}(\sqrt{\epsilon}R) - \frac{h^2}{24}V_x^2\right)\right]dx + \mathcal{O}(h^4)$$

ϵ is not a perturbative parameter and it can assume any positive value without affecting our results. Therefore we set $\epsilon = \frac{1}{4\alpha^2}$ which gives $2\alpha\sqrt{\epsilon} = 1$ and

$$\frac{1}{\epsilon}\phi_{Toda}(\sqrt{\epsilon}R) = \frac{e^{2\alpha\sqrt{\epsilon}R} - 2\alpha\sqrt{\epsilon}R - 1}{4\alpha^2\epsilon} = e^R - R - 1$$

$\mathcal{K}_{FPU}$ has the exact shape that is needed in the extension of Dubrovin's theorem. We can thus apply the formulas given above to a density j_0 of a Toda's first integral to obtain its second-order extension

$$\begin{aligned} j_2(V,R) = &-\frac{1}{6}e^R R_x V_x j_{03V}(V,R) - \frac{1}{12}e^R R_x^2 j_{0VVR}(V,R) - \frac{1}{24}V_x^2 j_{0VV}(V,R) \\ &- \frac{1}{12}V_x^2 j_{0VVR}(V,R) \end{aligned} \tag{3.1}$$

In this section, we look for conditions on a density

$$\begin{aligned} j_4 = &\alpha R_{xx}^2 + \beta R_{xx}V_{xx} + \gamma V_{xx}^2 + \delta R_{xx}V_x^2 + \epsilon R_x^2 V_{xx} + \mu R_x^4 + \nu R_x V_x^3 + \rho R_x^2 V_x^2 + \lambda R_x^3 V_x \\ &+ \omega V_x^4 + \frac{1}{2}\eta R_x^2 + \xi R_x V_x + \frac{1}{2}\zeta V_x^2 + \sigma; \end{aligned}$$

so that

$$\begin{aligned} J(V,R) = &J_0(V,R) + h^2 J_2(V,R) + h^4 J_4(V,R) = \\ &= \int \left[j_0(V,R) + h^2 j_2(V,R,V_x,R_x) + h^4 j_4(V,R,V_x,R_x,V_{xx},R_{xx}) \right] dx \end{aligned}$$

gives $\{J, \mathcal{K}_{FPU}\} = \mathcal{O}(h^6)$.

Theorem 3.1 (4th-order expansion). *Given the hamiltonian $\mathcal{K}_{FPU}$ and a first integral $J_0 = \int j_0 dx$ of the Toda chain, one can find an extension to the fourth order that satisfies $\{J, \mathcal{K}_{FPU}\} = \mathcal{O}(h^6)$. Moreover, the coefficients of j_4 satisfy the following formulas*

$$\begin{aligned} &\alpha = \frac{1}{120}e^{2R} j_{04V} - \frac{1}{720}e^R j_{0VVR}; \qquad \beta = \frac{1}{120}e^R j_{03V} + \frac{1}{60}e^R j_{03VR}; \\ &\gamma = \frac{1}{720}j_{0VV} + \frac{1}{180}j_{0VVR} + \frac{1}{120}e^R j_{04V}; \qquad \delta = \frac{j_{0VVR}}{1440} - \frac{1}{180}e^R j_{04V}; \\ &\epsilon = \frac{1}{120}e^R j_{03V} + \frac{1}{72}e^R j_{03VR}; \qquad \lambda = \frac{1}{540}e^R j_{03VR} - \frac{14e^{2R} j_{05V}}{2160} - \frac{1}{216}e^{2R} j_{05VR}; \\ &\mu = \frac{e^R j_{0VVR}}{2160} - \frac{1}{360}e^{2R} j_{04V} - \frac{17e^{2R} j_{04VR}}{4320} - \frac{1}{864}e^{3R} j_{06V}; \\ &\nu = -\frac{j_{03VR}}{1440} - \frac{1}{144}e^R j_{05V} - \frac{1}{216}e^R j_{05VR}; \qquad \rho = -\frac{7e^R j_{04V}}{1440} - \frac{1}{160}e^R j_{04VR} - \frac{1}{144}e^{2R} j_{06V}; \\ &\omega = -\frac{j_{04V}}{5760} - \frac{1}{864}e^R j_{06V} - \frac{j_{04VR}}{1080}; \qquad \eta = 0; \qquad \xi = 0; \qquad \zeta = 0; \end{aligned}$$

$\sigma_{RR} = \sigma_{VV} e^R + 3 j_{0VV} \Delta\beta R^2$

so that we end up with the density

$$j_4 = \alpha R_{xx}^2 + \beta R_{xx}V_{xx} + \gamma V_{xx}^2 + \delta R_{xx}V_x^2 + \epsilon R_x^2 V_{xx} + \mu R_x^4 + \nu R_x V_x^3 + \rho R_x^2 V_x^2 + \tag{3.2}$$

$$+ \lambda R_x^3 V_x + \omega V_x^4 + \sigma \tag{3.3}$$

Proof. (sketch) Similarly to the second-order extension, one has first to compute the Poisson brackets

$$\{J, \mathcal{K}_{FPU}\} = \{J_0, \mathcal{K}_0\} + h^2(\{J_2, \mathcal{K}_0\} + \{J_0, \mathcal{K}_2\}) + h^4(\{J_0, \mathcal{K}_4\} + \{J_2, \mathcal{K}_2\} + \{J_4, \mathcal{K}_0\})$$

and recalling that $\{J_0, \mathcal{K}_0\} = 0$ and that $h^2(\{J_2, \mathcal{K}_0\} + \{J_0, \mathcal{K}_2\}) = \mathcal{O}(h^4)$, one has only to compute its 4-th order term and to impose

$$\{J, \mathcal{K}_{FPU}\} = h^4(\{J_0, \mathcal{K}_4\} + \{J_2, \mathcal{K}_2\} + \{J_4, \mathcal{K}_0\}) = \mathcal{O}(h^6)$$

obtaining

$$\begin{aligned}
\{J, \mathcal{K}_{FPU}\} = h^4 \int \Bigg[& \frac{j_{0R}}{360} V_{5x} + (\beta V_x + 2\gamma R_x \phi''_{Toda}) V_{4x} + (2\alpha V_x + \beta \phi''_{Toda} R_x) R_{4x} - \frac{a}{12} V_{3x} R_{xx} - \\
& - \frac{b}{12} V_{xxx} V_{xx} + \left(4\gamma_R \phi''_{Toda} - \frac{a_R}{24}\right) V_{xxx} R_x^2 + \left(4\gamma_V \phi''_{Toda} + 2\beta_R - 2\epsilon - \frac{a_V}{12}\right) V_{xxx} R_x V_x + \\
& + \left(2\delta + 2\beta_V + \frac{c_R}{24} - \frac{b_V}{12}\right) V_{xxx} V_x^2 + 4\alpha_V R_{xxx} V_x^2 + (2\beta_V \phi''_{Toda} - 2\delta \phi''_{Toda} + 4\alpha_R) R_{xxx} R_x V_x + \\
& + (2\epsilon \phi''_{Toda} + 2\beta_R \phi''_{Toda}) R_{xxx} R_x^2 + (2\alpha_V + 2\beta_R - 2\epsilon) V_{xx} R_{xx} V_x + \\
& + \phi''_{Toda}(2\beta_V + 2\gamma_R - 2\delta) V_{xx} R_{xx} R_x + (5\delta_V + \beta_{VV} - 3\nu) V_{xx} V_x^3 + \\
& + (4\gamma_{RV} \phi''_{Toda} + \beta_{RR} - \epsilon_R - 3\lambda - 6\nu \phi''_{Toda}) V_{xx} R_x^2 V_x + \\
& + (2\gamma_{VV} \phi''_{Toda} + 4\delta_R + 2\beta_{RV} - 4\rho - 12\omega \phi''_{Toda} - 2\epsilon_V) V_{xx} R_x^2 V_x + \\
& + 2\phi''_{Toda}(\gamma_{RR} + \epsilon_V - \rho) V_{xx} R_x^3 + \phi''_{Toda}(\beta_{RR} + 5\epsilon_R - 3\lambda) R_{xx} R_x^3 + (2\delta_R + 2\alpha_{VV} - 2\rho) R_{xx} V_x^3 + \\
& + (2\delta + \gamma_R + \beta_V) V_{xx}^2 V_x + 3\gamma_V \phi''_{Toda} V_{xx}^2 R_x + \phi''_{Toda}(2\epsilon + \alpha_V + \beta_R) R_{xx}^2 R_x + 3\alpha_R R_{xx}^2 V_x + \\
& + (\beta_{VV} \phi''_{Toda} - \delta_V \phi''_{Toda} - 3\nu - 6\lambda + 4\alpha_{RV}) R_{xx} R_x V_x^2 + \\
& + (4\epsilon_V \phi''_{Toda} + 2\beta_{RV} \phi''_{Toda} - 2\delta_R \phi''_{Toda} - 4\rho \phi''_{Toda} + 4\alpha_{RR} - 12\mu) R_{xx} R_x^2 V_x + \\
& + (\delta_{VV} - \nu_V + \omega_R) V_x^5 + (2\delta_{RV} - 2\rho_V - 3\omega_V \phi''_{Toda}) V_x^4 R_x + \\
& + (\delta_{RR} - 3\lambda_V - 2\nu_V \phi''_{Toda} - \rho_R - 4\omega_R \phi''_{Toda}) V_x^3 R_x^2 + \\
& + (\epsilon_{VV} \phi''_{Toda} - 3\nu_R \phi''_{Toda} - \rho_R \phi''_{Toda} - 2\lambda_R - 4\mu_V) V_x^2 R_x^3 + (2\epsilon_{RV} \phi''_{Toda} - 2\rho_R \phi''_{Toda} - 3\mu_R) V_x R_x^4 + \\
& + (\mu_V \phi''_{Toda} - \lambda_R \phi''_{Toda} + \epsilon_{RR} \phi''_{Toda}) R_x^5 + \frac{\phi''_{Toda}}{2}(\eta_V - 2\xi_R) R_x^3 - \frac{1}{2}(\eta_R + 2\zeta_R \phi''_{Toda}) R_x^2 V_x \\
& - \frac{1}{2}(\zeta_V \phi''_{Toda} + 2\eta_V) R_x V_x^2 + \frac{1}{2}(\zeta_R - 2\xi_V) V_x^3 - \xi \phi''_{Toda} R_{xx} R_x - \xi V_{xx} V_x - \zeta \phi''_{Toda} V_{xx} R_x \\
& - \eta R_{xx} V_x + \sigma_R V_x + (\sigma_V \phi''_{Toda} + 3 j_{0V} \Delta\beta R^2) R_x \Bigg] dx + \mathcal{O}(h^6)
\end{aligned}$$

One calls I the integrand (which can be calculated via computer software) and uses the Corollary 2.1 to transform the problem in the two equations

$$E_R I = 0 \qquad E_V I = 0$$

from which one can obtain the equations that make the coefficient of j_4 vanish. These formulas are correct because they also appear in the fourth-order Toda hierarchy (see [2]). As mentioned previously, in [7] one can find more details on the calculations. □

3.1 Explicit extension and conjecture

In this subsection we will see the explicit extension of $j_0^{(2)}$, $j_0^{(3)}$ and $j_0^{(4)}$ and we will also describe the conjecture we will try to solve.
The two most important PDEs we have seen so far are

$$j_{0RR} = e^R j_{0VV} \tag{3.4}$$

$$\sigma_{RR} = \sigma_{VV} e^R + 3 j_{0VVV} \Delta\beta R^2 \tag{3.5}$$

The first gives us the first integrals $j_0^{(n)}$ of the Toda chain, which are equivalent to the continuum-limit extension of Henon's first integrals up to a multiplicative constant. See [6] for their definition in the case of finite N and appendix C for their extension and equivalence. The first five $j_0^{(n)}$ are

$$\begin{aligned}
j_0^{(2)} &= \frac{V^2}{2} + e^R \\
j_0^{(3)} &= \frac{V^3}{6} + V e^R \\
j_0^{(4)} &= \frac{V^4}{6} + 2V^2 e^R + e^{2R} \\
j_0^{(5)} &= \frac{V^5}{30} + \frac{2}{3} V^3 e^R + V e^{2R} \\
&\vdots
\end{aligned}$$

More generic formulas (separately for even n and odd n) are

$$j_0^{(2n)} = \sum_{l=0}^{n} C_n^l V^{2(n-l)} e^{lR}, \qquad j_0^{(2n+1)} = \sum_{l=0}^{n} B_n^l V^{2(n-l)+1} e^{lR}$$

where the coefficients are given by

$$C_n^l = \begin{cases} \frac{\prod_{m=l+1}^{n} m^2}{[2(n-l)]!} & \text{for } l = 0, \dots, n-1 \\ 1 & \text{for } l = n \end{cases} \qquad B_n^l = \begin{cases} \frac{\prod_{m=l+1}^{n} m^2}{[2(n-l)+1]!} & \text{for } l = 0, \dots, n-1 \\ 1 & \text{for } l = n \end{cases}$$

The second PDE allows us to fully describe j_4 and it is non-homogeneous, so the solutions must have the form $\sigma = \sigma_0 + \sigma_p$, where σ_0 is a solution of the homogeneous PDE $\sigma_{RR} = e^R \sigma_{VV}$ (i.e. a first integral) and σ_p is a particular solution of the entire PDE.

Proposition 3.2 (Extensions of $j_0^{(2)}$, $j_0^{(3)}$ and $j_0^{(4)}$)**.** *The 4-th order extensions of* $j_0^{(2)}$, $j_0^{(3)}$ *and* $j_0^{(4)}$ *to the FPU chain are given by the formulas*

$$
\begin{aligned}
j^{(2)} &= \frac{V^2}{2} + e^R - h^2\frac{1}{24}V_x^2 + h^4\left(\frac{\Delta\beta R^4}{4} + \frac{1}{720}V_{xx}^2\right)\\
j^{(3)} &= j_0^{(3)} + h^2\left(-\frac{1}{6}e^R R_x V_x - \frac{1}{24}VV_x^2\right) +\\
&\quad + h^4\left(\frac{1}{4}\Delta\beta R^4 V + \frac{1}{120}e^R R_{xx}V_{xx} + \frac{1}{120}e^R R_x^2 V_{xx} + \frac{1}{720}VV_{xx}^2\right)\\
j^{(4)} &= j_0^{(4)} + h^2\left(-\frac{2}{3}e^R V R_x V_x - \frac{1}{3}e^{2R}R_x^2 - \frac{1}{3}e^R V_x^2 - \frac{1}{24}\left(4e^R + 2V^2\right)V_x^2\right) +\\
&\quad + h^4\Bigg(\sigma(V,R) + \frac{1}{30}e^R V R_{xx}V_{xx} - \frac{7}{360}e^R R_{xx}V_x^2 + \frac{1}{36}e^{2R}R_{xx}^2 + \frac{1}{30}e^R V R_x^2 V_{xx}\\
&\quad - \frac{7}{360}e^R R_x^2 V_x^2 - \frac{1}{108}e^{2R}R_x^4 + \left(\frac{1}{720}\left(4e^R + 2V^2\right) + \frac{e^R}{18}\right)V_{xx}^2 - \frac{V_x^4}{1440}\Bigg)
\end{aligned}
$$

where $\sigma(V,R)$ *satisfies equation 3.5.*

Proof. We only need to find a suitable σ for the 4th-order extension, because the other terms have already been found previously. Let's see the first two extensions in detail:

- $j_0^{(2)}$: in this case the PDE reads

$$\sigma_{RR} = e^R\sigma_{VV} + 3\Delta\beta R^2$$

  This is solved setting $\sigma_0 = j_0^{(2)}$ and $\sigma_p = \frac{\Delta\beta}{4}R^4$, which is trivially a particular solution of the PDE. We have proved in another way that the extension of the unperturbed hamiltonian is, obviously, the perturbed hamiltonian.

- $j_0^{(3)}$:

$$\sigma_{RR} = e^R\sigma_{VV} + 3\Delta\beta V R^2$$

  Here we can simply set $\sigma_0 = j_0^{(3)}$ and $\sigma_p = \frac{\Delta\beta}{4}VR^4$.

- $j_0^{(4)}$ (sketch): in order to extend it, we have to solve

$$\sigma_{RR} = e^R\sigma_{VV} + 3\Delta\beta(2V^2 + 4e^R)R^2$$

  For this purpose we conjecture (ansatz) that a particular solution for equation 3.5 has the following form

$$\sigma_p = \Delta\beta[R^4P_2(V,e^R) + R^3P_3(V,e^R) + R^2P_4(V,e^R) + RP_5(V,e^R) + P_6(V,e^R)]$$

where the subscript indicates the maximum degree the polynomial can have. These are polynomials in which R appears only as e^R. With this ansatz, instead of solving the PDE we have now to solve the simpler system given by the 5 PDEs

$$\begin{cases} \partial_R^2 P_2 = e^R \partial_V^2 P_2 \\ 8\partial_R P_2 + \partial_R^2 P_3 = e^R \partial_V^2 P_3 \\ 12P_2 + 6\partial_R P_3 + \partial_R^2 P_4 = 3j_{0VV}^{(4)} + e^R \partial_V^2 P_4 \\ 6P_3 + 4\partial_R P_4 + \partial_R^2 P_5 = e^R \partial_V^2 P_5 \\ 2P_4 + 2\partial_R P_5 + \partial_R^2 P_6 = e^R \partial_V^2 P_6 \end{cases}$$

The first one gives simply $P_2 = j_0^{(2)}$, whereas the other four PDEs are non-homogeneous, thus they follow the same solution pattern described above. In the end we obtain (see [7])

$$P_2 = \frac{V^2}{2} + X \qquad P_3 = -8X \qquad P_4 = 48X \qquad P_5 = cj_0^{(5)} - 144X$$
$$P_6 = 192X + c\left(\frac{V^5}{15} - VX^2\right)$$

where c is a free parameter and we have set $X = e^R$.

□

We can now state the conjecture (contained in [7]) that we will try to solve. As mentioned above, its proof will be the core of our thesis.

Conjecture 3.1. *Every $j_0^{(n)}$ can be extended to be an approximated first integral of FPU chain up to the fourth order with σ_p that has the following form*

$$\sigma_p = \Delta\beta[R^4 P_{n-2}(V, e^R) + R^3 P_{n-1}(V, e^R) + R^2 P_n(V, e^R) + RP_{n+1}(V, e^R) + P_{n+2}(V, e^R)]$$

and where the polynomials are solutions of the following system of PDEs

$$\begin{cases} \partial_R^2 P_{n-2} = e^R \partial_V^2 P_{n-2} \\ 8\partial_R P_{n-2} + \partial_R^2 P_{n-1} = e^R \partial_V^2 P_{n-1} \\ 12P_{n-2} + 6\partial_R P_{n-1} + \partial_R^2 P_n = 3j_{0VV}^{(n)} + e^R \partial_V^2 P_n \\ 6P_{n-1} + 4\partial_R P_n + \partial_R^2 P_{n+1} = e^R \partial_V^2 P_{n+1} \\ 2P_n + 2\partial_R P_{n+1} + \partial_R^2 P_{n+2} = e^R \partial_V^2 P_{n+2} \end{cases} \tag{3.6}$$

4 Proof of conjecture

As a first attempt we tried to find solutions via induction, but we found the following:

Remark (Polynomials' dependency upon n) The polynomials that make up the system depend on the particular $j_0^{(n)}$ one is extending.

Proof. By contradiction, if we suppose induction is working, then the polynomials that make up 3.6 for n are known and they are also involved in the system for $n+1$:

$$\begin{cases} \partial_R^2 P_{n-1} = e^R \partial_V^2 P_{n-1} \\ 8\partial_R P_{n-1} + \partial_R^2 P_n = e^R \partial_V^2 P_n \\ 12 P_{n-1} + 6\partial_R P_n + \partial_R^2 P_{n+1} = 3 j_{0VV}^{(n+1)} + e^R \partial_V^2 P_{n+1} \\ 6P_n + 4\partial_R P_{n+1} + \partial_R^2 P_{n+2} = e^R \partial_V^2 P_{n+2} \\ 2P_{n+1} + 2\partial_R P_{n+2} + \partial_R^2 P_{n+3} = e^R \partial_V^2 P_{n+3} \end{cases}$$

From this we can observe that P_{n-1} solves both the second PDE for n and the first for $n+1$, so we have

$$8\partial_R P_{n-2} = e^R \partial_V^2 P_{n-1} - \partial_R^2 P_{n-1} = 0$$

and this tells us P_{n-2} must not depend on R. Moreover, we know that P_{n-2} solves the first PDE for n:

$$\partial_R^2 P_{n-2} = e^R \partial_V^2 P_{n-2} = 0 \quad \Rightarrow \quad \partial_V^2 P_{n-2} = 0 \quad \Rightarrow \quad P_{n-2} = aV + b$$

so our polynomial must have a specific form and must not depend on R, and it also has to be a first integral of Toda chain of degree $n-2$. This is possible just for $n=3$, where $P_1 = V$, and not $\forall n$, so we found an absurd. $\square$

This proposition tells us the polynomials are not "fixed" as we change first integral and suggests we should write a superscript $P_i^{(n)}$ to indicate this dependency, but we will not do it to avoid heavier notation. Also, there will never be confusion about the first integral we are extending, because we will never have to study a simultaneous extension of two of them.

Let's move on now and let us rewrite the system of PDEs using $X = e^R$ and the operator ∂_X instead of R and ∂_R:

$$X = e^R \quad \Rightarrow \quad \partial_R = \frac{\partial X}{\partial R}\partial_X \quad \Rightarrow \quad \partial_R = X\partial_X \quad \Rightarrow \quad \partial_R^2 = X\partial_X + X^2\partial_X^2$$
$$\Rightarrow \quad \partial_R^2 - e^R\partial_V^2 = X\partial_X + X^2\partial_X^2 - X\partial_V^2$$

We can then write

$$\begin{cases}(X\partial_X + X^2\partial_X^2)P_{n-2} = X\partial_V^2 P_{n-2}\\ 8X\partial_X P_{n-2} + (X\partial_X + X^2\partial_X^2)P_{n-1} = X\partial_V^2 P_{n-1}\\ 12P_{n-2} + 6X\partial_X P_{n-1} + (X\partial_X + X^2\partial_X^2)P_n = 3j_{0VV}^{(n)} + X\partial_V^2 P_n\\ 6P_{n-1} + 4X\partial_X P_n + (X\partial_X + X^2\partial_X^2)P_{n+1} = X\partial_V^2 P_{n+1}\\ 2P_n + 2X\partial_X P_{n+1} + (X\partial_X + X^2\partial_X^2)P_{n+2} = X\partial_V^2 P_{n+2}\end{cases}$$

and with few modifications we obtain

$$\begin{cases}(X\partial_X + X^2\partial_X^2 - X\partial_V^2)P_{n-2} = 0\\ (X\partial_X + X^2\partial_X^2 - X\partial_V^2)P_{n-1} = -8X\partial_X P_{n-2}\\ (X\partial_X + X^2\partial_X^2 - X\partial_V^2)P_n = -12P_{n-2} - 6X\partial_X P_{n-1} + 3j_{0VV}^{(n)}\\ (X\partial_X + X^2\partial_X^2 - X\partial_V^2)P_{n+1} = -6P_{n-1} - 4X\partial_X P_n\\ (X\partial_X + X^2\partial_X^2 - X\partial_V^2)P_{n+2} = -2P_n - 2X\partial_X P_{n+1}\end{cases} \tag{4.1}$$

which shows immediately how the 5 PDEs have similar shapes: they all share the same operator on the left-hand side and differ just for the non-homogeneous term on the right-hand side. Moreover, we already know the general solution of the first PDE:

$$P_{n-2} = j_0^{(n-2)} = \begin{cases}\sum_{l=0}^{\frac{n}{2}-1} C^l_{\frac{n}{2}-1} V^{2(\frac{n}{2}-1-l)} X^l & \text{if even n}\\ \sum_{l=0}^{\frac{n-3}{2}} B^l_{\frac{n-3}{2}} V^{2(\frac{n-3}{2}-l)+1} X^l & \text{if odd n}\end{cases}$$

so we only need to solve the other four. We recall that the system concerns polynomials in X and V that can be written in all generality as

$$A = \sum_{i,j=0}^{m} a_{ij} V^i X^j$$

where a_{ij} are simply constant coefficients. Setting proper degrees, our main ansatz for the polynomials will be

$$P_{n-2} = j_0^{(n-2)} \qquad P_{n-1} = \sum_{i,j=0}^{n-1} p_{ij} V^i X^j \qquad P_n = \sum_{i,j=0}^{n} q_{ij} V^i X^j$$
$$P_{n+1} = \sum_{i,j=0}^{n+1} r_{ij} V^i X^j \qquad P_{n+2} = \sum_{i,j=0}^{n+2} s_{ij} V^i X^j$$

We can now state the main result found in this thesis

Theorem 4.1 (Proof of conjecture 3.1)**.** *The system of PDEs admits a particular solution* $\forall n \in \mathbb{N}$ *that has the following form*

- *If even* n

$$P_{n-2} = \frac{n^2}{16} j_0^{(n-2)} = \frac{n^2}{16} \sum_{l=0}^{\frac{n}{2}-1} C^l_{\frac{n}{2}-1} V^{2(\frac{n}{2}-1-l)} X^l$$

$$P_{n-1} = \sum_{m=2}^{\frac{n}{2}} p_{n-2m,m-1} V^{n-2m} X^{m-1} \qquad P_n = \sum_{m=2}^{\frac{n}{2}} q_{n-2m,m-1} V^{n-2m} X^{m-1}$$

$$P_{n+1} = \sum_{m=1}^{\frac{n}{2}} r_{n-2m,m-1} V^{n-2m} X^{m-1} \qquad P_{n+2} = \sum_{m=1}^{\frac{n}{2}} s_{n-2m,m-1} V^{n-2m} X^{m-1}$$

- *If odd* n

$$P_{n-2} = \frac{(n-1)^2}{16} j_0^{(n-2)} = \frac{(n-1)^2}{16} \sum_{l=0}^{\frac{n-3}{2}} B^l_{\frac{n-3}{2}} V^{2(\frac{n-3}{2}-l)+1} X^l$$

$$P_{n-1} = \sum_{m=2}^{\frac{n-3}{2}+1} p_{n-2m,m-1} V^{n-2m} X^{m-1} \qquad P_n = \sum_{m=2}^{\frac{n-3}{2}+1} q_{n-2m,m-1} V^{n-2m} X^{m-1}$$

$$P_{n+1} = \sum_{m=1}^{\frac{n-3}{2}+1} r_{n-2m,m-1} V^{n-2m} X^{m-1} \qquad P_{n+2} = \sum_{m=1}^{\frac{n-3}{2}+1} s_{n-2m,m-1} V^{n-2m} X^{m-1}$$

and the coefficients that make up the polynomials are given by the following recursive formulas on m*:*

- P_{n-1}

$$p_{n-2(m+1),m} = -\frac{n^2}{2m} C^m_{\frac{n}{2}-1} + \frac{(n-2m)(n-2m-1)}{m^2} p_{n-2m,m-1} \qquad \textit{if even } n$$

$$p_{n-2(m+1),m} = -\frac{(n-1)^2}{2m} B^m_{\frac{n-3}{2}} + \frac{(n-2m)(n-2m-1)}{m^2} p_{n-2m,m-1} \qquad \textit{if odd } n$$

and $p_{n-2,0} = 0$ *as boundary condition.*

- P_n

$$q_{n-2(m+1),m} = -\frac{6}{m} p_{n-2(m+1),m} + \frac{(n-2m)(n-2m-1)}{m^2} q_{n-2m,m-1}$$

and $q_{n-2,0} = 0$ *as boundary condition.*

- P_{n+1}

$$r_{n-2(m+1),m} = -\frac{6}{m^2} p_{n-2(m+1),m} - \frac{4}{m} q_{n-2(m+1),m} + \frac{(n-2m)(n-2m-1)}{m^2} r_{n-2m,m-1}$$

- P_{n+2}

$$s_{n-2(m+1),m} = -\frac{2}{m^2} q_{n-2(m+1),m} - \frac{2}{m} r_{n-2(m+1),m} + \frac{(n-2m)(n-2m-1)}{m^2} s_{n-2m,m-1}$$

In the even case $m = 1, \dots, \frac{n}{2} - 1$ and $n \geq 4$, whereas in the odd case $m = 1, \dots, \frac{n-3}{2}$ and $n \geq 5$.

Proof. For the sake of simplicity, we will suppose even n, the case of odd n being analogous, with differences just in the sums and indexes extremes.

- **Second PDE**. We use the ansatz made above for P_{n-2} and P_{n-1}. We also use $\frac{n^2}{16}$ as a multiplicative constant for P_{n-2}. Its utility will become clear further on. Now, the action of the operator $X\partial_X + X^2\partial_X^2 - X\partial_V^2$ on a monomyal V^iX^j gives

$$(X\partial_X + X^2\partial_X^2 - X\partial_V^2)(V^iX^j) = j^2V^iX^j - i(i-1)V^{i-2}X^{j+1}$$

and coefficients are just carried through the calculations undisturbed. With some similar manipulation we obtain that the PDE becomes

$$\sum_{i,j=0}^{n-1} \left(j^2V^iX^j - i(i-1)V^{i-2}X^{j+1}\right) p_{ij} = -\frac{n^2}{2} \sum_{l=1}^{\frac{n}{2}-1} C^l_{\frac{n}{2}-1} l V^{2(\frac{n}{2}-1-l)} X^l =$$
$$= -\frac{n^2}{2} C^1_{\frac{n}{2}-1} V^{n-4}X - n^2 C^2_{\frac{n}{2}-1} V^{n-6}X^2 + \cdots - \frac{n^2}{2}\left(\frac{n}{2} - 1\right) X^{\frac{n}{2}-1}$$

The first term of the right-hand side has $V^{n-4}X$ and it must be balanced by analogous monomials in the left-hand side. If we take a look at this, we see that this is possible if we choose $(i,j) = (n-4, 1)$ for the first term and $(i,j) = (n-2, 0)$ for the second. This means we have the equation

$$p_{n-4,1}V^{n-4}X - (n-2)(n-3)p_{n-2,0}V^{n-4}X = -\frac{n^2}{2} C^1_{\frac{n}{2}-1} V^{n-4}X$$
$$\Rightarrow \quad p_{n-4,1} - (n-2)(n-3)p_{n-2,0} = -\frac{n^2}{2} C^1_{\frac{n}{2}-1}$$

The same reasoning applied to the second term of the right-hand side

$$-n^2 C^2_{\frac{n}{2}-1} V^{n-6} X^2$$

tells us that we have to choose $p_{n-6,2}$ and $p_{n-4,1}$ in the left-hand side, so that we obtain the equation

$$\begin{aligned}4p_{n-6,2}V^{n-6}X^2 - (n-4)(n-5)p_{n-4,1}V^{n-6}X^2 &= -n^2C^2_{\frac{n}{2}-1}V^{n-6}X^2\\ \Rightarrow \quad 4p_{n-6,2} - (n-4)(n-5)p_{n-4,1} &= -n^2C^2_{\frac{n}{2}-1}\end{aligned}$$

We can now repeat the procedure for every term of the right-hand side, obtaining for $m = 1, \dots, \frac{n}{2} - 1$

$$\begin{aligned}m^2p_{n-2(m+1),m} - (n-2m)(n-2m-1)p_{n-2m,m-1} &= -\frac{n^2}{2}mC^m_{\frac{n}{2}-1}\\ \Rightarrow \quad p_{n-2(m+1),m} &= -\frac{n^2}{2m}C^m_{\frac{n}{2}-1} + \frac{(n-2m)(n-2m-1)}{m^2}p_{n-2m,m-1}\end{aligned}$$

This is a recursive formula that gives a coefficient when the previous is known. The ones not involved in the recursion can be set to zero and we will see that the fourth PDE will provide us the equation $p_{n-2,0} = 0$, so that coefficients are always known $\forall n \in \mathbb{N}$ without arbitrariness. In the end we can write

$$P_{n-1} = \sum_{m=2}^{\frac{n}{2}} p_{n-2m,m-1}V^{n-2m}X^{m-1}$$

- **Third PDE**. We have to use the ansatz for P_{n-2} and the formula just written for P_{n-1}. At this point we can see why we introduced $\frac{n^2}{16}$: thanks to this coefficient $-12P_{n-2}$ becomes exactly equal to $3j^{(n)}_{0VV}$, thus the non-homogeneous part simplifies and we are left just with $-6X\partial_X P_{n-1}$. Without this coefficient the terms cancel out only for $n = 4$ and $n = 5$, so that it becomes impossible to solve the system for $n > 5$ because of spurious monomials. At the end the PDE becomes

$$\sum_{i,j=0}^{n} \left(j^2V^iX^j - i(i-1)V^{i-2}X^{j+1}\right)q_{ij} = -6\sum_{m=1}^{\frac{n}{2}-1} p_{n-2(m+1),m}mV^{n-2(m+1)}X^m$$

At this point we repeat the procedure above: we take every term of the right-hand side and we balance it with proper monomyals coming from the left-hand side, obtaining the recursive formula

$$q_{n-2(m+1),m} = -\frac{6}{m}p_{n-2(m+1),m} + \frac{(n-2m)(n-2m-1)}{m^2}q_{n-2m,m-1}$$

Here again we will see that the fifth PDE will provide us $q_{n-2,0} = 0$, so that the coefficients are always fixed $\forall n \in \mathbb{N}$ without external arbitrariness and we can use them to construct the polynomial

$$P_n = \sum_{m=2}^{\frac{n}{2}} q_{n-2m,m-1}V^{n-2m}X^{m-1}$$

- **Fourth PDE**. The non-homogeneous term this time is $-6P_{n-1} - 4X\partial_X P_n$. If we substitute the ansatz and we manipulate it, it becomes

$$-6\sum_{m=1}^{n/2} p_{n-2m,m-1}V^{n-2m}X^{m-1} - 4\sum_{m=1}^{\frac{n}{2}-1} q_{n-2(m+1),m}mV^{n-2(m+1)}X^m$$

that gives the equation

$$\sum_{i,j=0}^{n+1} \left(j^2V^iX^j - i(i-1)V^{i-2}X^{j+1}\right) r_{ij} = -6\sum_{m=1}^{n/2} p_{n-2m,m-1}V^{n-2m}X^{m-1}$$
$$- 4\sum_{m=1}^{\frac{n}{2}-1} q_{n-2(m+1),m}mV^{n-2(m+1)}X^m$$

If we choose now the term with $m = 1$ in the right-hand side we have

$$-6p_{n-2,0}V^{n-2}$$

this term cannot be balanced on the left, so we must have $p_{n-2,0} = 0$. The other terms on the right-hand side give the recursive formula

$$r_{n-2(m+1),m} = -\frac{6}{m^2}p_{n-2(m+1),m} - \frac{4}{m}q_{n-2(m+1),m} + \frac{(n-2m)(n-2m-1)}{m^2}r_{n-2m,m-1}$$

- **Fifth PDE**. This is analogous to the fourth:

$$\sum_{i,j=0}^{n+2} \left(j^2V^iX^j - i(i-1)V^{i-2}X^{j+1}\right) s_{ij} = -2\sum_{m=1}^{\frac{n}{2}} q_{n-2m,m-1}V^{n-2m}X^{m-1}$$
$$- 2\sum_{m=1}^{\frac{n}{2}-1} mr_{n-2(m+1),m}V^{n-2(m+1)}X^m$$

and with similar passages it gives $q_{n-2,0} = 0$ and the recursive formula

$$s_{n-2(m+1),m} = -\frac{2}{m^2}q_{n-2(m+1),m} - \frac{2}{m}r_{n-2(m+1),m} + \frac{(n-2m)(n-2m-1)}{m^2}s_{n-2m,m-1}$$

We observe that the coefficients $r_{n-2,0}$ and $s_{n-2,0}$ are not fixed, so they introduce an arbitrariness in the polynomials P_{n+1} and P_{n+2}. Coherence with P_{n-1} and P_n suggests to impose $r_{n-2,0} = s_{n-2,0} = 0$.
The polynomials we have found are trivially solutions of their PDEs because of the construction we have carried out. □

4.1 Explicit results

We want to see now what polynomials are given by the formulas above for some value of n. Of course, in the case $n = 4$ we expect to find the same we have seen before.

- $n = 4$. In this case, the index m can only have the value 1, so we have just an equation for every polynomial and the only non-zero coefficients are $p_{0,1}$, $q_{0,1}$, $r_{0,1}$ and $s_{0,1}$. We also agree to set $p_{2,0} = q_{2,0} = r_{2,0} = s_{2,0} = 0$. The recursive formulas yield the following linear system

$$\begin{cases} p_{0,1} = 2p_{2,0} - 8 \\ q_{0,1} = 2q_{2,0} - 6p_{0,1} \\ r_{0,1} = -6p_{0,1} - 4q_{0,1} + 2r_{2,0} \\ s_{0,1} = -2q_{0,1} - 2r_{0,1} + 2s_{2,0} \end{cases} \Rightarrow \begin{cases} p_{0,1} = -8 \\ q_{0,1} = -6p_{0,1} \\ r_{0,1} = -6p_{0,1} - 4q_{0,1} \\ s_{0,1} = -2q_{0,1} - 2r_{0,1} \end{cases} \Rightarrow \begin{cases} p_{0,1} = -8 \\ q_{0,1} = 48 \\ r_{0,1} = -144 \\ s_{0,1} = 192 \end{cases}$$

$$\Rightarrow P_{n-2} = \frac{n^2}{16} j_0^{(2)} = \frac{V^2}{2} + X \qquad P_{n-1} = -8X \qquad P_n = 48X \qquad P_{n+1} = -144X$$
$$P_{n+2} = 192X$$

We can immediately see that these are identical to the polynomials found before, the only difference being that we don't have any free parameter. This happens because we set to zero the coefficients that possibly can create them.

- $n = 5$. Here again we have only $m = 1$, but this time the non-zero coefficients are $p_{1,1}$, $q_{1,1}$, $r_{1,1}$ and $s_{1,1}$. The linear system reads

$$\begin{cases} p_{1,1} = 6p_{3,0} - 8 \\ q_{1,1} = 6q_{3,0} - 6p_{1,1} \\ r_{1,1} = -6p_{1,1} - 4q_{1,1} + 6r_{3,0} \\ s_{1,1} = -2q_{1,1} - 2r_{1,1} + 6s_{3,0} \end{cases} \Rightarrow \begin{cases} p_{1,1} = -8 \\ q_{1,1} = -6p_{1,1} \\ r_{1,1} = -6p_{1,1} - 4q_{1,1} \\ s_{1,1} = -2q_{1,1} - 2r_{1,1} \end{cases} \Rightarrow \begin{cases} p_{1,1} = -8 \\ q_{1,1} = 48 \\ r_{1,1} = -144 \\ s_{1,1} = 192 \end{cases}$$

$$\Rightarrow P_{n-2} = \frac{V^3}{6} + VX \qquad P_{n-1} = -8VX \qquad P_n = 48VX \qquad P_{n+1} = -144VX$$
$$P_{n+2} = 192VX$$

we see that we obtain the same polynomials as before, just with VX instead of X.

- $n = 6$. Here $m = 1, 2$ and we have two non-zero coefficients for every polynomial:

$$\begin{cases} p_{2,1} = -36 \\ p_{0,2} = \frac{1}{4}\left(2p_{2,1} - 36\right) \\ q_{2,1} = -6p_{2,1} \\ q_{0,2} = \frac{1}{4}\left(2q_{2,1} - 12p_{0,2}\right) \\ r_{2,1} = -6p_{2,1} - 4q_{2,1} \\ r_{0,2} = \frac{1}{4}\left(-6p_{0,2} - 8q_{0,2} + 2r_{2,1}\right) \\ s_{2,1} = -2q_{2,1} - 2r_{2,1} \\ s_{0,2} = \frac{1}{4}\left(-2q_{0,2} - 4r_{0,2} + 2s_{2,1}\right) \end{cases} \Rightarrow \begin{cases} p_{2,1} = -36 \\ p_{0,2} = -27 \\ q_{2,1} = 216 \\ q_{0,2} = 189 \\ r_{2,1} = -648 \\ r_{0,2} = -\frac{1323}{2} \\ s_{2,1} = 864 \\ s_{0,2} = 999 \end{cases}$$

$$\Rightarrow P_{n-2} = \frac{9}{4}\left(\frac{V^4}{6} + 2V^2X + X^2\right) \qquad P_{n-1} = -36V^2X - 27X^2$$

$$P_n = 216V^2X + 189X^2 \qquad P_{n+1} = -648V^2X - \frac{1323}{2}X^2 \qquad P_{n+2} = 864V^2X + 999X^2$$

5 Conclusions

As preannounced in the abstract, we managed to solve the conjecture and we ended up proving that for every first integral of the Toda chain there exist a fourth-order extension which is an approximated first integral of the FPU chain. This extension can also be written explicitly. In order to extend a generic $j_0^{(n)}$ to the FPU chain, one has to follow these simple steps:

1. Calculate second-order extension $j_2^{(n)}$ using formula 3.1;

2. Calculate fourth-order extension $j_4^{(n)}$ (σ excluded) using expression 3.2 and theorem 3.1;

3. Calculate σ using the formulas in theorem 4.1 to complete the extension.

Further developments of this result could be

- Study extension up to the sixth-order: this implies a lot more computation but could as well find when and how motions of Toda and FPU chains start to differ.

- Study extension for lattices in greater dimension

A Cauchy estimates

Let's recall a simple result from basic complex calculus:

Proposition A.1 (Cauchy integral formula)**.** *If $f : D \subset \mathbb{C} \to \mathbb{C}$ is an analytic function and $z_0 \in D$, then the following holds*

$$\frac{1}{2\pi i}\oint_{\mathcal{C}_r} \frac{f(z)}{(z-z_0)^{s+1}}dz = \frac{f^{(s)}(z_0)}{s!}$$

where $\mathcal{C}_r = \{z \in D | z = z_0 + re^{i\phi}, \phi \in \mathbb{S}^1\}$ is a circle of radius r and centre z_0 completely contained in D.

Proof. If $z_0 \in D$ and f is analytic in $D \subset \mathbb{C}$, we have by definition that $\forall z \in D$

$$f(z) = \sum_{j\geq 0} \frac{f^{(j)}(z_0)}{j!}(z-z_0)^j$$

and we also have $dz = rie^{i\phi}d\phi$ from the definition of $\mathcal{C}_r$, with $\phi \in [0, 2\pi[$. We can thus write

$$\frac{1}{2\pi i}\oint_{\mathcal{C}_r} \frac{f(z)}{(z-z_0)^{s+1}}dz = \frac{1}{2\pi i}\oint_{\mathcal{C}_r} \sum_{j\geq 0} \frac{f^{(j)}(z_0)}{j!}(z-z_0)^{j-s-1}dz =$$
$$= \sum_{j\geq 0} \frac{f^{(j)}(z_0)}{j!}\int_0^{2\pi} r^{j-s-1}e^{i(j-s-1)\phi}rie^{i\phi}d\phi = \sum_{j\geq 0} \frac{f^{(j)}(z_0)}{j!}\frac{1}{2\pi}r^{j-s}\int_0^{2\pi} e^{i(j-s)\phi}d\phi = \frac{f^{(s)}(z_0)}{s!}$$

In the second-last passage we used the fact that $e^{i(j-s)\phi} = \delta_{js}$, so that in the sum only the term with $j = s$ survives. □

We can immediately use this result to obtain the so-called Cauchy estimates, which describe how derivatives are bounded in the analytic domain: we rename $z_0 \to z$, $z \to \xi$ and take the modules of both sides in the formula above

$$\frac{|f^{(s)}(z)|}{s!} \leq \frac{1}{2\pi}\oint_{\mathcal{C}_r} \frac{|f(\xi)|}{|\xi - z|^{s+1}}rd\phi = \frac{1}{2\pi}\oint_{\mathcal{C}_r} \frac{|f(\xi)|}{r^s}d\phi \leq \frac{2\pi M(r)}{2\pi r^s} = \frac{M(r)}{r^s}$$

from which

$$|f^{(s)}(z)| \leq s!\frac{M(r)}{r^s} \quad \text{with} \quad M(r) = \sup_{\xi\in\mathcal{C}_r} |f(\xi)|$$

The next result is again quite basic:

Proposition A.2 (Maximum principle)**.** *If $f : D \subset \mathbb{C} \to \mathbb{C}$ is analytic in D, then its maximum is reached on the boundary of D.*

Proof. By contradiction, we suppose z is a local maximum point inside the domain in which f is analytic. We take s=1 and use Cauchy integral formula:

$$f(z) = \frac{1}{2\pi i} \oint_{\mathcal{C}_\rho} \frac{f(\xi)}{\xi - z} d\xi$$

Now, by definition z is such that

$$|f(z)| > |f(\xi)| \quad \forall \xi \in \mathring{\mathcal{C}}_\rho \quad \forall \rho$$

This implies

$$|f(z)| \leq M(\rho) \quad \text{with } M(\rho) = \sup_{\mathcal{C}_\rho} |f(\xi)|$$

which is absurd. □

Now, take $u(x)$ an analytic periodic function with $x \in \frac{\mathbb{R}}{\mathbb{Z}}$. In order to apply Cauchy estimates, we immerge the function in $\mathbb{C}$ obtaining its analytical extension $u(z)$. Thanks to Schwarz symmetric principle we have $u(\overline{z}) = \overline{u(z)}$. Indeed, using Taylor series expansion for $u(z)$ we can write

$$u(z) = \sum_{j \geq 0} \frac{u^{(s)}(x)}{s!}(z-x)^s \quad \Rightarrow \quad u(\bar{z}) = \sum_{j \geq 0} \frac{u^{(s)}(x)}{s!}(\bar{z}-x)^s = \sum_{j \geq 0} \overline{\frac{u^{(s)}(x)}{s!}} \overline{(z-x)^s} = \overline{u(z)}$$

If $u(z)$ is analytical in the strip $\Omega_\sigma = \{x \in \mathbb{C} || Im(x)| \leq \sigma\}$, we can extend this up to the imaginary part of the first singularity. On the other hand, maximum principle says the maximum is reached on the boundary, so if we agree to call

$$M(\sigma) = \max_{Im(z)=\sigma} |u(z)|$$

using Cauchy estimates we can write

$$|u^{(s)}(x)| \leq s! \frac{M(\sigma)}{\sigma^s} \quad \forall x \in \frac{\mathbb{R}}{\mathbb{Z}}$$

which is the formula used to estimate functions V and R in previous sections.

B Hamiltonian perturbation theory results

Let's consider a perturbed integrable hamiltonian:

$$H_\lambda = h + \lambda H_1 + \lambda^2 H_2 + \dots$$

with h integrable. If J_0 is a first integral of h then $\{h, J_0\} = 0$ and if we calculate its total derivative along the flow of H_λ we have

$$\frac{dJ_0}{dt} = \dot{J}_0 = \{J_0, H_\lambda\} = \{J_0, h\} + \{J_0, \lambda H_1\} + \dots = \lambda\{J_0, H_1\} + \lambda^2\{J_0, H_2\} + \mathcal{O}(\lambda^3)$$

Introducing $\tau = \lambda t$ as a re-scaling of time gives

$$\frac{dJ_0}{d\tau} = \{J_0, H_1\} + \mathcal{O}(\lambda)$$

so J_0 varies on a time scale of $\mathcal{O}(1)$ in τ and $\mathcal{O}(\frac{1}{\lambda})$ in t. We want now to see if we can find a function $J_1(H_1)$ such that $J_0 + \lambda J_1(H_1)$ varies on a time scale of $\mathcal{O}(\frac{1}{\lambda^2})$ in t. To this purpose, in all generality, we can define $J_\lambda = J_0 + \lambda J_1 + \lambda^2 J_2 + \dots$ and impose

$$\{J_\lambda, H_\lambda\} = \left\{ \sum_{i\geq 0} \lambda^i J_i, \sum_{j\geq 0} \lambda^j H_j \right\} = \sum_{i,j\geq 0} \lambda^{i+j}\{J_i, H_j\} = \sum_{k\geq 0} \lambda^k \left(\sum_{i+j=k} \{J_i, H_j\} \right) = 0$$
$$\iff \sum_{i+j=k} \{J_i, H_j\} = 0 \quad \forall k \geq 0$$

which gives

$$\begin{aligned}
&(k=0) \qquad \{J_0, H_0\} = 0 \\
&(k=1) \qquad \{J_0, H_1\} + \{J_1, H_0\} = 0 \quad \Rightarrow \quad L_h J_1 + \{J_0, H_1\} = 0 \\
&(k=2) \qquad \{J_0, H_2\} + \{J_1, H_1\} + \{J_2, h\} = 0 \quad \Rightarrow \quad L_h J_2 = -\{J_1, H_1\} - \{J_0, H_2\} \\
&\quad \dots \qquad\quad \dots
\end{aligned}$$

where $L_h := \{\cdot, h\}$ is the operator that gives the Poisson brackets with respect to h.
We recall now a simple result on hamiltonian flows:

Lemma B.1 (Exchange lemma)**.** *For any function F and any hamiltonian G one has*

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

Proof. Define $\tilde{F}(s) := F \circ \phi_G^s$ and observe that $\tilde{G}(s) = G \circ \phi_G^s = G$ and $\tilde{F}(0) = F$. The derivative of $\tilde{F}$ with respect to the flow of G now reads

$$\dot{\tilde{F}} = \{F, G\} \circ \phi_G^s = \widetilde{L_G F} \quad \Rightarrow \quad \ddot{\tilde{F}} = \widetilde{L_G^2 F} \quad \Rightarrow \quad \dots \quad \Rightarrow \quad \frac{d^n \tilde{F}}{ds^n} = \widetilde{L_G^n F} \quad \forall n \geq 0$$

and if we calculate the Taylor expansion of $\tilde{F}(s)$ we obtain

$$\tilde{F}(s) = \sum_{n\geq 0} \frac{s^n}{n!} \frac{d^n \tilde{F}}{ds^n}\bigg|_{s=0} = \sum_{n\geq 0} \frac{s^n L_G^n}{n!} F = e^{sL_G} F$$

□

Proposition B.1. *The $k = 1$ equation above is solved $\iff$ $\{J_0, \overline{H_1}^{(h)}\} = 0$, with the over-line signifying time average on the unperturbed flow of h.*

Proof. We use exchange lemma to write

$$L_h J_1 + \{J_0, H_1\} = 0 \iff L_h J_1 \circ \phi_h^s = \{H_1, J_0\} \circ \phi_h^s \iff e^{sL_h} L_h J_1 = e^{sL_h}\{H_1, J_0\}$$

and we suppose h is such that the exponential is bounded. If now we integrate the left-hand side of the last equation and we divide by t we have

$$\Rightarrow \frac{1}{t}\int_0^t e^{sL_h} L_h J_1 ds = \frac{1}{t}\int_0^t \frac{d}{ds}(e^{sL_h} J_1) ds = \frac{(e^{tL_h} - 1) J_1}{t} \to 0 \quad \text{for } t \to \infty$$

Applying the same passages to the right-hand side yields

$$0 = \lim_{t\to\infty} \frac{1}{t}\int_0^t e^{sL_h}\{H_1, J_0\} ds = \lim_{t\to\infty} \frac{1}{t}\int_0^t \{H_1, J_0\} \circ \phi_h^s ds = \lim_{t\to\infty} \frac{1}{t}\int_0^t \{H_1 \circ \phi_s^h, J_0\} ds =$$
$$= \{\overline{H_1}^{(h)}, J_0\}$$

that is the thesis. □

We could as well find similar results for higher k that make sure the condition

$$\sum_{i+j=k} \{J_i, H_j\} = 0$$

is satisfied, so that J_k exists. But, if $\exists k \geq 2$ such that the sum above is not zero, then we're facing an obstacle to the extension of J_λ. If this happens, then $J_\lambda^{(k-1)} = J_0 + \lambda J_1 + \cdots + \lambda^{k-1} J_{k-1}$ cannot be extended anymore and we can conclude that $\dot{J}_\lambda^{(k-1)} = \{J_\lambda^{(k-1)}, H_\lambda\} = \mathcal{O}(\lambda^k)$. This means $J_\lambda^{(k-1)}$ varies on a time scale of $\mathcal{O}(\frac{1}{\lambda^k})$ in t or $\mathcal{O}(\lambda^k)$ in τ.

C Continuum extension of Henon's first integrals

In his article [6] Henon defines the following first integrals for the n-particles Toda chain:

$$J_m = \sum_{i=1}^{n} \sum_{p,\alpha_j,\beta_j} A(\alpha_0, \dots, \alpha_p, \beta_0, \dots, \beta_{p-1}) u_i^{\alpha_0} u_{i+1}^{\alpha_1} \dots u_{i+p}^{\alpha_p} X_i^{\beta_0} X_{i+1}^{\beta_1} \dots X_{i+p-1}^{\beta_{p-1}} \tag{C.1}$$

where $m = 1, \dots, n$ and the coordinates are $u_i = \dot{x}_i$ and $X_i = e^{-(x_{i+1}-x_i)}$. The second sum is intended on every p, α_j, $\beta_j \in \mathbb{N}$ such that $\beta_j \geq 1$ and

$$\sum_{j=0}^{p} \alpha_j + 2 \sum_{j=0}^{p-1} \beta_j = m$$

and the coefficients are given by

$$A(\alpha_0, \dots, \alpha_p, \beta_0, \dots, \beta_{p-1}) = \prod_{j=0}^{p} \frac{(\alpha_j + \beta_{j-1} + \beta_j - 1)!}{\alpha_j!} \prod_{j=0}^{p-1} \frac{1}{\beta_j!(\beta_j - 1)!}$$

According to the article, the first five J_m are

$$J_1 = \sum_{i=1}^{n} u_i \qquad J_2 = \sum_{i=1}^{n} \left[\frac{1}{2} u_i^2 + X_i \right] \qquad J_3 = \sum_{i=1}^{n} \left[\frac{1}{3} u_i^3 + (u_i + u_{i+1}) X_i \right]$$

$$J_4 = \sum_{i=1}^{n} \left[\frac{1}{4} u_i^4 + (u_i^2 + u_i u_{i+1} + u_{i+1}^2) X_i + \frac{1}{2} X_i^2 + X_i X_{i+1} \right]$$

$$J_5 = \sum_{i=1}^{n} \left[\frac{1}{5} u_i^5 + (u_i^3 + u_i^2 u_{i+1} + u_i u_{i+1}^2 + u_{i+1}^3) X_i + (u_i + u_{i+1}) X_i^2 + (u_i + 2u_{i+1} + u_{i+2}) X_i X_{i+1} \right]$$

and we can notice the first coefficient in the sum is $\frac{1}{m}$. A simple calculation using the formula for A shows this is the case $\forall m$.

Proposition C.1. *When extended to the continuum case $n \to \infty$, Henon's first integrals are equivalent to $J_0^{(m)} = \int j_0^{(m)} dx$ up to a multiplicative constant. This is $mC_{\frac{m}{2}}^0 = \frac{\left(\frac{m}{2}!\right)^2}{(m-1)!}$ in the case of even m and $mB_{\frac{m-1}{2}}^0 = \frac{\left(\frac{m-1}{2}!\right)^2}{(m-1)!}$ in the case of odd m.*

Proof. We want to extend the general formula C.1 to the continuum case. We start by defining $h = \frac{1}{n}$ and interpolating the coordinates u and X with two smooth functions V and $\tilde{X}$ in the following way:

$$u_i(t) = V(hi, t) = V(x, t) \qquad X_i(t) = \tilde{X}(x, t)$$

$$u_{i+1}(t) = V(h(i+1), t) = V(x + h, t) \qquad X_{i+1}(t) = \tilde{X}(x + h, t)$$

$$\dots$$

$$u_{i+p}(t) = V(x + ph, t) \qquad X_{i+p-1}(t) = \tilde{X}(x + (p-1)h, t)$$

We are interested in the case of h small, so we can use Taylor expansions

$$V(x+jh,t) = V(x,t) + \frac{\partial V}{\partial x}(x,t)jh + \mathcal{O}(h^2) \quad \text{for } j = 1, \dots, p$$
$$\tilde{X}(x+jh,t) = \tilde{X}(x,t) + \frac{\partial \tilde{X}}{\partial x}(x,t)jh + \mathcal{O}(h^2) \quad \text{for } j = 1, \dots, p-1$$

and taking the limit $h \to 0$ (which means $n \to \infty$) we are left only with the first terms. Also, the first sum in formula C.1 becomes $\int dx$ and we can write

$$J_m = \int \sum_{p,\alpha_j,\beta_j} A(\alpha_0, \dots, \alpha_p, \beta_0, \dots, \beta_{p-1}) V^{\sum_{j=0}^{p} \alpha_j} \tilde{X}^{\sum_{j=0}^{p-1} \beta_j} dx$$

We use now the constraints seen above to define

$$l := \sum_{j=0}^{p-1} \beta_j \quad \Rightarrow \quad \sum_{j=0}^{p} \alpha_j = m - 2l$$

Because of the limit operation, we can say that the coefficients A "aggregate" and end up depending only on m and l. Now, in the case of even m we have $l \in \{0, \dots, \frac{m}{2}\}$ whereas in the case of odd m we have $l \in \{0, \dots, \frac{m-1}{2}\}$ and we can write

$$J_m = \int \sum_{l=0}^{\frac{m}{2}} A(m,l) V^{m-2l} \tilde{X}^l dx \quad \text{for even m}$$
$$J_m = \int \sum_{l=0}^{\frac{m-1}{2}} A(m,l) V^{m-2l} \tilde{X}^l dx \quad \text{for odd m}$$

These two formulas are similar to the ones we have written in section 3.1 for $j_0^{(2m)}$ and $j_0^{(2m+1)}$ if we agree that $\tilde{X} = e^R$ and rewrite them using m instead of $2m$ and $2m+1$. Also, here we are considering the entire first integrals (not just their densities), so this motivates the presence of the integral sign.
We will show now that the two sets of first integrals are equivalent up to a multiplicative constant that depends on m, so that $A(m,l)$ is nothing but a re-scaling of $C(m,l)$ or $B(m,l)$. To do so, we take advantage of the first five J_m. Their continuum extensions are

$$J_1 = \int V dx \qquad J_2 = \int \left[\frac{V^2}{2} + \tilde{X}\right] dx \qquad J_3 = \int \left[\frac{V^3}{3} + 2V\tilde{X}\right] dx$$
$$J_4 = \int \left[\frac{V^4}{4} + 3V^2\tilde{X} + \frac{3}{2}\tilde{X}^2\right] dx \qquad J_5 = \int \left[\frac{V^5}{5} + 4V^3\tilde{X} + 6V\tilde{X}^2\right] dx$$

The first two are equal to $J_0^{(1)}$ and $J_0^{(2)}$ while the others can be transformed in $J_0^{(m)}$ multiplying by $\frac{1}{2}$, $\frac{2}{3}$ and $\frac{1}{6}$ respectively. In all generality, the first coefficient for J_m is $\frac{1}{m}$ while the first for $J_0^{(m)}$ is $C^0_{\frac{m}{2}}$ in the case of even m and $B^0_{\frac{m-1}{2}}$ in the case of odd m. We can thus conclude that $mC^0_{\frac{m}{2}}$ and $mB^0_{\frac{m-1}{2}}$ are the multiplicative coefficients needed to transform J_m in $J_0^{(m)}$. Finally, if we use the explicit formulas for $C^0_{\frac{m}{2}}$ and $B^0_{\frac{m-1}{2}}$ we can immediately obtain that these coefficients are $\frac{\left(\frac{m}{2}!\right)^2}{(m-1)!}$ in the case of even m and $\frac{\left(\frac{m-1}{2}!\right)^2}{(m-1)!}$ in the case of odd m. $\square$

D Wolfram Mathematica code

- Functional derivative of a density $f(u)$ (up to order 5)

```
funder[f_,u_]:=Sum[(-1)^n*Dt[D[f,D[u[x],{x,n}]],{x,n}],{n,0,5}];
```

- Poisson brackets of two densities $f_1(u,v)$ and $f_2(u,v)$

```
PP[f1_,f2_,u_,v_]:=funder[f1,u]*Dt[funder[f2,v],x]
+funder[f1,v]*Dt[funder[f2,u],x];
```

- Coefficients C_n^l and B_n^l

```
c[n_,l_]:=Piecewise[{{Product[m^2,{m,l+1,n}]/(2(n-l))!,l!= n},
{1,l==n}}];
b[n_,l_]:=Piecewise[{{Product[m^2,{m,l+1,n}]/(2(n-l)+1)!,l!=n},
{1,l==n}}];
```

- First integrals of Toda chain

```
j0even[V_,R_,n_]:=Sum[c[n/2,l]V^(2(n/2-l))E^(lR),{l,0,n/2}];
j0odd[V_,R_,n_]:=Sum[b[(n-1)/2,l]V^(2((n-1)/2-l)+1)E^(lR),
{l,0,(n-1)/2}];
```

- Densities for Dubrovin's theorem

```
f00=f0[u[x],v[x]];
f1=p[u[x],v[x]]v'[x];
f2=1/2(a[u[x],v[x]]u'[x]^2+2b[u[x],v[x]]u'[x]v'[x]
+c[u[x],v[x]]v'[x]^2);
h0=1/2v[x]^2+\[Phi][u[x]];h2=-1/24\[Phi]''[u[x]]u'[x]^2+O[h]^3;
```

- Densities for the extension of Dubrovin's theorem

```
j00=j0[V[x],R[x]];
j2=1/2 (a[V[x],R[x]]R'[x]^2+2b[V[x],R[x]]R'[x]V'[x]+
+c[V[x],R[x]]V'[x]^2)+p[V[x],R[x]]R'[x]+q[V[x],R[x]]V'[x]+d[V[x],R[x]];
K0=1/2V[x]^2+\[Phi][R[x]];
K2=\[Psi]1[R[x]]-1/24V'[x]^2+O[h]^3;
```

- Densities for harmonic oscillator case

```
j00=j0[V[x],R[x]];
j2=1/2(a[V[x],R[x]]R'[x]^2+2b[V[x],R[x]]R'[x]V'[x]+
+c[V[x],R[x]]V'[x]^2)+p[V[x],R[x]]R'[x]+q[V[x],R[x]]V'[x]+d[V[x],R[x]];
K0=1/2V[x]^2+\[Phi][R[x]]/.{\[Phi][R[x]]->1/2\[Omega]R[x]^2};
K2=\[Psi]1[R[x]]-1/24V'[x]^2+O[h]^3;
```

- Densities for the 4-th order extension of first integrals

```
j00:=j0[V[x],R[x]];
j2:= 1/2(a[V[x],R[x]]R'[x]^2+2b[V[x],R[x]]R'[x]V'[x]
+c[V[x],R[x]]V'[x]^2);
j2var=-1/12D[j0[V[x],R[x]],{V[x],2},{R[x],1}]E^R[x]R'[x]^2
-1/6D[j0[V[x],R[x]],{V[x],3}]E^R[x]R'[x]V'[x]
-1/12D[j0[V[x],R[x]],{V[x],2},{R[x],1}]V'[x]^2
-1/24D[j0[V[x],R[x]],{V[x],2}]V'[x]^2;
j4:=\[Alpha][V[x],R[x]](R''[x])^2+\[Beta][V[x],R[x]]R''[x]V''[x]
+\[Gamma][V[x],R[x]](V''[x])^2+\[Delta][V[x],R[x]]R''[x](V'[x])^2
+\[Epsilon][V[x],R[x]]V''[x](R'[x])^2+\[Mu][V[x],R[x]](R'[x])^4
+\[Nu][V[x],R[x]]R'[x](V'[x])^3+\[Rho][V[x],R[x]](R'[x]V'[x])^2
+\[Lambda][V[x],R[x]](R'[x])^3V'[x]+\[Omega][V[x],R[x]](V'[x])^4
+1/2\[Eta][V[x],R[x]]R'[x]^2+\[Xi][V[x],R[x]]R'[x]V'[x]
+1/2\[Zeta][V[x],R[x]]V'[x]^2+\[Sigma][V[x],R[x]];
K0=1/2V[x]^2+\[Phi]toda[R[x]];
K0var=1/2V[x]^2+E^R[x]-R[x]-1;
K2=-1/24(V'[x])^2;
K4=1/720(V''[x])^2+1/4\[Epsilon]0\[CapitalDelta]\[Beta]R^4;
```

- Ansatz for σ

```
\[Sigma][V_,R_]:=\[CapitalDelta]\[Beta](R^4P[n][V,E^R]+R^3P[m][V,E^R]
+R^2P[i][V,E^R]+RP[j][V,E^R]+P[k][V,E^R]);
```

- System of PDEs for σ

```
D[P[n-2][V,R],{R,2}]==E^RD[P[n-2][V,R],{V,2}];
8D[P[n-2][V,R],R]+D[P[n-1][V,R],{R,2}]==E^RD[P[n-1][V,R],{V,2}];
12P[n-2][V,R]+6D[P[n-1][V,R],R]+D[P[n][V,R],{R,2}]==E^RD[P[n][V,R],{V,2}]
+3D[j04[V,R],{V,2}];
6P[n-1][V,R]+4D[P[n][V,R],R]+D[P[n+1][V,R],{R,2}]==E^RD[P[n+1][V,R],{V,2}];
2P[n][V,R]+2D[P[n+1][V,R],R]+D[P[n+2][V,R],{R,2}]==E^RD[P[n+2][V,R],{V,2}];
```

- Recursion formulas associated with the PDEs

  - Even n case

```
Subscript[p,n-2,0]=Subscript[q,n-2,0]=Subscript[r,n-2,0]=
Subscript[s,n-2,0]=0;
For[m=1,m<=n/2-1,m++,Print[Column[{Subscript[p,-2(1+m)+n,m]
=(-(1/2)mn^2c[-1+n/2,m]+(-1-2m+n)(-2m+n)Subscript[p,-2m+n,-1+m])/m^2,
Subscript[q,-2(1+m)+n,m]=(-6mSubscript[p,-2(1+m)+n,m]+(-1-2m+n)(-2m+n)
Subscript[q,-2m+n,-1+m])/m^2,Subscript[r,-2(1+m)+n,m]=
(-6Subscript[p,-2(1+m)+n,m]-4mSubscript[q,-2(1+m)+n,m]+(-1-2m+n)(-2m+n)
Subscript[r,-2 m+n,-1+m])/m^2,Subscript[s,-2(1+m)+n,m]=
(-2Subscript[q,-2(1+m)+n,m]-2mSubscript[r,-2(1+m)+n,m]+(-1-2m+n)(-2m+n)
Subscript[s,-2m+n,-1+m])/m^2}]]];
```

  - Odd n case

```
Subscript[p,n-2,0]=Subscript[q,n-2,0]=Subscript[r,n-2,0]=
Subscript[s,n-2,0]=0;
For[m=1,m<=(n-3)/2,m++,Print[Column[{Subscript[p,-2(1+m)+n,m]=
(-(1/2)m(-1+n)^2b[1/2 (-3+n),m]+(-1-2m+n)(-2m+n)
Subscript[p,-2m+n,-1+m])/m^2,Subscript[q,-2(1+m)+n,m]=
(-6mSubscript[p,-2(1+m)+n,m]+(-1-2m+n)(-2m+n)
Subscript[q,-2m+n,-1+m])/m^2,Subscript[r,-2(1+m)+n,m]=
(-6Subscript[p,-2(1+m)+n,m]-4mSubscript[q,-2(1+m)+n,m]
+(-1-2m+n)(-2m+n) Subscript[r,-2m+n,-1+m])/m^2,
Subscript[s,-2(1+m)+n,m]=(-2Subscript[q,-2(1+m)+n,m]
-2mSubscript[r,-2(1+m)+n,m]+(-1-2m+n)(-2m+n)
Subscript[s,-2m+n,-1+m])/m^2}]]]
```

E Acknowledgments

Alla fine di questo percorso di sei anni vorrei innanzitutto ringraziare i miei genitori e la mia famiglia per il loro supporto costante. Un grazie enorme poi a tutti gli amici che ho incontrato lungo questa strada, anche a quelli che purtroppo non vedo più per un motivo o per l'altro. Grazie agli amici di Padova e di Vicenza, grazie a Francesca, al gruppo di Cittadella, agli amici e agli insegnanti di musica di Camisano e Curtarolo. Grazie alla dott. Schiarante, ai coinquilini di galleria San Bernardino. Grazie ai proff. Benettin e Ponno e a Giuseppe Orsatti per la disponibilità e per l'aiuto durante le tesi.
L'amore e l'affetto che tutti voi mi avete dimostrato vale sicuramente più di ogni bene materiale e di ogni successo si possa ottenere. Un grazie infinite insomma a tutti quelli che ci sono stati e hanno preso parte al mio percorso e alla mia crescita. Vi voglio bene.

Luca

References

[1] D. Bambusi and A. Ponno. “On metastability in FPU”. In: *Comm. Math. Phys.* 264 (2006), pp. 539–561.

[2] G. Carlet, B. Dubrovin, and Y. Zhang. “The extended Toda hierarchy”. In: *Moscow Math Journal* 4 (2004), pp. 313–332.

[3] Boris Dubrovin. “On universality of critical behaviour in hamiltonian PDEs”. In: *American Mathematical Society Translations* 224 (2008).

[4] E. Fermi, J. Pasta, and S. Ulam. “Studies of non linear problems”. In: *LASL Report LA-1940. Reprinted in 'Collected Papers of E.Fermi', V.II, University Of Chicago Press* (1965).

[5] H. Flaschka. “The Toda Lattice. II. Existence of integrals”. In: *Physical Review B* 9 (1974), p. 1924.

[6] M. Henon. “Integrals of the Toda lattice”. In: *Physical Review B* 9 (1974), p. 1921.

[7] Giuseppe Orsatti. “Dubrovin's approach to the FPU problem (Unpublished thesis)”. 2019. URL: `http://tesi.cab.unipd.it/63320/1/Tesi_LM_P_Orsatti_Giuseppe.pdf`.

[8] M. Toda. “Vibration of a chain with nonlinear interaction”. In: *J. Phys. Soc. Japan* 22 (1967).