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Report

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First of all I would like to thank professor C. Simó for supervising me during research project, professor A. Jorba along with whole organizing committee for inviting me to the DocCourse in Computational Methods in Dynamical Systems and Applications held at Institut de Mathemátiques de la Universitat de Barcelona. I also like to thank all the lecturers who gave introductory courses during first month for inspiration and presentation of very interesting research problems.

1 Introduction

So far in my research I was dealing with the dissipative partial differential equations (PDEs) exhibiting energy dissipation, which is in contrast to the conservation of energy in conservative PDEs (cPDEs).

Examples of the dissipative PDEs (dPDEs) are

- The heat equation, modeling heat distribution over a domain.
- The Burgers equation, derived originally as a model of turbulence phenomena, later on successfully used to model gas dynamics and acoustic phenomena.
- The Navier-Stokes equations, famous equations with many mathematical problems related, describing fluid flow.
- The Kuramoto-Shivasinsky equation, modelling flame propagation.

Only the first one being linear.

Examples of the cPDEs are

- The wave equation, it is not hard to guess, modelling wave propagation.
- The Korteweg-deVries equation (KdV equation), modeling solitary waves.
- The sine-Gordon equation, nonlinear version of Klein-Gordon equation.

In this report we present summary of the project that focused on the specific form of KdV equation. More closely speaking, firstly, we describe the finite dimensional genesis of this equation, how it is derived, we show that it is a limit of finite dimensional structures and we present an attempt in understanding the foundations of the equation by describing the dynamics of those finite dimensional structures.

2 Motivation

We motivate the work by the fact that the dynamics of conservative equations is in general much different than that of dissipative ones. When the energy of a system stays trapped inside rather than escapes away a lot of interesting phenomena is being born. Moreover if we introduce perturbation to the system we may expect appearance of ergodicity and chaos, both describing the widely studied phenomena of the system escaping deterministic behavior and being no longer predictable. Due to the KAM theorem still some portion of determinability will prevail after introduction of a perturbation, having form of the islands in the sea of ergodicity.

3 Notation

We will use symbol q for describing both discrete values of displacement, denoted by q_i and a function $q\colon \mathbb{R} \to \mathbb{R}$.

4 Method of deriving cPDEs

4.1 Lattices

One of the methods of deriving cPDEs, we would like to focus on, considers a cPDEs as the limit of equations describing interaction among n particles, when $n \to \infty$.

Definition 1 *Let $n \in \mathbb{N}$, $n > 1$.*
We call a lattice a set (partially ordered) of n interacting particles placed on a circle, where every particle interacts only with its closest neighbours.
We attach to i-th particle two values $\{q_i, p_i\}$, where p_i is its momentum and q_i is its displacement from equilibrium position.

Definition 2 *$f(q_i - q_{i+1})$ is force of interaction in between i-th and $i+1$-th particle and $u(q_i - q_{i+1})$ is its potential, $u\colon \mathbb{R} \to \mathbb{R}$, $f\colon \mathbb{R} \to \mathbb{R}$ are regular functions.*

Dynamics on a lattice is considered as Hamiltonian system with Hamiltonian in form

$$H = \sum \frac{p_i}{2} + \sum u\left(q_i - q_{i+1}\right) \tag{1}$$

Therefore equations of motion take form of the system

$$\begin{cases} \frac{dq_i}{dt} = p_i \\ \frac{dp_i}{dt} = -f\left(q_i - q_{i+1}\right) + f\left(q_{i-1} - q_i\right) \end{cases}, \quad i = 0, \ldots, n-1. \tag{2}$$

First start with presenting a few types of lattices, one linear and two nonlinear, with different forcing function f.

1. In the simplest case, interpreted as lattice of particles connected by springs obeying Hooke's law u is a quadratic function, f is linear, equations of motion take following form

   $$\begin{cases} \frac{dq_i}{dt} = p_i \\ \frac{dp_i}{dt} = q_{i+1} + q_{i-1} - 2q_i \end{cases}, \quad i = 0, \ldots, n-1. \tag{3}$$

   This system is integrable.

2. Second degree polynomial forcing function f gives rise to Fermi-Pasta-Ulam lattice (FPU lattice). Numerical investigation in 50's was source of the famous FPU problem, essentially it revealed behavior of this system which was completely out of authors expectations. Question of integrability of this lattice will be answered later on.

3. Case that will be subject of our further investigation is the Toda lattice with exponential forcing function. $f(x) = a\left(1 - e^{bx}\right)$. Surprisingly it turned out to be integrable. Even more surprisingly if we replace exponentials by infinite series and truncate them at any given level we obtain not integrable system. In particular force from FPU lattice can be viewed as approximation of exponential function up to second order, thus as a colorally we deduce that FPU lattice is not integrable.

4.2 Passing with number of particles to the limit.

In this section we describe a technique of passing to the limit with number of particles and we present the limit (dPDEs). We assumed that all particles are of uniform mass 1, thus in passing to the limit we need to introduce some kind of normalization of masses. In fact instead of normalizing the masses we will scale time equivalently. First of all we assume that there is a smooth 1-periodic function q defined on the circle that approximates the displacements i.e. $q_i(t) = q\left(t, 2\pi\frac{i}{n}\right)$ as $n \to \infty$, introducing scaling of time results in $q_i(t) = q\left(nt, 2\pi\frac{i}{n}\right)$. We will not present all the steps needed to derive cPDE from a lattice, but rather an outline.

Having approximation q, the equation $\ddot{q}_i = -f\left(q_i - q_{i+1}\right) + f\left(q_{i-1} - q_i\right)$ is equivalent to

$$n^2 \frac{\partial^2 q(nt,x)}{\partial t^2} = -f(q(nt,x) - q(nt, x + \frac{2\pi}{n})) + f(q(nt, x - \frac{2\pi}{n}) - q(nt,x)), \quad (4)$$

at points $x = 2\pi \frac{i}{n}$, $i = 0, \ldots, n$. Then we Taylor expand $q(nt, x + \frac{2\pi}{n})$. This step wipes out terms $q(nt,x)$ in (4), rest is dependant on $\varepsilon = \frac{2\pi}{n}$. We perform truncation of terms having ε over given order, and depending on the level at which we performed truncation we receive different cPDEs. We present briefly what one receives for linear and nonlinear cases. We have respectively

1. Linear force lattice - the wave equation $q_{tt} = q_{xx}$. It is integrable system, with infinite number of integrals.
2. Nonlinear - depending on the level of approximation in (4)
   - the wave equation $q_{tt} = aq_{xx} + O\left(\frac{1}{n}\right)$,
   - the Boussinesq equation $q_{tt} = \left[q + q^2 + q_{xx}\right]_{xx} + O\left(\frac{1}{n^3}\right)$,
   - subject of our further investigation the Korteweg-deVries equation

$$q_t = q \cdot q_x + \frac{1}{2} q_{xxx} \quad (5)$$

5 KdV equation

In this section we focus on (5) and present a brief survey of rigorous knowledge regarding it and what phenomena are embedded in this equation. Firstly, we address the latter, because it was somehow indicator to what can be proved by rigorous means. The equation admits solutions in form of soliton waves. By soliton it is meant a solitary wave that travels at its own speed and its shape remains unchanged. Numerical experiments performed back in 60's revealed an astonishing feature of solitons, basically they almost do not interact during collisions. After collision the velocities and amplitudes remains unchanged, only what is being changed is the separation distance between solitons.

This behavior gave a hint that there has to be present in KdV equation infinite number of invariant quantities, some kind of memory that allows solitons to remember their shape. It led to the discovery of infinite set of integrals of motion for this equation, see e.g. [Mk].

6 Undesirable effects

In this and in the following chapters we focus on the Toda lattice and KdV equation, and analyze this model from dynamical systems point of view. First of all, Toda lattice is an integrable system, as well as KdV equation, however having infinite degrees of freedom it posses also infinite number of integrals. One of the consequences of this fact is that the motion can be described by simple means, as we already have explained that in the case of KdV equation the motion takes form of solitons, whereas in the Toda lattices particle and momenta motion is quasi-periodic. This is due to the simplicity of the model. However this model is of little relevance to the reality, because of strong assumption that masses of all particles are equal to 1. We never find a system with bodies of exactly equal masses in the world that surround us. In next chapter we get rid of this "undesirable effect".

7 Modification of the model

In this section we propose a modification to the original model, such that resulting model will be free of what we called in the previous section "undesirable effect". Our modification is to introduce lack of homogeneity to the particle masses. For our purpose, we change masses of particles by introducing a perturbation to the particle masses.

Definition 3 *Inhomogeneous Toda lattice is a Toda lattice consisting particles having masses satisfying the law $m_i = 1 + \delta \sin 2\pi \frac{i}{n}$, where m_i is mass of the i-th particle, δ is the perturbation parameter.*

In the case of inhomogeneous Toda lattice motion equations (2) are slightly changed into

$$\begin{cases} \frac{dq_i}{dt} = p_i \\ \frac{dp_i}{dt} = ae^{-b(q_{i+1}-q_i)} - ae^{-b(q_i-q_{i-1})} \end{cases} \quad ,i = 0, \ldots, n-1 \tag{6}$$

Now very important question arise, what is the limit PDE of this system? We give answer shortly, but do not provide here detailed analysis, similar to the one presented in Section 4.2 plus some specific scaling.

Definition 4 *Continuous approximation of particle masses (3) is a continuous function $m\colon \mathbb{R} \to [1-\delta, 1+\delta]$, defined by $m(x) = 1 + \delta \sin 2\pi x$.*

Under assumption that there is a smooth 1-periodic function q defined on the circle that approximates the displacements i.e. $q_i(t) = q\left(t, 2\pi \frac{i}{n}\right)$ as $n \to \infty$ the limit PDE of (6) is

$$q_t + \frac{\delta}{2} \sin 2\pi x \, q_x + \frac{m(x)}{2} q_{xxx} + m(x) q \cdot q_x = 0 \tag{7}$$

The inhomogeneous Toda lattice is not integrable for three particles [Si2]. We have predicted "interesting" dynamics embodied by this system, in the sense that the motion is not anymore deterministic, and starting at some value of the perturbation parameter δ the system shows some part of ergodic behavior. Goal of our research is to examine inhomogeneous Toda lattice varying the number of particles and searching for behaviour that is invariant to changing number of particles. This, we hope, will be transfered to the limit case, which is perturbed KdV equation. (7).

8 Examination of inhomogeneous Toda lattice

8.1 Lyapunov exponents

In order to get an outlook of dynamics of (6) we used Lyapunov Characteristic Exponents as dynamics indicator, see e.g. [Sk]. For our purposes we have been approximating only maximal Lyapunov characteristic exponent. Basically it gives asymptotic behaviour of separation between two orbits that were started at points in some distance from each other.

Definition 5 *The quantity*

$$\chi_1(x_0, \xi_0) = \limsup_{t\to\infty} \frac{\log ||\xi(t)||}{t}$$

is called maximal Lyapunov Characteristic Exponent (mLCE) of (6). Where x_0 is an initial value, $\xi(t)$ is a deviation vector at time t and $||\xi_0|| = 1$, evolution of deviation vectors is governed by variational equation i.e. $\dot{\xi} = D^2H(q,p)\cdot\xi$.

Meaning of this quantity is as follows: if $\chi_1(x_0, \xi_0) > 0$ it guarantees that given orbit is chaotic, on contrary if $\chi_1(x_0, \xi_0) = 0$ the orbit is regular. In our approach we approximate (5) by numerical algorithm. We use the approximate value $\overline{\chi_1(x_0, \xi_0)} = \frac{\log ||\xi t||}{t}$ to predict the value of $\chi_1(x_0, \xi_0)$.

Definition 6 *The sum*

$$S_n = \log ||\xi_1|| + \log\frac{||\xi_2||}{||\xi_1||} + \log\frac{||\xi_3||}{||\xi_2||} + \cdots + \log\frac{||\xi_n||}{||\xi_{n-1}||}, \quad \xi_i = \xi(i\tau)$$

is called the n-th Lyapunov sum.

Using this approach we have to answer many questions. First, we cannot use infinite time, when should we stop calculations? Second, we have to perform thresholding in order to having an approximation, determine if mLCE is zero or positive. Last but not least question, how to make huge amount of data finish in reasonable time? We address them in the next section.

8.2 Numerical approximation

To answer first two questions, we determined by rule of thumb suitable values of T, being maximum time, and $\widetilde{\chi_1}$, being the threshold value. We have established $\widetilde{\chi_1} = 10^{-3}$, and then performed bunch of numerical simulations to look for T such that if $\chi_1 = 0$ then $\overline{\chi_1(x_0, \xi_0)} = \frac{\log ||\xi(t)||}{t}$ will most likely drop under $\widetilde{\chi_1}$ before time T. Thus T established at $T = 20000$. To address the last question, one of the implemented techniques was to do linear least-squares fitting of the Lyapunov sums (6) in order to determine if sums are growing linearly, because then if fit is good enough (5) is positive and we can stop calculating. There is also important issue how to avoid $||\xi_i||$ being out of range of representable fixed-point numbers, which may happen very quickly for chaotic orbits. To address this we simply normalize ξ_i at each time $i\tau$.

Still, at first shot we implemented Taylor algorithm solving simultaneously motion equations (6) and variational equations (5) using fast automatic differentiation library FADBAD [FADBAD]. It became obvious that this approach can not be used in practice due to very poor efficiency. Time of calculating a $\chi_1(x_0, \xi_0)$ for (6) with thirty particles and $T = 15000$ was six minutes on a PC. Then we become aware that such calculations could be made feasible by using Taylor solver with variable step size using custom implementation of fast automatic differentiation formulas that omits recalculating things. Doing so we reduced total time of calculating mentioned $\chi_1(x_0, \xi_0)$ for thirty particles down to six seconds. figure 8.2 presents striking difference between both mentioned approaches.

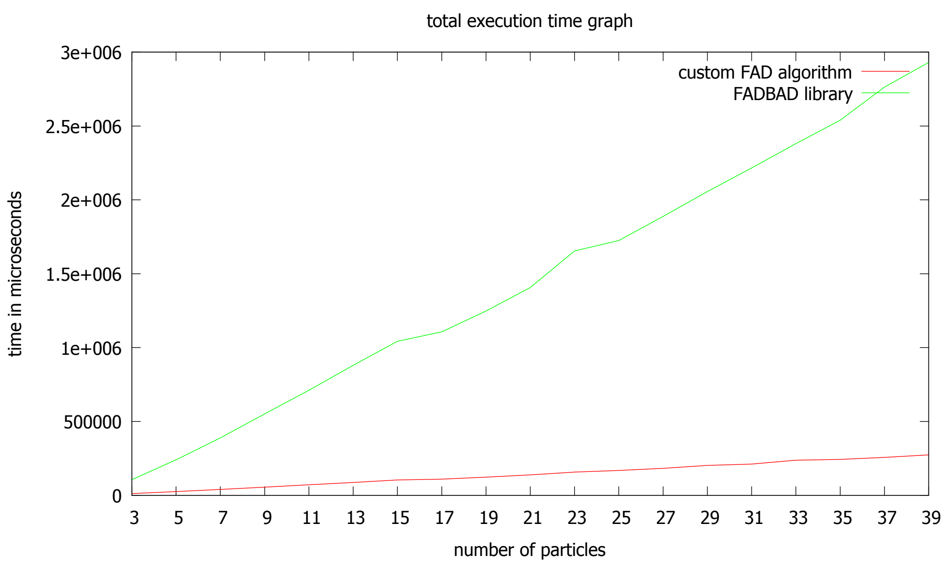

Figure 1:

9 Transition region

We performed experiment, which aimed at finding values of perturbation parameter δ^- and δ^+, such that if $\delta < \delta^-$ we will with high probability have $\chi_1(x_0, \xi_0, \delta, n) = 0$ and for $\delta > \delta^+$ we will have $\chi_1(x_0, \xi_0, \delta, n) > 0$. Basically speaking over δ^+ there is chaos, whereas under δ^- is determiniability. We present results on figure 9. By high probability we mean that for three random initial conditions we get expected quantities. We are aware that number of samples should be increased to refine this results, but with three particles already calculations were very time consuming. All of the initial conditions had normalized energy, we mean $H = 5$. For three particles very suprisingly we have not detected chaos at this energy level. The results give us hope that there is a universal parameter δ that is in the transition region for all amounts of particles.

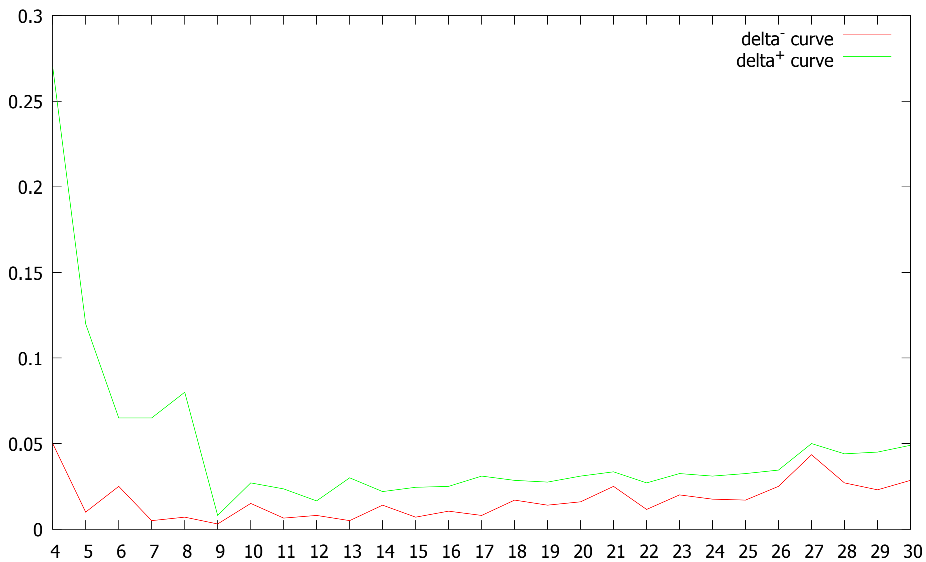

Figure 2:

10 Future

In this last section we present our future goals. First of all we are going to look at the transition region for all high number of particles up to 100 to predict what is going to happen in the limit case. Then having this knowledge we are going to search in this region hyperbolic periodic (quasi-periodic) orbits and then examine if homo/heteroclinic phenomena is present in indicated region. Having this knowledge we will move our attention to the limit PDE (7). Moreover to make numerical calculations fast enough to realize those tasks our algorithms will be parallelized to make them perform on a computer cluster.

References

[CF] G. Casati, J. Ford, *Stochastic transition in the unequal-mass Toda lattice*, Physical Review A 12:4 pp. 1702-1709 (1975).

[FADBAD] FADBAD, C++ library for automatic differentation, www.fadbad.com.

[FST] J. Ford, S. D. Stoddard, J. S. Turner, *On the Integrability of the Toda Lattice*, Progress of Theoretical Physics Vol. 50 pp. 1547-1560 (1973).

[JZ] A. Jorba, M. Zou, *A software package for the Numerical Integration of ODEs by means of High-Order Taylor Methods*, Experimental Mathematics 14:1 pp. 99-117 (2005).

[Kr] M. Kruskal, *Nonlinear wave equations*, Lecture Notes in Physics Vol. 38 pp. 310-354 (1974).

[Mk] H.P. McKean, *Integrable Systems and Algebraic Curves*, Lecture Notes in Mathematics Vol. 755, pp. 83-200 (1978).

[Si1] C. Simó, *On the Analytical and Numerical Approximation of Invariant Manifolds*, Les Methodes Modernes de la Mecanique Celeste (Course given at Goutelas, France, 1989), D. Benest and C. Froeschle (eds.), 285-329, Editions Frontieres, Paris, 1990.

[Si2] C. Simó, communication.

[Sk] Ch. Skokos, *The Lyapunov Characteristic Exponents and Their Computation*, Lecture Notes in Physics Vol. 790 pp.63-135 (2010).