KdV equation and energy sharing in FPU

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Abstract

We address the problem of equipartition in a long FPU chain. After giving a precise relation between FPU and KdV we use the latter equation to show that, corresponding to initial data *à la Fermi*, the time average of the energy on the k-th mode decreases exponentially with k/N. The result persists in the thermodynamic limit.

We study here the Fermi-Pasta-Ulam (FPU) α-chain for a large number N of particles and initial data in which only the first Fourier mode is excited. We show that the KdV is a normal form of the system that allows to describe the dynamics for quite long times (explicitly given). We use the KdV in order to show that, for such times, the time average of the energy in the k-th linear mode decreases exponentially with k/N. All the estimates depend only on the specific energy of the initial datum and thus persist in the limit where both the energy E and N tend to infinity with E/N fixed (thermodynamic limit).

1 Introduction

We study here the Fermi, Pasta and Ulam (FPU) problem concerning the distribution of energy among the Fourier modes of long anaharmonic chains. The origin of the problem is well known: FPU (see [1]) observed a lack of equipartition in the time evolution of the normal modes of the chain, at least when the energy is initially concentrated on the first mode. Moreover they observed that the time average of the energy on the k-th mode tends to stabilize after a short time interval. Since the appearing of the FPU work a question is open: is this phenomenon relevant for the foundations of statistical mechanics? The main point concerns the existence of the lack of equipartition in the so called thermodynamics limit, i.e. when the number of particles tends to infinity and the initial energy per particle is kept fixed.

To answer the question huge numerical computations have been done and different behaviours have been observed depending on the kind of initial data considered and on the kind of observable measured. The starting point of the present paper are the numerical observations by Berchialla, Galgani and Giorgilli [6]. Such authors, following FPU, observed that when one considers an initial datum with all the energy concentrated on the first Fourier mode, the energy rapidly flows to a nearby *packet* and then the evolution is essentially frozen. Actually, the idea that a frozen state is quickly formed, and that a subsequent approach to equilibrium would occur over an extremely larger time scale was first proposed in the paper [3]. What was added in the paper [6] is a rather precise description of the phenomenon, showing that it seems to depend only on intensive quantities, like the specific energy and the relative wave number (k/N) of the modes involved, as is expected in the thermodynamic limit.

In the present paper we give a theoretical explanation (not yet a rigorous proof) of the formation and stabilization of the packet in the thermodynamic limit. More precisely we obtain that the dynamics presents three characteristic time scales: A first short time scale over which the packet is formed; a subsequent quite long time scale over which the packet persists; and a third much longer time scale over which we are unable to make previsions, but over which a slow evolution towards equipartition could happen.

Our explanation is based on the relation between the FPU model and the Kortweg de Vries equation (KdV). First of all we use the tools of modern rigorous perturbation for PDEs [13] in order to show that a pair of decoupled KdV equations constitute the resonant normal form of the FPU in the region of the phase space where only long wave states are present. Here we give, at least in a simple situation, a precise statement concerning the relation between the PDEs and the original FPU model. In particular it turns out that the KdV allows to approximate in a good way the solutions of the FPU over a long but finite time scale. This is the time scale over which we are able to make previsions.

We recall that the existence of a relation between the FPU and KdV is known since a long time [2]. As a variant with respect to the standard approach we obtain here that two KdVs with periodic boundary conditions on a normalized annulus can be used to approximate a long (FPU) chain. As pointed out above, such a description can be made rigorous also for initial data of interest for the thermodynamic limit. Moreover, it turns out that the KdVs obtained have a small dispersion, precisely that there is a coefficient N^{-2} in front of the term with the third derivative.

Then we use the KdV in order to study the dynamics of the FPU. We start from the remark that, for large N, the term with the third derivative can be neglected and thus the KdV reduces to a Burgers equation. It is well known that any solution of the Burgers equation develops a singularity in finite times; correspondingly one sees a fast transfer of energy to the low frequency Fourier modes (formation of the packet). Afterwards, when the third derivative of the solution grows, the term with the third derivative becomes active with the consequences that energy stops flowing. This is the metastable part of the dynamics in which the packet does not change its shape. In particular we show that, due to the fact that the solution of the KdV is analytic in space, one always has exponential decay of the energy with the index k of the Fourier mode. More precisely we show that the time average of the energy on the k-th mode decays with k/N. This procedure is a generalization to the FPU of a method introduced in the paper [3], which in turn is inspired by a work of Frisch and Morf [4] in hydrodynamics. The present paper is also strongly related to the papers [8, 9, 10]

2 Relation between KdV and FPU

We consider the Hamiltonian system

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

$$U(x) = \frac{x^2}{2} + \frac{x^3}{3} \quad , \quad (2)$$

$$q_{n+2N} = q_n \quad , \quad p_{n+2N} = p_n \quad , \quad (3)$$

where $\boldsymbol{q} = (q_{-N}, \ldots, q_{N-1})$ and $\boldsymbol{p} = (p_{-N}, \ldots, p_{N-1})$ are the two sets of canonical conjugate variables. The Hamiltonian (1) is known as the Fermi, Pasta and Ulam (FPU) α-model (with $\alpha = 1$). Due to the periodic boundary conditions (3), the total linear momentum of the system is preserved. So one can restrict oneself to the case $\sum_n p_n = \sum_n q_n = 0$.

In the appendix we will present a procedure based on normal form which allows to deduce the KdV as a normal form for the FPU. Here we just give the final result of such a procedure, namely we describe how solving the KdV one gets informations on the FPU.

Thus, consider the following couple of KdV equations

$$\xi_t = \frac{1}{N^2}\frac{1}{24}\,\xi_{xxx} + \frac{\sqrt{\epsilon}}{\sqrt{2}}\,\xi\xi_x \ , \tag{4}$$

$$\eta_t = -\frac{1}{N^2}\frac{1}{24}\,\eta_{xxx} - \frac{\sqrt{\epsilon}}{\sqrt{2}}\,\eta\eta_x \ , \tag{5}$$

with periodic boundary conditions on $[-\pi, \pi]$. As will be clear in a while, ϵ plays the role of specific energy.

Given an analytic initial datum $\xi_0(x), \eta_0(x)$ with zero average, consider the corresponding solution $\xi(x,t), \eta(x,t)$. To such a solution we associate *an approximate solution* $q^{\rm app}$ of the FPU namely

$$\begin{aligned} q_j^{\rm app}(t) - q_{j+1}^{\rm app}(t) &\equiv r_j^{\rm app}(t) \\ &:= \sqrt{\epsilon}\left(\xi\left(\frac{j+t}{N}, \frac{t}{N}\right) + \eta\left(\frac{j-t}{N}, \frac{t}{N}\right)\right) \end{aligned} \tag{6}$$

which due to the condition $\sum_j q_j^{\rm app} = 0$ is uniquely defined. The relation with a true solution of the FPU system can be made precise. As an example we state now a theorem that can be obtained by applying methods similar to those of [12] (a paper with a detailed proof of a more precise result is in preparation).

Theorem 2.1. *There exist constants $C_1, C_2, T > 0$ such that, provided $\epsilon + N^{-4} < C_1$, then the solution $q(t)$ of the FPU model (1) with initial data $(q_j^{\rm app}(0), \dot{q}^{\rm app}{}_j(0))$ fulfills*

$$\left|q_j(t) - q_j^{\rm app}(t)\right| \leqslant C_2\sqrt{\epsilon}\left(\sqrt{\epsilon} + N^{-2}\right) \tag{7}$$

for all times t fulfilling

$$|t| \leqslant \frac{TN}{\sqrt{\epsilon}} \tag{8}$$

We want to stress here that for the deduction one does not perform any limit to the continuum. Here one has only to assume that i) the specific energy ϵ is small, and ii) N is very large.

Since we are interested in studying the evolution of the (time average of the) energy distribution of the modes of the FPU we give the relation between the spectrum of the functions ξ, η and the spectrum of the FPU. Consider the Fourier series of $r_j^{\rm app} \equiv q_j^{\rm app} - q_{j+1}^{\rm app}$, this is given by

$$\hat{r}_k^{\rm app} = \frac{1}{\sqrt{2N}}\sum_{j=-N}^{N-1} r_j^{\rm app} e^{-ijk\frac{\pi}{N}} \tag{9}$$

while the Fourier coefficients of the function ξ are given by

$$\hat{\xi}_k = \frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi} \xi(x) e^{-ixk} dx \tag{10}$$

and similarly for η. Inserting explicitly the time dependence, the relation between the two objects is given by

$$\begin{aligned} \hat{r}_k^{\rm app}(t) &= \sqrt{\frac{2N}{2\pi}}\sum_{l\in\mathbb{Z}}(\hat{\xi}_{k+2Nl}(t)e^{-it(k+2Nl)} \\ &\qquad + \hat{\eta}_{k+2Nl}(t)e^{it(k+2Nl)}) \\ &\simeq \sqrt{\frac{2N}{2\pi}}(\hat{\xi}_k(t)e^{-itk} + \hat{\eta}_k(t)e^{itk}) \end{aligned}$$

The last line is a good approximation of the complete expression if the spectrum of both ξ and η decreases fast with k.

Finally define the energy of the k-th mode by $E_k = (\hat{p}_k^2 + \omega_k^2\hat{q}_k^2)/2$ where as usual $\hat{p}_k$ is the Fourier coefficient of p_j and $\omega_k = 2\sin(\frac{k\pi}{2(N+1)})$ are the frequencies of the FPU. Thus, on the approximate solution one has

$$E_k(t) \sim N\epsilon\left(|\hat{\xi}_k|^2 + |\hat{\eta}_k|^2 + 2\Re(\hat{\xi}_k^*\hat{\eta}_k e^{i2kt})\right) \tag{11}$$

whose time average converges to $N\epsilon(|\hat{\xi}_k|^2 + |\hat{\eta}_k|^2)$. Thus, denoting by $\bar{E}_k(t)$ the time average at time t of the energy of the k–th mode then one has

$$\frac{\bar{E}_k(t)}{E_{tot}} \overset{t\to\infty}{\to} C\left(|\hat{\xi}_k|^2 + |\hat{\eta}_k|^2\right) \tag{12}$$

where E_{tot} is the total energy and C is a constant which in particular is independent of N.

3 Analysis of the KdV and spectrum of the FPU

The dynamics is thus reduced to the study of two uncoupled KdV. So we consider only one of them (that for the ξ variable).

We consider an initial datum with all the energy on the first linear mode. This is given by

$$\xi(x,0) = \cos(x) \ . \tag{13}$$

For large N one has that initially the term in ξ_{xxx} is negligible and the equation reduces to a Burgers Equation (BE):

$$\xi_t = \sqrt{\epsilon}\xi\xi_x \ , x \in [-\pi,\pi] \ . \tag{14}$$

One can easily show that the solution of (14) has a shock at a finite time given by

$$t_S \approx \frac{1}{\sqrt{\varepsilon}} \ . \tag{15}$$

At such a time ξ_x becomes infinite at $x = -\pi/2$ and the wave profile looks sawtooth-like. If one considers the analytic extension of the equation in the space variable, $x \to z \in \mathbb{C}$ and the corresponding solution $\xi(z,t)$, one has that at $t = 0^+$ a logarithmic singularity is generated and approaches the the real axis reaching it at t_S. Now it is well known that, if $\sigma(t)$ denotes the distance of the singularity of $\xi(z,t)$ from the real axis, the k-th Fourier coefficient $\hat{\xi}_k$ of ξ is estimated by

$$\left|\hat{\xi}_k\right| \leqslant \sqrt{2\pi} M e^{-\sigma(t)|k|} \ , \tag{16}$$

where M is the maximum of ξ in the strip of analyticity of width 2σ centered on the real axis. It is easily shown that for the (BE) equation (14) with initial datum (13),

$$M_{BE} \approx e^{\sigma(t)} \ . \tag{17}$$

Since $\sigma(t)$ approaches zero as $t \to t_S$, one realizes that energy is progressively transfered to all the Fourier modes in a finite time.

However as the singularity approaches the real axis the size of the term ξ_{xxx} increases and one has to take into account the effects of the corresponding term in the KdV. Indeed it is well known that the solution of the KdV equation (with analytic initial datum) is analytic for all times, see e.g. [15].

To continue the discussion we recall that if the solution is analytic in a strip $\sigma(t)$ and has maximum in such a strip given by M_{KdV} then one has

$$\frac{1}{N^2}|\xi_{xxx}| \leqslant \frac{1}{N^2}\frac{6M_{KdV}}{\sigma^3(t)} \tag{18}$$

and

$$\sqrt{\epsilon}|\xi\xi_x| \leqslant \sqrt{\epsilon}\frac{M^2_{KdV}}{\sigma(t)} \ . \tag{19}$$

Thus, as a first approximation one can think that the singularity stops approaching the real axis when the two quantities (18,19) are equal. To obtain an estimate simply replace M_{KdV} with M_{BE} given in (17). Within such an approximation, equality occurs when the singularity $\sigma(t)$ reaches a critical value σ_c solving the equation

$$\frac{6}{N^2\sqrt{\epsilon}} = e^{\sigma_c}\sigma_c^2$$

For large N, the solution is approximatively given by

$$\sigma = \frac{\sqrt{6}}{N\epsilon^{1/4}} \ .$$

Thus, going back to the FPU, one gets that the time average of the energy of the k-th mode, for t large, but smaller than $N/\sqrt{\epsilon}$, fulfills

$$\frac{\bar{E}_k(t)}{E_{tot}} \leqslant C e^{-\frac{\sigma_0}{\epsilon^{1/4}}\frac{k}{N}} \tag{20}$$

with constants C and σ_0 independent of N and of the specific energy ϵ.

It has to be pointed out here that from the estimate (20) one realizes that the quantities characterizing the phenomenon are intensive: they depend only on the specific energy $\varepsilon = E/N$. Thus, at least at a formal level, such estimates hold in the thermodynamic limit $E \to \infty$, $N \to \infty$ with $\varepsilon = E/N$ fixed.

The numerical results available in the literature are in agreement with the above predictions. The scaling $k_c \sim \varepsilon^{1/4}$ was observed both by Berchialla et al. [6] and by Biello et al. [7]. In both these works an exponential tail of the kind (20) in the FPU energy spectrum was observed.

4 Discussion

The problem we leave open here concerns mainly the estimate of the effects of the errors that is done in approximating the FPU with a couple of KdVs. Given for granted that such effects are relevant only on a time scale longer than the fast relaxation time of the KdV (to be verified in future works), the problem posed is whether deviations from KdV become relevant over power law time scales, $t \sim 1/\varepsilon^a$, or over stretched exponential ones, i.e. $t \sim e^{1/\varepsilon^a}$. The second seems to be the case, as conjectured first in [3], and numerically confirmed in [16] and [17]; see also [18] and [19]. The possibility that the relaxed states observed in FPU experiments might be actually meta equilibrium states was clearly stated for the first time, to our knowledge, in [20]. We think that the theoretical explanation of such a two time scale scenario *à la Parisi* constitutes the future challenge in the field.

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A Appendix: Deduction of the KdV

Let $p(x)$, $q(x)$, $x \in [-N, N]$ be interpolating functions for p_n and q_n, namely periodic functions with zero average such that $q(n) = q_n$ and $p(n) = p_n$ for any integer n. If the dynamics of the interpolating functions is controlled by the Hamiltonian

$$H(q,p) = \int_N^N \left(\frac{p^2}{2} + U((e^{\partial_x} - 1)q) \right) dx \qquad (21)$$

where e^{∂_x} is the translation operator, namely $[e^{\partial_x} q](x) = q(x+1)$, then the q_n's fulfill the FPU equations. We recall that the equations of motion of (21) are given by $\dot z = J \frac{\delta H}{\delta z}$, where $z = (q,p)$, and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

is the Poisson tensor, while $\frac{\delta H}{\delta z} \equiv \left(\frac{\delta H}{\delta q}, \frac{\delta H}{\delta p} \right)$ is the L^2 gradient of the Hamiltonian.

Remark that on the space of functions with zero average the operator $e^{\partial_x} - 1$ is invertible, so it is natural to introduce a new variable $\Phi(x)$ and a new momentum $r(x)$ by

$$r = -(e^{\partial_x} - 1)q \ , \quad p = (e^{\partial_x} - 1)\Phi \ ,$$

Moreover we are interested in long–wave–small–amplitude initial data, so we consider solutions of the form

$$r(x) = \sqrt{2\epsilon}\, u(\mu x) \ , \quad \Phi(x) = \sqrt{2\epsilon}\, v(\mu x) \qquad (22)$$

with u, v periodic functions of period 2π, μ a small parameter which in order to preserve the periodicity of the original variables has to fulfill $\mu = K/2N$ with some integer K. Finally ϵ has the meaning of specific energy. In the new variables (and rescaling time to μt) the Hamiltonian takes the form

$$H(\Phi, r) = \int_{-\pi}^{\pi} \left(\frac{u^2}{2} + \frac{[(e^{\mu\partial_x} - 1)v]^2}{2} + \sqrt{2\epsilon}\frac{u^3}{3} \right) dx \qquad (23)$$

We make now a non canonical change of variables which simplifies the main part of the Hamiltonian correspondingly we change the Poisson tensor. Thus introduce the variables

$$\xi := \frac{u + v_x}{\sqrt{2}} \ , \quad \eta := \frac{u - v_x}{\sqrt{2}} \qquad (24)$$

so that the Hamiltonian takes the form

$$H(\xi, \eta) = \int_{-\pi}^{\pi} \left[\frac{\xi^2 + \eta^2}{2} + \mu^2 \frac{[\partial_x(\xi - \eta)]^2}{4} \right] dx + \int_{-\pi}^{\pi} \sqrt{\epsilon} \left[\frac{(\xi + \eta)^3}{6} \right] dx + \text{h.o.t.} \ . \qquad (25)$$

where h.o.t. denotes higher order terms. Denoting $X = (\xi, \eta)$, the equation of motion takes the form

$$X_t = J \frac{\delta H}{\delta X} \ , \qquad (26)$$

where the Poisson tensor J is now

$$J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \partial_x \ . \tag{27}$$

For completeness we write down the main part of the equation of motion (26) explicitly by components:

$$\xi_t = \left[\xi - \mu^2 \frac{\partial_{xx}}{2} (\xi - \eta) + \frac{\sqrt{\epsilon}}{2} (\xi + \eta)^2 \right]_x \ ,$$
$$\eta_t = - \left[\eta - \mu^2 \partial_{xx} (\eta - \xi) + \frac{\sqrt{\epsilon}}{2} (\xi + \eta)^2 \right]_x \tag{28}$$

Changes of variables similar to the ones performed above and leading to the symplectic structure of the KdV equation were used in reference [5] in the framework of the water wave problems.

The Hamiltonian (25) appears as a perturbation of the linear Hamiltonian

$$H_0(X) := \int_{-\pi}^{\pi} \frac{\xi^2 + \eta^2}{2}$$

whose Hamilton equations are $\xi_t = \xi_x$, $\eta_t = -\eta_x$ the flow of which is periodic. So it is natural to use averaging theory in order to transform the Hamiltonian (25) into a simpler system. We recall that the formal procedure is as follows: consider a Hamiltonian system with Hamiltonian

$$H(X) = H_0(X) + P(X) + Q(X) \ , \tag{29}$$

with $H_0 \gg P \gg Q$ (Q representing here the h.o.t. of eq. (25)), and denote by $\Phi^t(\xi, \eta)$ the flow of the linearized system, namely

$$\Phi^t(\xi, \eta)(x) := (\xi(x + t), \eta(x - t)) \ .$$

Then (see e.g. [14] or [13]) one can construct a canonical change of coordinates such that in the new coordinates the Hamiltonian (29) takes the form

$$H_0(X) + \langle P \rangle (X) + h.o.t \tag{30}$$

where

$$\langle P \rangle (X) := \frac{1}{2\pi} \int_0^{2\pi} P[\Phi^s(X)] ds \tag{31}$$

$$\equiv \int_{-\pi}^{\pi} \left[-\mu^2 \frac{\xi_x^2 + \eta_x^2}{48} + \sqrt{\epsilon} \frac{(\xi^3 + \eta^3)}{6\sqrt{2}} \right] dx \ . \tag{32}$$

The equations of motion of $H_0 + \langle P \rangle$ are

$$\xi_t = \xi_x + \frac{1}{24} \xi_{xxx} + \frac{1}{\sqrt{2}} \xi \xi_x \ , \tag{33}$$

$$\eta_t = -\eta_x - \frac{1}{24} \eta_{xxx} - \frac{1}{\sqrt{2}} \eta \eta_x \ , \tag{34}$$

i.e. two KdV equations in translating frames. Passing to the translating frames one gets the two standard uncoupled KdVs. Going back to the variables of the FPU one gets the construction of the approximate solution of the FPU as given in sect. 2.

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