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Dynamics of the Fermi-Pasta-Ulam system

A. GIORGILLI

Univ. degli Studi di Milano, Dipt. di Matematica
Milano
Italy

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by Antonio Giorgilli

This document contains the pages presented at the Advanced Workshop on Anderson Localization, Nonlinearity and Turbulence: a Cross–Fertilization, Gargnano (Trieste), august 26 – september 3, 2010.

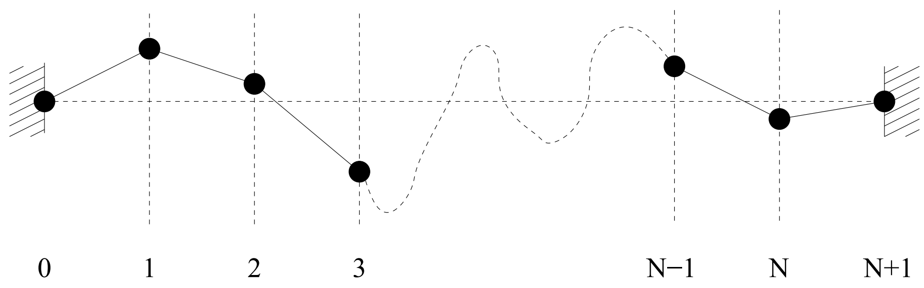
The pages with the movies can not be included in a text, of course. I apologize for the inconvenience.

An introductory text on which these pages are based may be found in:

The Fermi-Pasta-Ulam problem: a status report, G. Gallavotti ed., Lect. Not. Phys, **728** Springer, Berlin Heidelberg (2008).

FPU ?

RICOMINCIO DA TRE !



Work in progress, in collaboration with

Luisa Berchialla
Andrea Carati
Simone Paleari
Antonio Ponno
Dario Bambusi
Luigi Galgani
Tiziano Penati

and with contributions of many others.

The FPU paradox

The question

"The ergodic behaviour of such systems was studied with the primary aim of establishing, experimentally, the rate of approach to the equipartition of energy among the various degrees of freedom of the system"

$$\overline{E}_j = \frac{1}{T}\int_0^T E_j(t)dt \longrightarrow \frac{E}{N}$$

where E_j is the harmonic energy of the normal modes and E is the total energy.

The model

- The Hamiltonian

$$H(x,y) = \sum_{j=1}^{N} \frac{y_j^2}{2} + V(x_0,\ldots,x_{N+1})$$

- Fixed ends condition

$$x_0(t) = x_{N+1}(t) = 0$$

- Potential energy

$$V(x_0,\ldots,x_{N+1}) = \frac{1}{2}\sum_{j=0}^{N}(x_{j+1}-x_j)^2 + \frac{\alpha}{3}\sum_{j=0}^{N}(x_{j+1}-x_j)^3 + \frac{\beta}{4}\sum_{j=0}^{N}(x_{j+1}-x_j)^4$$

α, β arbitrary parameters.

- Normal modes

$$x_j = \sqrt{\frac{2}{N+1}} \sum_{k=0}^{N} q_k \sin \frac{jk\pi}{N+1} \ , \quad j = 1, \ldots, N$$

$$y_j = \sqrt{\frac{2}{N+1}} \sum_{k=0}^{N} p_k \sin \frac{jk\pi}{N+1} \ , \quad j = 1, \ldots, N$$

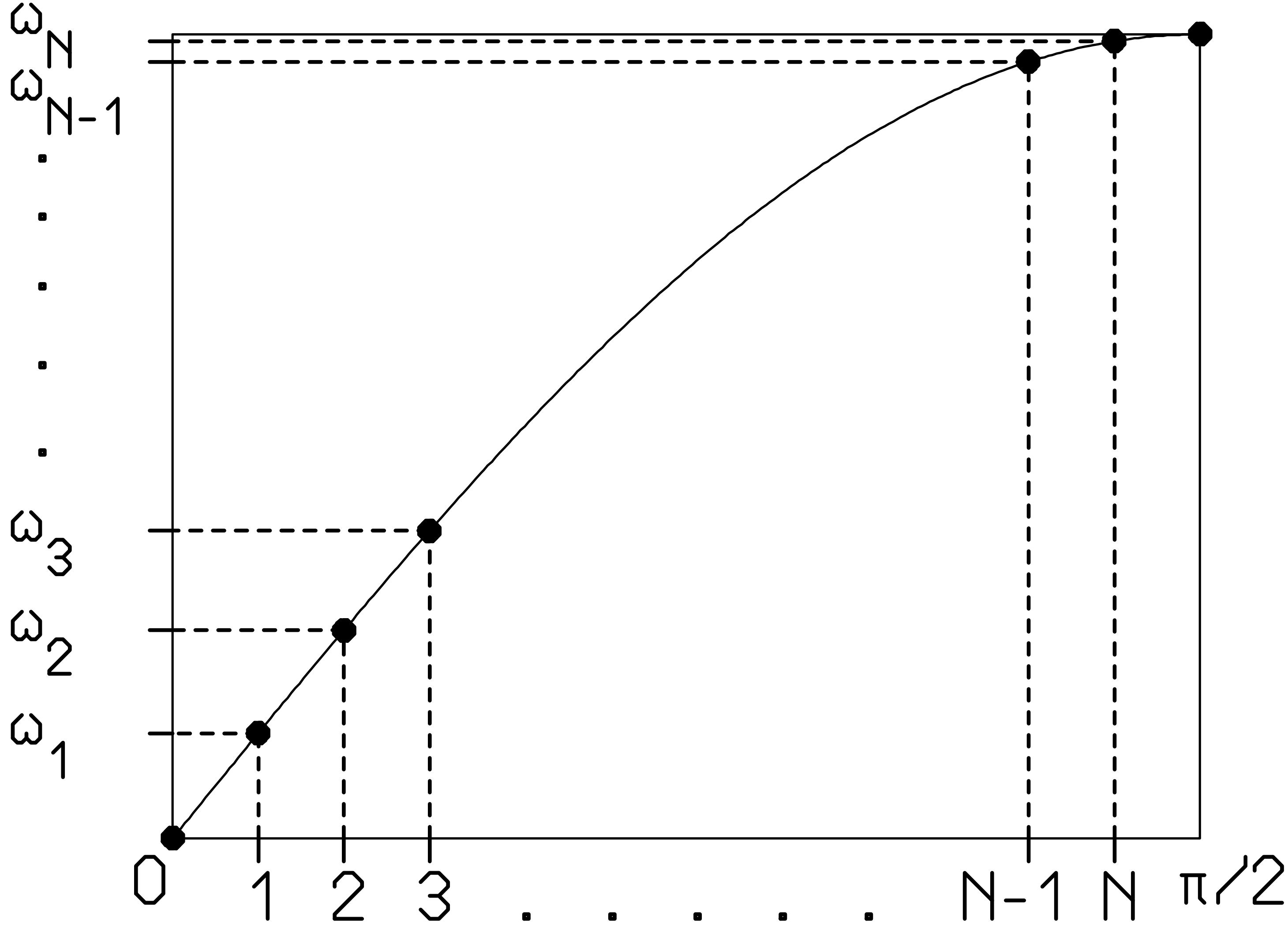
- Transformed Hamiltonian

$$H(q,p) = \frac{1}{2} \sum_{k=1}^{N} \left(p_k^2 + \omega_k^2 q_k^2 \right) + \alpha V_3(q) + \beta V_4(q)$$

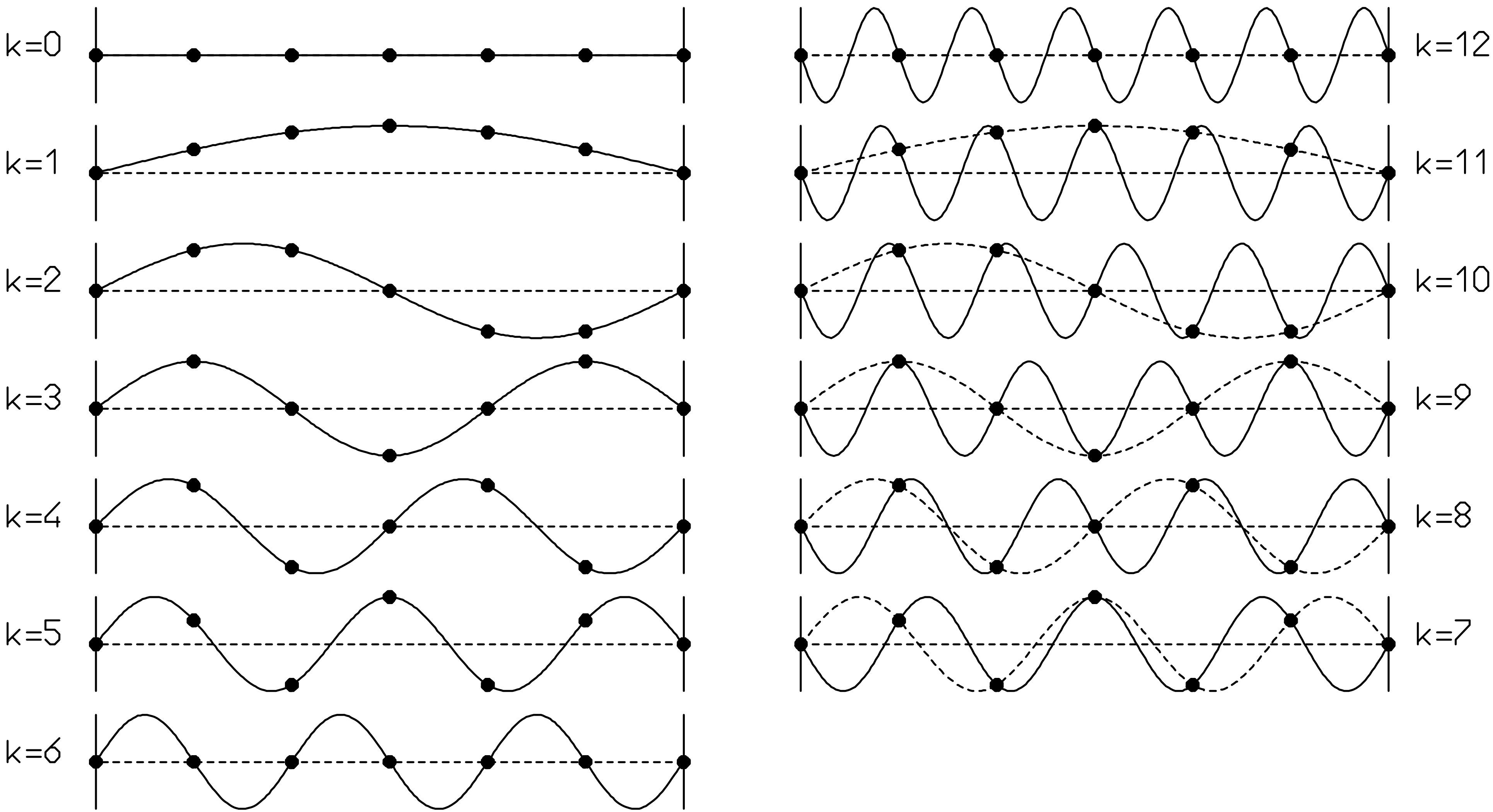
- The spectrum

$$\omega_k = 2 \sin \frac{k\pi}{2(N+2)} \ , \quad k = 1, \ldots, N$$

The spectrum of the linear chain



The normal modes of the linear chain



The beginning

"After the war, during one of his frequent summer visits to Los Alamos, Fermi became interested in the development and potentialities of the electronic computing machines."

. . . .

"We decided to try a selection of problems for heuristic work where in absence of closed analytic solutions experimental work on a computing machine would perhaps contribute to the understanding of properties of solutions".

. . . .

"In addition, such experiments on computing machines would at least have the virtue of having the postulates clearly stated".

. . . .

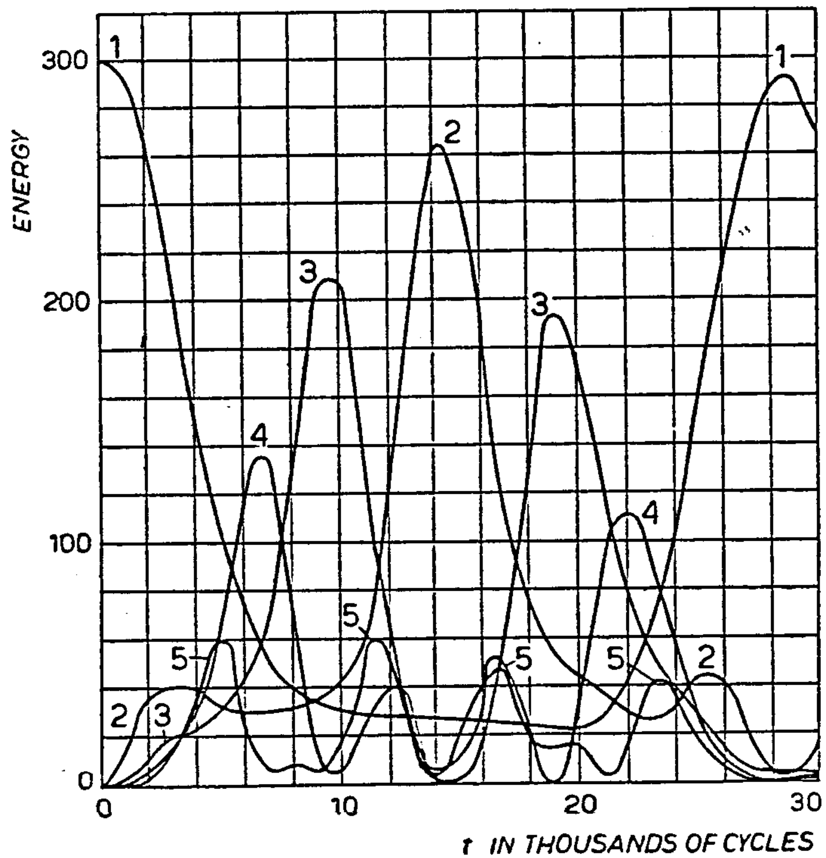
"One could venture a guess that one motive in the selection of problems could be traced in Fermi's early interest in ergodic theory".

S. Ulam

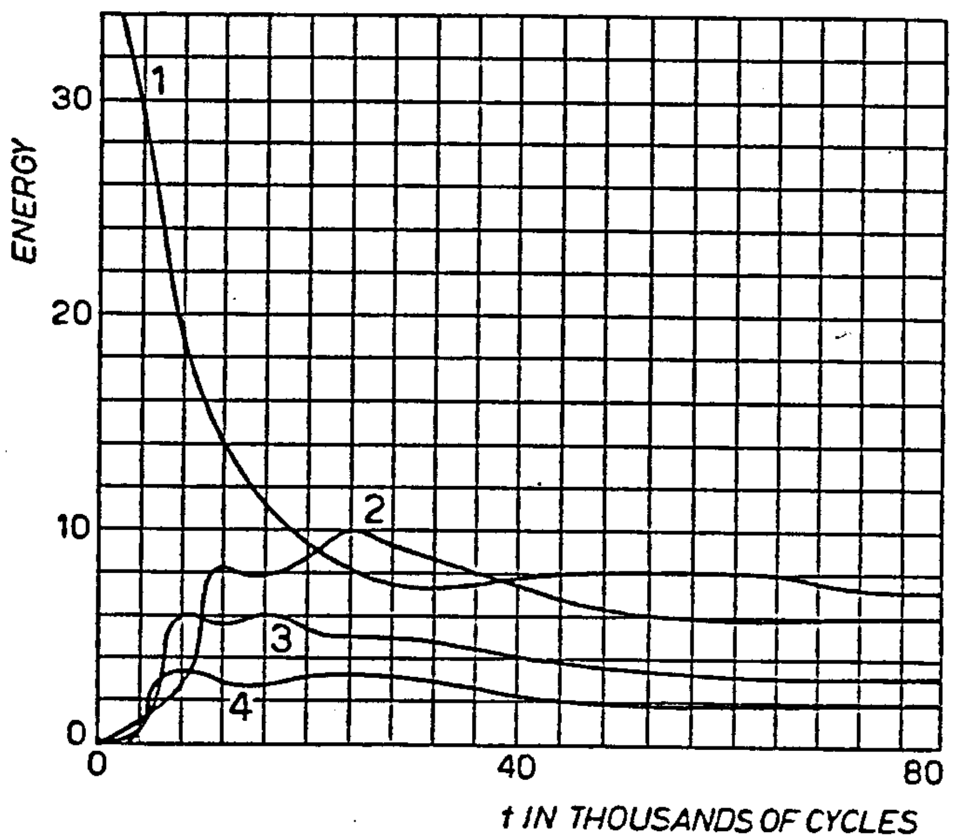
The answer of Fermi, Pasta and Ulam

"Let us say here that the results of our computations show features which were, from the beginning, surprising to us. Instead of a gradual, continuous flow of energy from the first mode to higher modes, all of the problems show an entirely different behaviour. (...) Instead of a gradual increase of all the higher modes, the energy is exchanged, essentially, among only a certain few. It is, therefore, very hard to observe the rate of 'thermalization' or mixing in our problem, and this was the initial purpose of the calculation".

The FPU experiment revisited



The time evolution of the harmonic energies. The figure is a reproduction of the first one of the original FPU report. Here, $N = 32$ (with $\alpha = 1/4$, $\beta = 0$)), and the energy was given initially just to the lowest frequency mode. One sees that the energy, instead of flowing to all the 32 modes, remains confined within a packet of low–frequency modes, namely modes 1 up to 5.



Time–averaged harmonic energies $\overline{E}_k$ vs. time. The figure is a reproduction of the last one of the original FPU report.

The prehistory

Ergodicity

Hamiltonian system

$$H(p,q) = h(p) + \varepsilon f(p,q)$$

with p the action variables, q the angles, ε a small parameter.

- Time average of a dynamical variable $f(p,q)$:

$$\langle f \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T f\big(p(t), q(t)\big) dt$$

- Phase average over the surface Σ_E of constant energy:

$$\overline{f} = \int_{\Sigma_E} f(p,q) d\sigma$$

- The system is ergodic if $\langle f \rangle = \overline{f}$ almost everywhere on Σ_E

Ergodicity and equipartition

Hamiltonian in the neighbourhood of an elliptic equilibrium expanded in power series

$$H(x,y) = H_2(x,y) + H_3(x,y) + H_4(x,y) + \ldots$$

where

$$H_2(x,y) = \sum_j \frac{\omega_j}{2}(x_j^2 + y_j^2)$$

- In action–angle variables p, q

  $$x_j = \sqrt{2p_j}\cos q_j \ , \quad y_j = \sqrt{2p_j}\sin q_j$$

  takes the form

  $$H(p,q) = h(p) + \varepsilon f(p,q)$$

  with

  $$h(p) = \sum_j \omega_j p_j$$

Ergodicity and equipartition

QUESTION

Does the perturbation make the system ergodic for any ε?

For the FPU system equipartition follows from ergodicity:

$$\overline{E}_j = \frac{1}{T}\int_0^T E_j(t)dt \longrightarrow \frac{E}{N}$$

where $E_j = \omega_j p_j$ is the harmonic energy of the normal modes and E is the total energy.

Non–integrability theorem of Poincaré

Let

$$H(p,q) = h(p) + \varepsilon f(p,q)$$

be analytic and satisfy

(i) non degeneration

$$\det\left(\frac{\partial^2 h}{\partial p_j \partial p_k}\right) \neq 0$$

(i.e., the frequencies $\omega_j = \frac{\partial h}{\partial p_j}$ are *non–isochronous*);

(ii) genericity: the coefficient $f_k(p)$ Fourier expansion of the perturbation

$$f(p,q) = \sum_{k\in\mathbf{Z}^n} f_k(p) e^{i\langle k,\omega\rangle}$$

are not identically zero on the surface $\langle k, \omega(p)\rangle = 0$.

Then there are no analytic first integrals independent of H.

(Poincaré, Méthode Nouvelles, Tome I, Ch. VIII)

Generalization by Fermi

Let

$$H(p,q) = h(p) + \varepsilon f(p,q)$$

be as in Poincaré's theorem.
Then there is no analytic invariant surface of dimension $2n-2$ embedded in the surface Σ_E of constant energy.

- Fermi's conclusion: the energy surface can not be decomposed in two invariant subsets of positive measure, hence the motions is ergodic on Σ_E.
- *but:* he *assumes* that the surface of separation is *analytic* (or at least smooth), which needs not be true.

(E. Fermi: Physikalische Zeitschrift **24**, 1923.)

Two conjectures

The conjecture of Izrailev – Chirikov (1966)

There is an energy threshold below which the system is not ergodic, due to the existence of a set of invariant tori of positive measure (Kolmogorov's theorem).

but:

- For increasing N the the spectrum becomes more and more resonant.
- Due to resonance overlapping the exchange of energy among modes becomes more and more effective.
- The threshold for applicability of Kolmogorov's theorem decreases (very rapidly!) to zero when N tends to infinity.
- Thus, ergodicity is recovered in the thermodynamic limit $N \to \infty$.

(see also Kantz (1989); Kantz, Livi and Ruffo (1994), Shepelyansky (1997), Casetti, Cerruti–Sola, Pettini and Cohen (1997), among others.)

The conjecture of Bocchieri – Scotti – Bearzi – Loinger (1970)

There is threshold in specific energy below which the system is not ergodic.

- Based on calculations with the Lennard–Jones potential.
- The threshold remains positive in the thermodynamic limit, being related to *specific energy* E/N.

(see also Galgani and Scotti (1972), Cercignani, Galgani and Scotti (1972), Livi, Pettini, Ruffo, Sparpaglione and Vulpiani (1985), among others.)

Kolmogorov's theorem and invariant tori

The theorem of Kolmogorov

Hamiltonian:

$$H(p,q) = h(p) + \varepsilon f(p,q) \ .$$

Assume:

(i) non–degeneration, i.e.,

$$\det\left(\frac{\partial^2 h}{\partial p_j \partial p_k}\right) \neq 0 \ ;$$

(ii) the *unperturbed* system possesses an invariant torus p^* with diophantine (non resonant) frequencies $\lambda = \omega(p^*)$, i.e.,

$$\bigl|\langle k,\lambda\rangle\bigr| \geq \gamma |k|^{-\tau} \quad \text{for } 0 \neq k \in \mathbf{Z}^n$$

with some constants $\gamma > 0$ and $\tau \geq n-1$.

If ε is small enough, $\varepsilon < \varepsilon^*$ say, then the perturbed system possesses an invariant torus carrying quasi–periodic motions with frequencies λ .

Applicability of Kolmogorov's theorem to the FPU system

- Non degeneration hypothesis: the unperturbed (quadratic part) of the Hamiltonian is isochronous, so it is degenerate.
- Non–resonance: what about resonances in the FPU spectrum?
- Threshold for applicability ε^*: what about the dependence on the number N of particles?

Removing the non–degeneration

Give the Hamiltonian

$$H(x,y) = \sum_{j=1}^{N} \frac{\omega_j}{2}(x_j^2 + y_j^2) + H_3(x,y) + H_4(x,y) + \ldots$$

the *Birkhoff normal form* up to degree 4

$$H^{(4)}(x,y) = H_2(x,y) + Z_4(x,y) + \ldots$$

where

$$H_2 = \sum_{j=1}^{N} \omega_j p_j \ , \quad Z_4 = \sum_{i,j} a_{i,j} p_i p_j \ , \quad p_j = \frac{x_j^2 + y_j^2}{2} \ .$$

- If the spectrum has no resonances up to order 4, i.e.,

  $$\langle k, \omega \rangle \neq 0 \quad \text{for } 0 < |k| \leq 4$$

  then $H^{(4)}$ for the FPU β model is non degenerate (Nishida, 1971).

- *but...:* does the FPU spectrum satisfy the non resonance condition?

Resonances in the FPU spectrum

Frequencies in the FPU spectrum

$$\omega_j = \sin \frac{j\pi}{2(N+1)}$$

- The frequencies are rationally independent if and only if $N+1$ is either prime or a power of 2 (Hemmer, 1959).
- In all other case there are resonance relation, including resonances of order 4; e.g.:

$$\begin{aligned}
\sin(\pi/6) + \sin(3\pi/14) - \sin(\pi/14) - \sin(5\pi/14) &= 0 \ , \quad N+1 = 42 \ , \\
\sin(\pi/6) + \sin(13\pi/30) - \sin(7\pi/30) - \sin(3\pi/10) &= 0 \ , \quad N+1 = 30 \ , \\
\sin(\pi/2) + \sin(\pi/10) - \sin(\pi/6) - \sin(3\pi/10) &= 0 \ , \quad N+1 = 30 \ .
\end{aligned}$$

- However, resonant term *do not* occur at order 4 in the FPU periodic β model, due to symmetries (Rink and Verhulst, 2000; Rink, 2006).

Energy threshold for the FPU chain

Thus, Komogorov's theorem applies to the FPU periodic β model if the energy E is small enough.

but . . . : How small?

- The parameter is $\varepsilon \sim \varrho$, the convergence radius of the Birkhoff's normal form;
- thus, $\varepsilon \sim \sqrt{E}$, the square root of the energy (may be $\varepsilon \sim \sqrt{E/N}$?);
- the best available estimates for Kolmogorov's theorem give $\varepsilon^* \sim C^{-N}$ with $C > 1$.

Kolmogorov's theorem applies for every finite N, but will likely become useless for very large N.

The metastability scenario

Exponential stability for an elliptic equilibrium

The Hamiltonian around the equilibrium

$$H(x,y) = H_2(x,y) + H_3(x,y) + \ldots$$
$$H_2(x,y) = \sum_j \frac{\omega_j}{2}(x_j^2 + y_j^2)\ .$$

$H_s(x,y)$ a homogeneous polynomial of degree s.

Birkhoff normal for at order r:

$$Z(x,y) = H_0(x,y) + Z_1(x,y) + \ldots + Z_r(x,y) + \mathcal{F}^{(r+1)}(x,y)$$

with

- Z_s a function of $p_j = \frac{x_j^2+y_j^2}{2}$ only (i.e., integrable);
- $\mathcal{F}^{(r+1)}(x,y)$ of degree at least $r+1$.

General result

- Assume $\left|\langle k,\omega\rangle\right| \geq \gamma|k|^{-\tau}$ with $\gamma > 0$ and $\tau > N-1$ (diophantine condition).
- In a polydisk $\Delta_{\varrho} = \{(x,y)\ :\ x_j^2 + y_j^2 \leq \varrho^2 R_j^2\}$ get

$$\left|\mathcal{F}^{(r+1)}(x,y)\right| \leq (r!)^{\tau+1} B^r \varrho^{r+3}$$

- the transformation to normal form is generally divergent: use truncation.
- optimize r as a function of ϱ and get

$$r \sim \frac{1}{\varrho^{1/(\tau+1)}}\ ,\quad \left|\mathcal{F}^{(r_{\rm opt})}(x,y)\right| \sim \exp\bigl(-(1/\varrho)^{1/(\tau+1)}\bigr)$$

  (exponential estimate of Nekhoroshev's type).
- The actions p_j of the system are almost constant up to time

$$T_{\rm stab} \sim \exp\bigl((1/\varrho)^{1/(\tau+1)}\bigr)\ .$$

If not eternity, this is a considerable slice of it (Littlewood).

The resonant case

Birkhoff normal for at order r:

$$Z(x,y) = H_0(x,y) + Z_1(x,y) + \ldots + Z_r(x,y) + \mathcal{F}^{(r+1)}(x,y)$$

with

$$\{H_0, Z_s\} = 0 \qquad \text{(resonant normal form)}$$

- Let $\mathcal{M} = \{k \in \mathbf{Z}^N \ : \ \langle k, \omega \rangle = 0\}$ (the *resonance module*).
- In action–angle variables p, q the normal form $Z_1, \ldots, Z_r$ depends only on $p_1, \ldots, p_n$ and $\langle k, q \rangle$ with $k \in \mathcal{M}$.
- There are $N - \dim \mathcal{M}$ approximate first integrals

$$\Phi = \sum_{j=1}^{n} \alpha_j p_j \ , \quad \alpha \perp \mathcal{M}$$

  which are independent of H.

Exponential estimate for the resonant case

- Change the diophantine condition to

$$\bigl|\langle k,\omega\rangle\bigr| \ge \gamma |k|^{-\tau} \quad \text{for } k \notin \mathcal{M}$$

  with $\gamma > 0$ and $\tau > n - \dim \mathcal{M} - 1$.
- The relevant quantity is *the number of rationally independent frequencies* $m = n - \dim \mathcal{M}$
- The approximate first integrals Φ remain almost constant up to time

$$T_{\rm stab} \sim \exp\bigl((1/\varrho)^{1/(\tau+1)}\bigr) \ .$$

- Remark: $\tau + 1 \sim m$.

Resonance may increase stability.

(Benettin, Galgani and Giorgilli, 1989)

Example: the FPU chain with alternatig masses

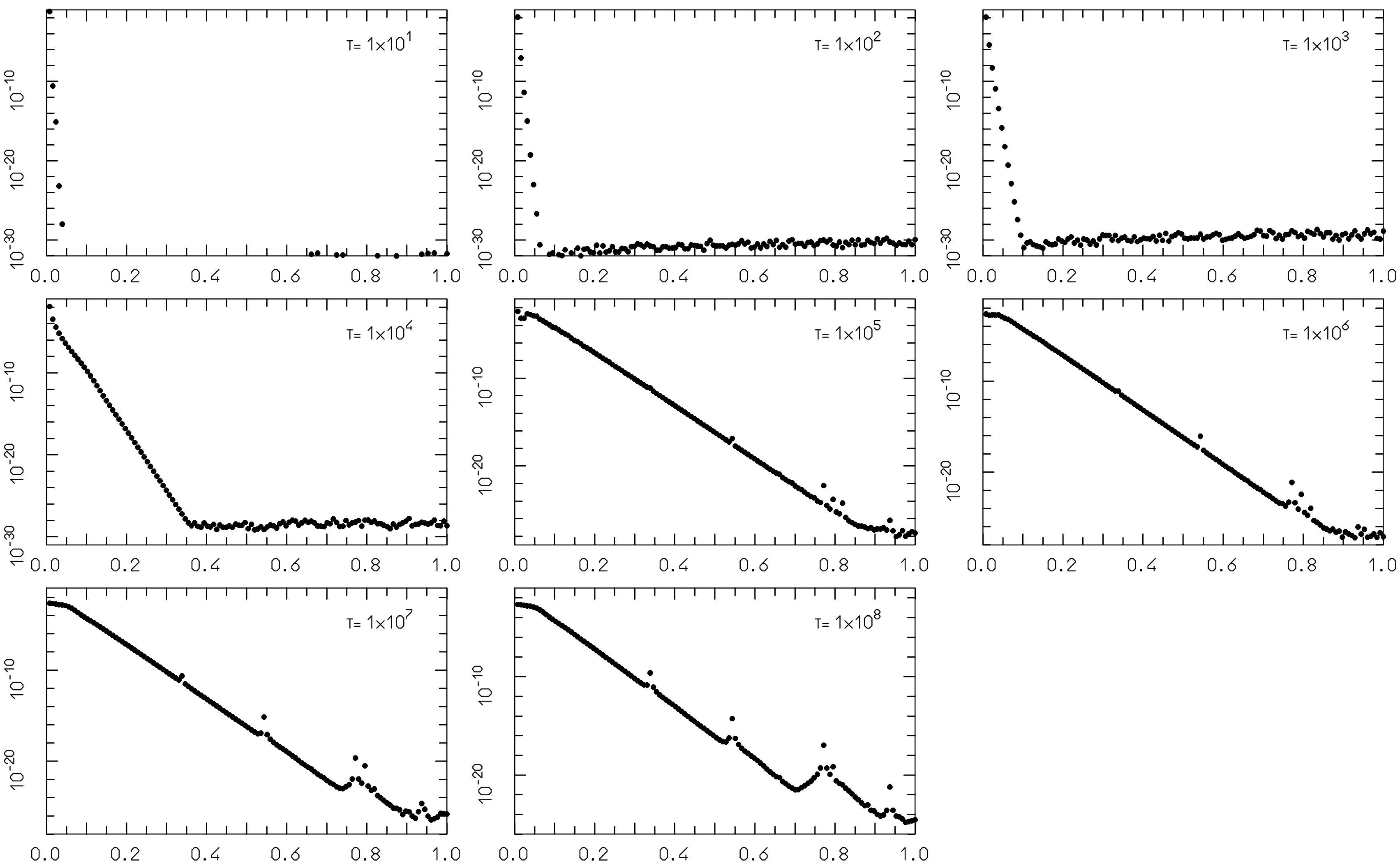
- The spectrum splits into
  - "acoustic" frequencies $\leq \omega$
  - "optical" frequencies $> \Omega \gg \omega$

- The energy flow (acoustic modes) $\longrightarrow$ (optical modes) is exponentially slow.

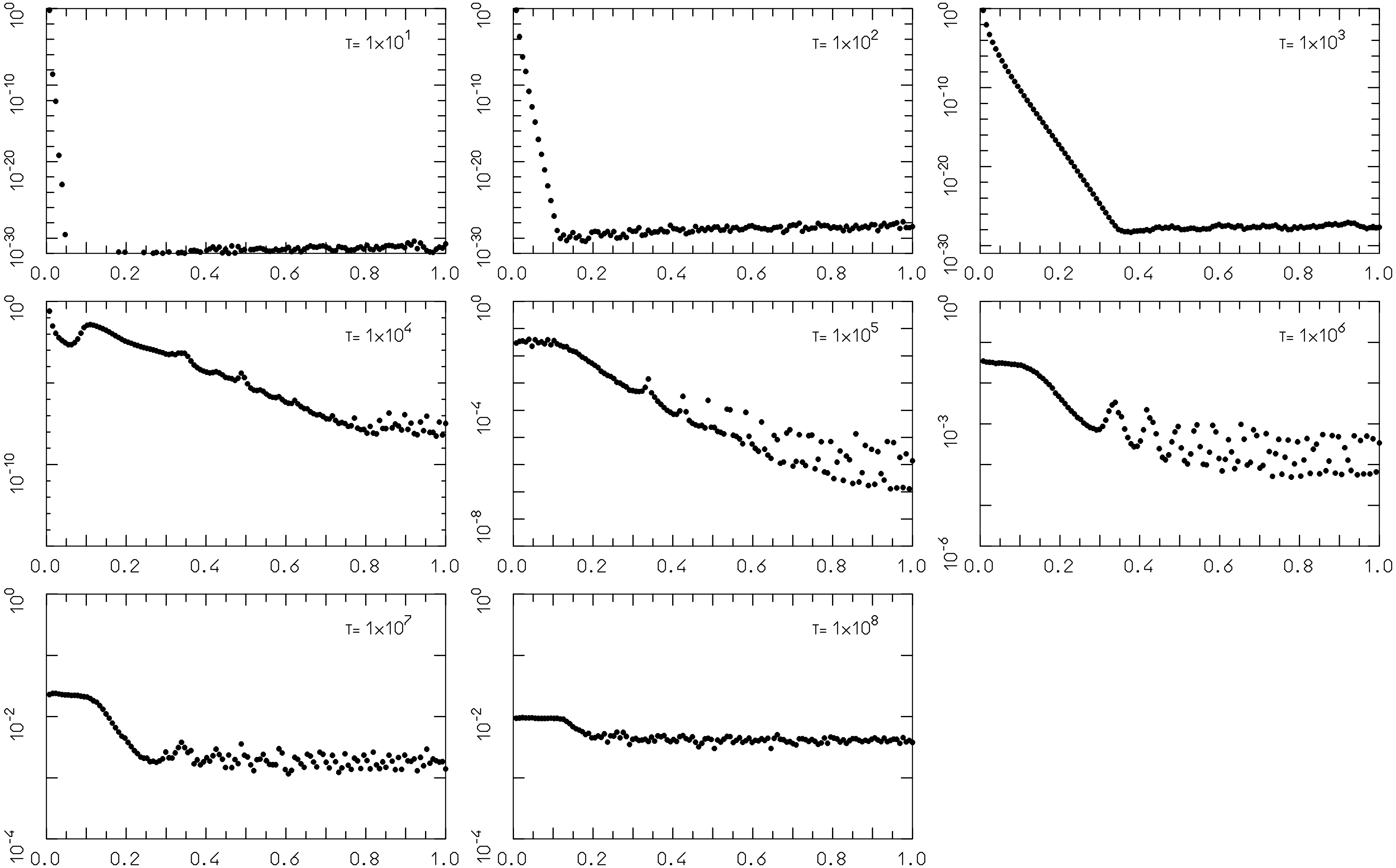
- Relaxation time: $T_{\mathrm{r}} \sim \exp(\Omega/\omega)$.

- Theoretical estimate (Benettin, Galgani and Giorgilli, 1989) confirmed by numerical calculations (Galgani, Giorgilli, Martinoli and Vanzini, 1992).

- Further Analytical results for $N \to \infty$, but typically with fixed *total* energy or with very particular initial conditions (Benettin, Fröhlich and Giorgilli, 1988; Bambusi and Giorgilli, 1993; Ponno and Bambusi, 2004; Bambusi and Ponno, 2006)

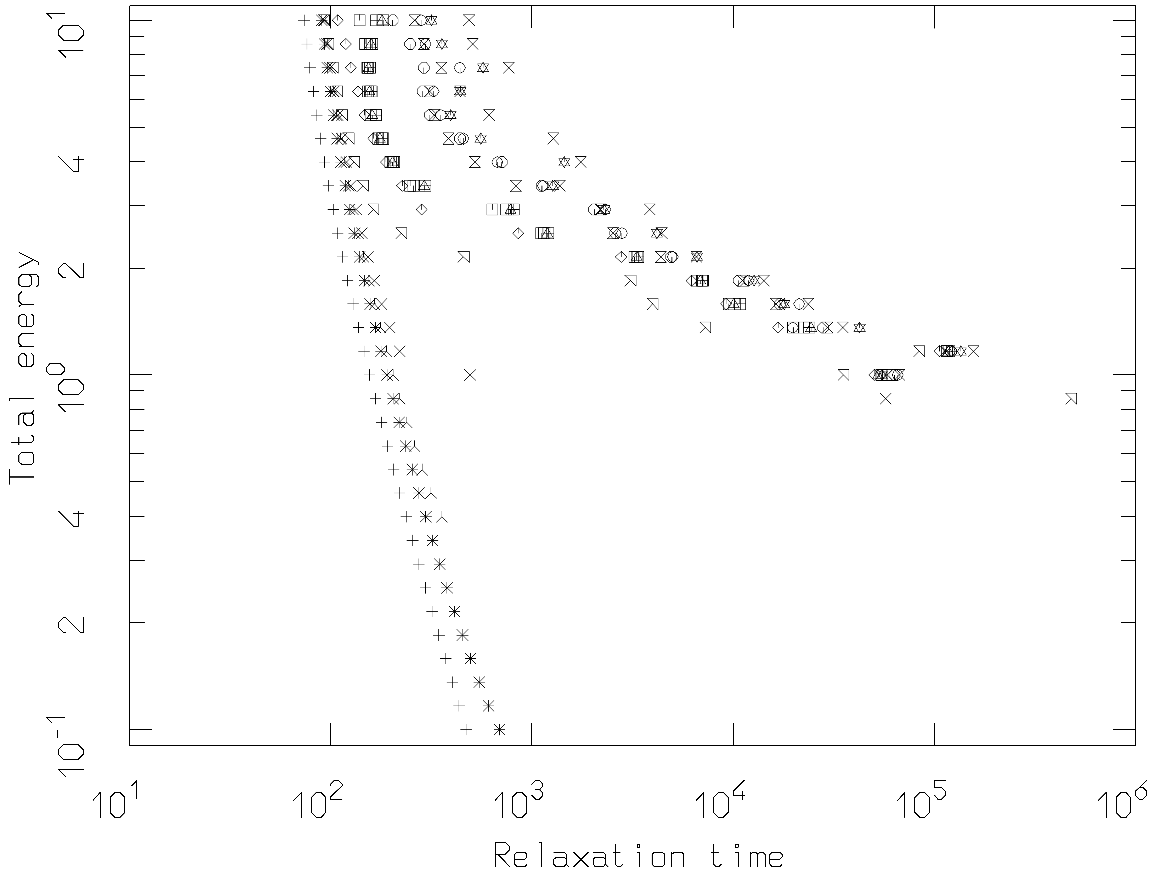


The spectrum at several times $(10, 10^2, \cdots, 10^8)$. $N = 127$, $\varepsilon = 1 \times 10^{-4}$).



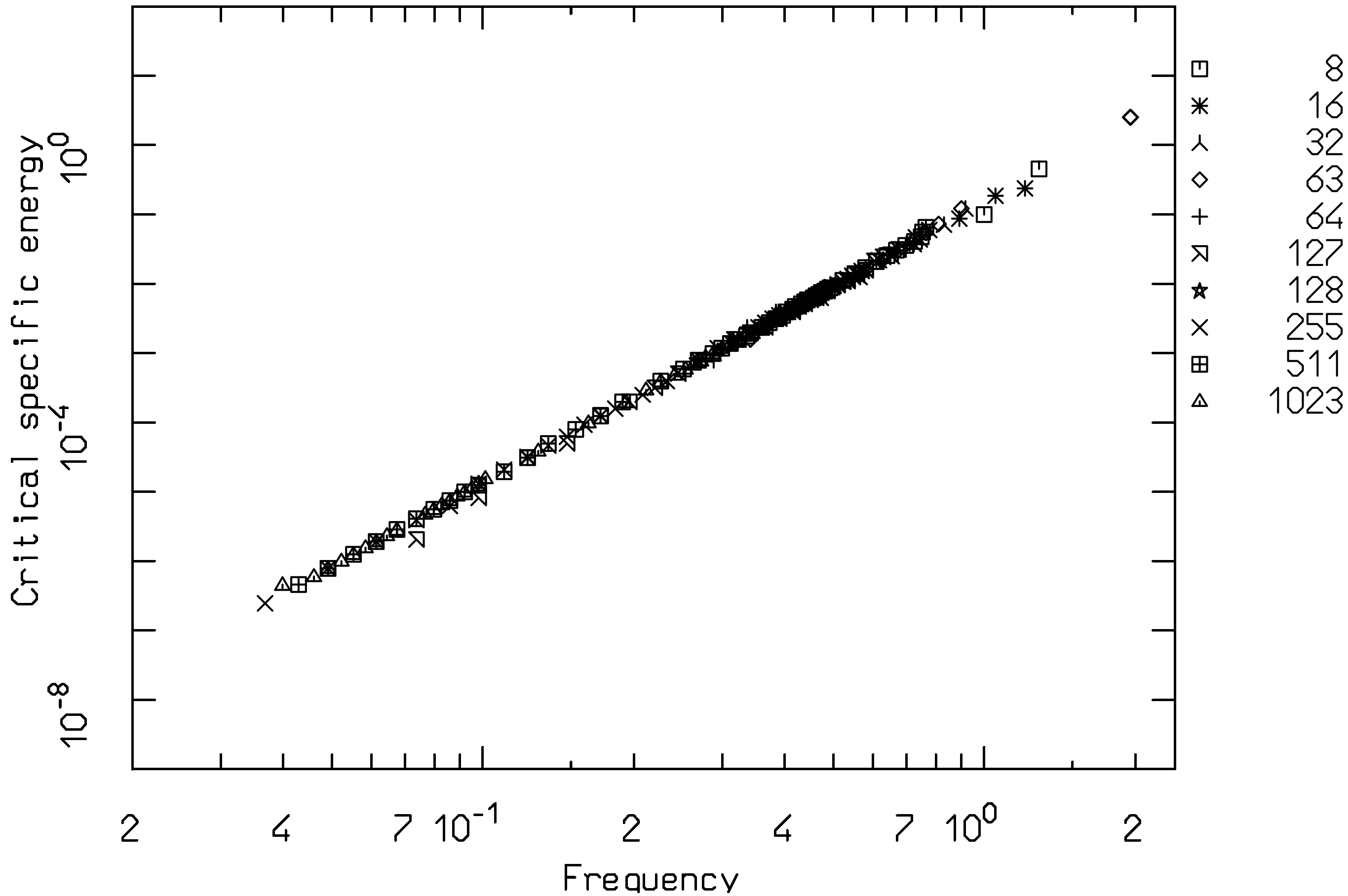
The spectrum at several times $(10, 10^2, \cdots, 10^8)$. $N = 127$, $\varepsilon = 1 \times 10^{-3}$).

The relation between critical time and energy



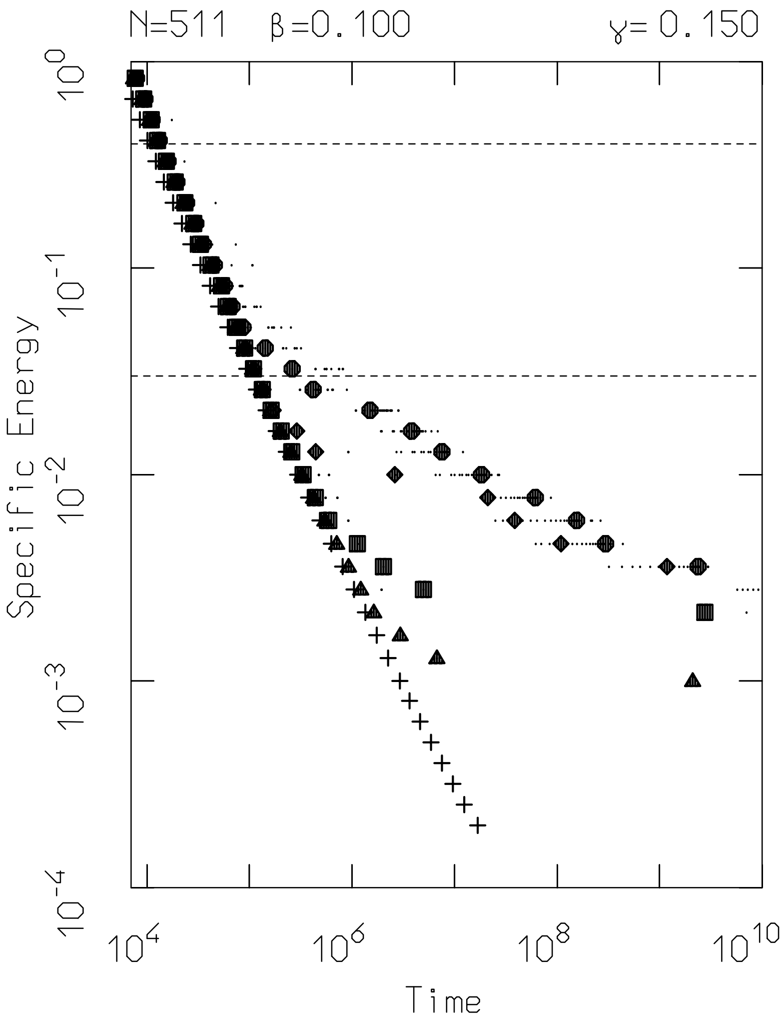
- A *natural packet* is formed in a short time.
- The flow of energy towards higher moded requires a long time.
- *Critical value of the energy: the point where the destruction time for a packet detaches from the left group.*

The critical energy as a function of the frequency

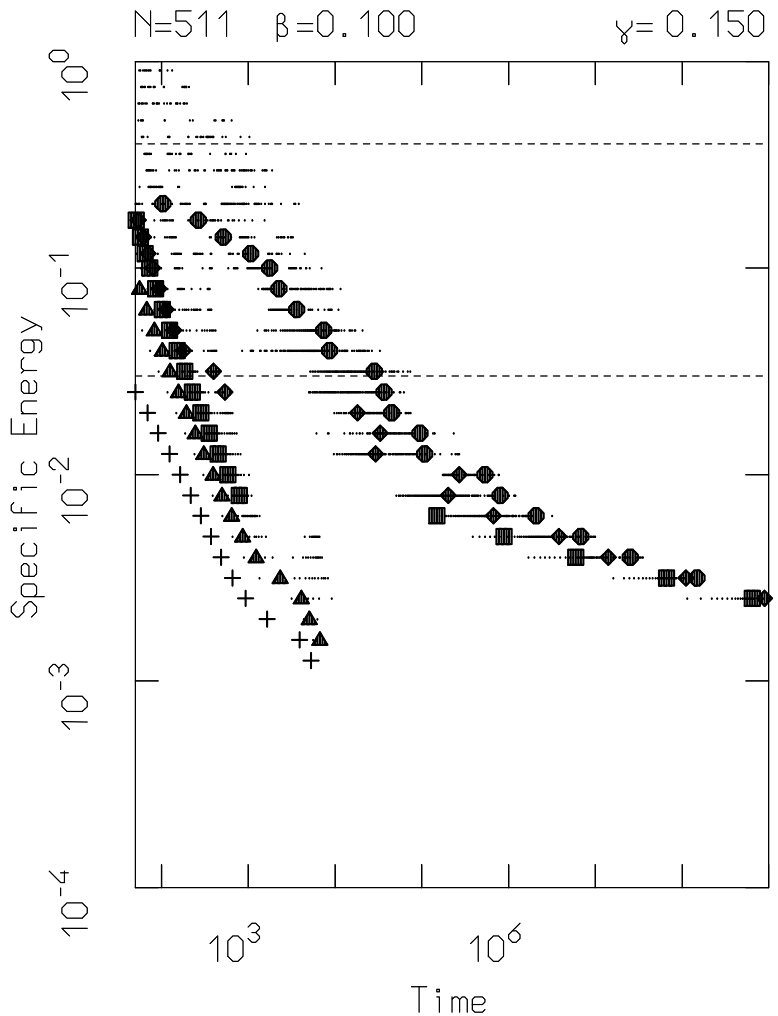


- *N ranging from 8 to 1023.*
- *The natural packet extends up to the mode of frequency ω only if the specific energy is greater that $\mathcal{E}_c(\omega)$.*

The ”packets” for theβ model

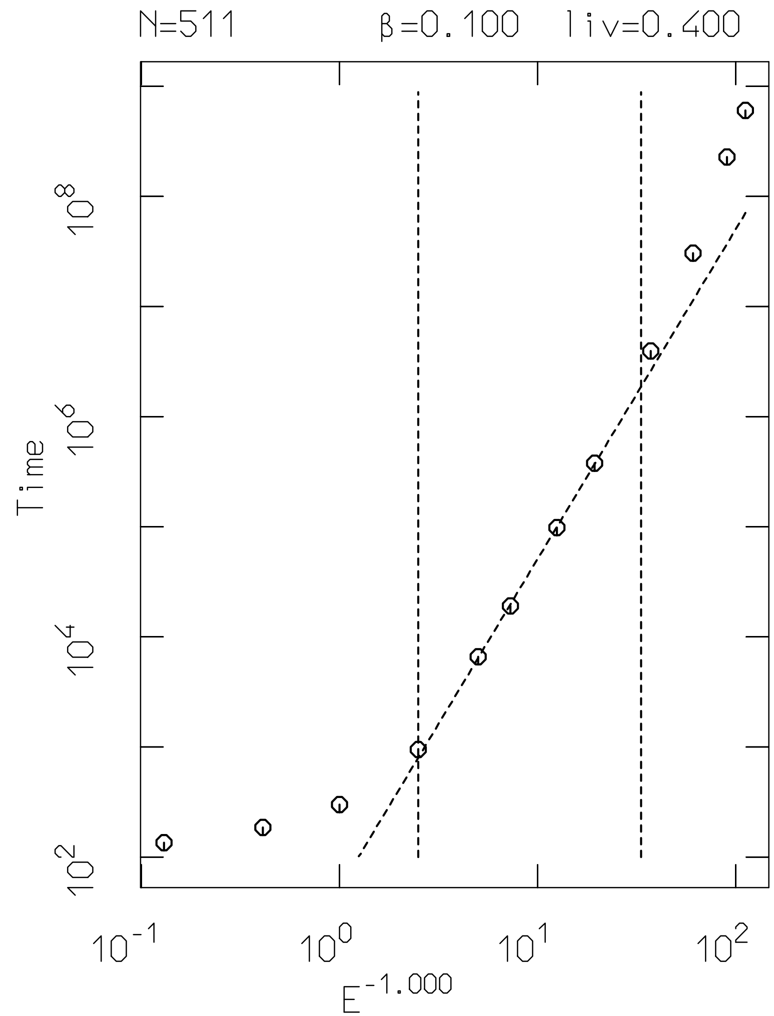


Mode 1 initially excited

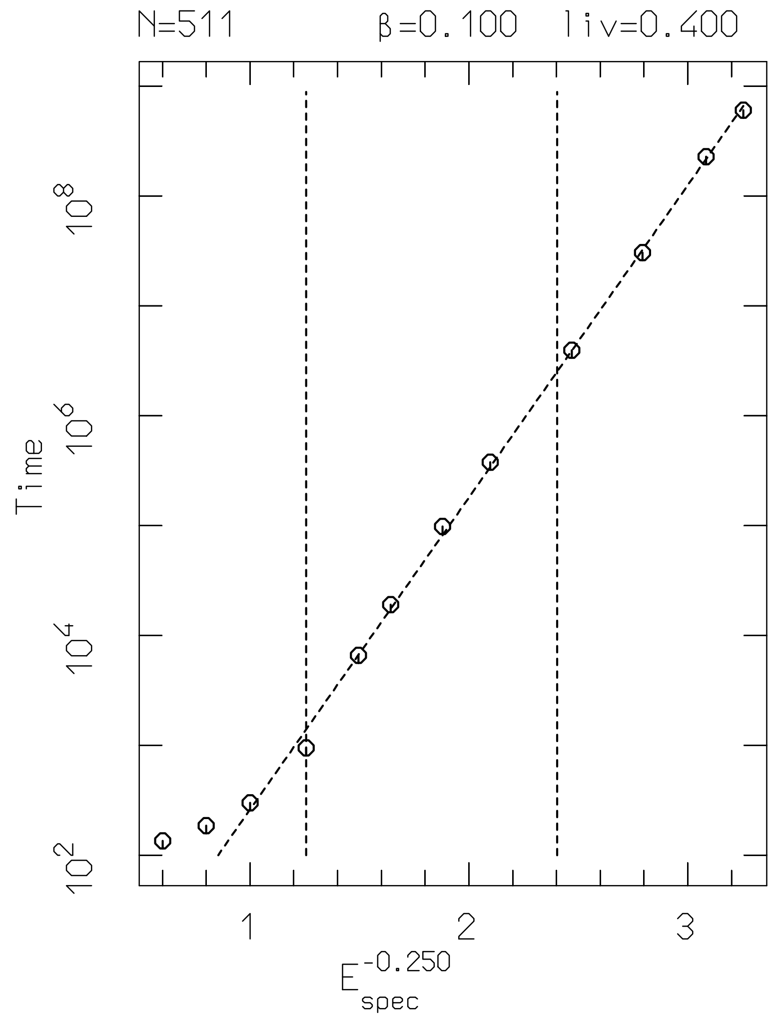


Modes 8–40 initially excited

The exponential estimate

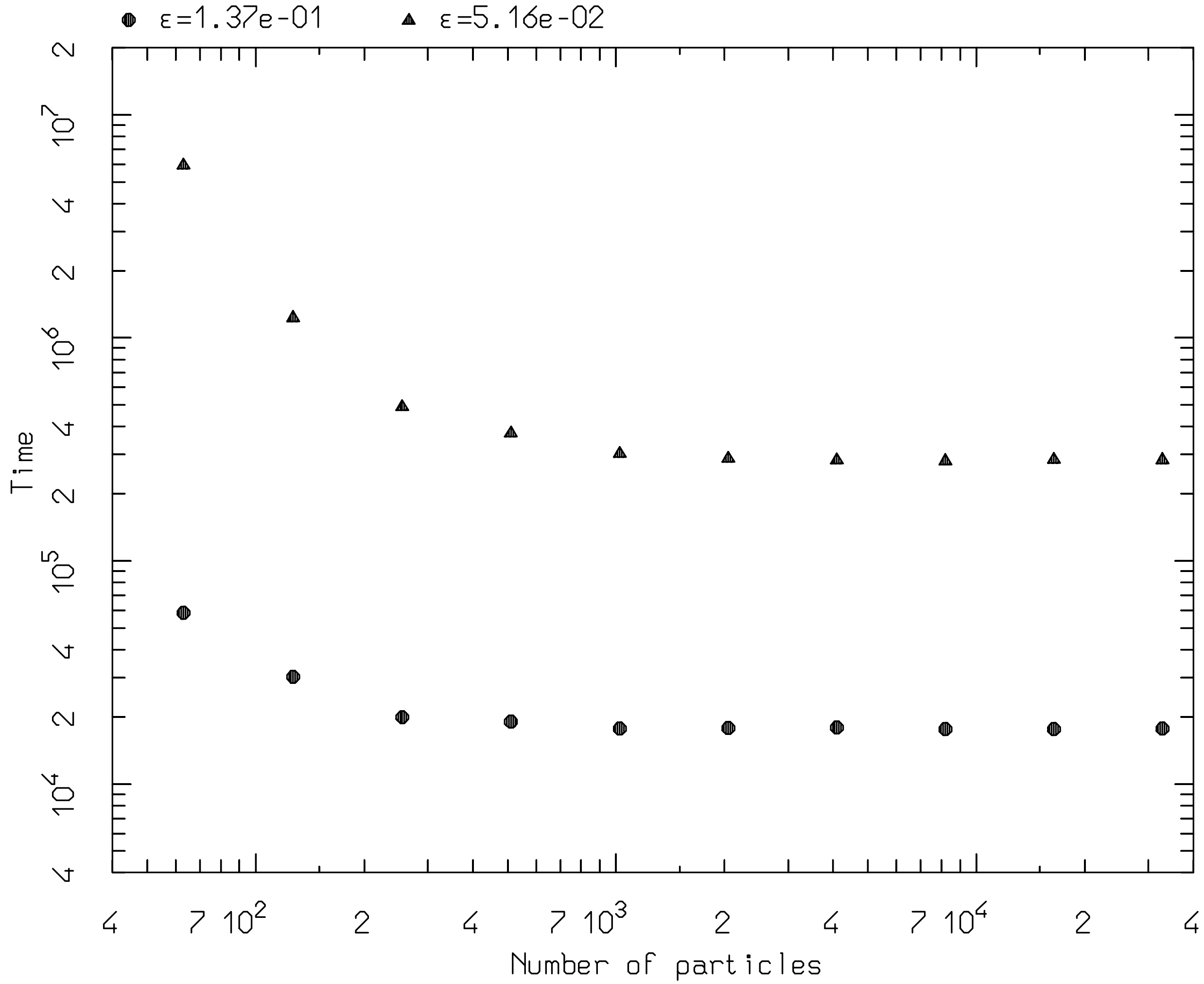


$T_{\mathrm{r}} \sim \varepsilon^{-3}$



$T_{\mathrm{r}} \sim \exp(\varepsilon^{-1/4})$

The dependence of the critical time on n



A few open questions

A few open questions

The question raised by Fermi, Pasta and Ulam is not yet answered.

- *Does the metastability scenario apply to generic initial conditions?*
  (see A. Carati, L. Galgani, A. Giorgilli and S. Paleari: FPU phenomenon for generic initial data, Phys. Rev. E **76**, *(2007)).*

- *Can we produce estimates for the relaxation time independent of N using statistical methods?*
  (see A. Carati: An averaging theorem for Hamiltonian dynamical systems in the thermodynamic limit, Journal of Statistical Physics **128**, *(2007)).*

- *Does the metastability scenario persist for lattices of FPU type in dimension 2 or 3?*
  (see G. Benettin and G. Gradenigo: A study of the Fermi-Pasta-Ulam problem in dimension two, CHAOS **18**, *(2008)).*