The Fermi-Pasta-Ulam Problem: from weak to strong chaos

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Rio de Janeiro, March 4, 2010

Outline: the main characters

- The Fermi-Pasta-Ulam problem: a review
- The discovery of the stochasticity thresholds
- Nonextensive statistical mechanics: Tsallis distribution at the edge of chaos
- Numerical analysis: perturbation of exact solutions

The origins of FPU problem

Consider a system governed by the Hamiltonian

$$H(\mathrm{I}, \phi) = H_0(\mathrm{I}) + \epsilon H_1(\mathrm{I}, \phi)$$

where $\mathrm{I} = (I_1, \ldots, I_M)$ are the action variables and $\phi = (\phi_1, \ldots, \phi_M)$ are the phase variables. If $\epsilon = 0$ the system is integrable, there are M independent first integrals (the actions I_i) and the motion evolves on M-dimensional tori.

In a seminal work, Acta Math. **13**, 1 (1890) H. Poincaré showed that generally a system with $\epsilon \neq 0$ does not possess analytic first integrals other than energy.

In 1923, in "Dimostrazione che in generale un sistema meccanico normale è quasi Ergodico", Phys. Zeitschrift 24, 261 (1923), Fermi proved the following statement:

for generic perturbations H_1 and $M > 2$, there cannot exist, on the $2M - 1$ dimensional constant-energy surface, even a single smooth[5] surface of dimension $2M - 2$ that is analytical in the variables (I, ϕ) and ϵ. From this result, Fermi argued that generic (non-integrable) Hamiltonian systems are ergodic.

STUDIES OF NON LINEAR PROBLEMS

E. Fermi, J. Pasta, and S. Ulam

Document LA-1940 (May 1955).

Abstract.

A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom.

The last few examples were calculated in 1955. After the untimely death of Professor E. Fermi in November, 1954, the calculations were continued in Los Alamos.

The model

E. Fermi, J. Pasta, S. Ulam, M. Tsingou

(T. Dauxois, Physics Today 61, 2008 on the role of M. Tsingou).

The Hamiltonian:

$$H(x_1, \cdots, x_N, p_1, \cdots, p_N) = \frac{1}{2}\sum_{j=1}^{N} p_j^2 + \sum_{j=1}^{N+1} V(x_{j+1} - x_j)$$

$$V(x) = \frac{1}{2}x^2 + \frac{\alpha}{2}x^3 + \frac{\beta}{3}x^4$$

In the original study, N=32, all masses and the harmonic constants have been set equal to 1

This model can be interpreted as a one-dimensional crystal, i.e. a chain of equal particles with ***nearest-neighbours*** *nonlinear interactions and fixed ends.*

The linearized system can be transformed into a system of uncoupled linear oscillators **(normal modes)**

$$H_2 = \sum_{k=1}^{N} E_k \qquad E_k = \omega_k I_k \qquad \omega_k = 2\sin\frac{k\pi}{2(N+1)}$$

The "FPU paradox"

- **Classical equilibrium mechanics:** the statistical properties of an isolated system at a given energy E are described by the microcanonical measure or equivalently by the Gibbs measure in the whole phase space for $T=T(E)$.
- **Equipartition theorem.** In the harmonic limit

$$< E_k >_E = E/N \equiv \epsilon \ , \quad k = 1, \dots, N$$

where $\epsilon = E/N$ is the specific energy

The result does not change qualitatively for a **slightly anharmonic system** and for a small temperature T, because the anharmonic corrections do vanish in the limit

$$\alpha, \beta \to 0 \text{ or } T \to 0 \text{ (i.e., } \epsilon \to 0)$$

- **Dynamical dichotomy**

Harmonic case. The system is integrable: N integrals.

Anharmonic case. for $\alpha \neq 0$ or $\beta \neq 0$ No integrals: the system is expected,

to be **ergodic, no matter how small the perturbation could be.**

The relaxation time

$f : M \to \mathbb{R}$ dynamical variable on the phase space M

$< f >_E$ microcanonical expectation value

$\{g^t\}_{t\in \mathbb{R}}, \; g^t : M \to M$ flow induced by the equations of motion

$\overline{f}(t,x)$ "time average" of f with initial datum $x \in M$

$$\overline{f}(t,x) = \frac{1}{t}\int_0^t f(g^s x)\,\mathrm{d}s$$

Ergodicity of the microcanonical distrubution:

$$\overline{f}(t,x) \to < f >_E \quad \text{as} \quad t \to \infty$$

J. Von Neumann (PNAS, 18, 263 (1932))

Relaxation time: the time τ such that, for $t \geq \tau$, the time-average essentially coincides with the phase average.

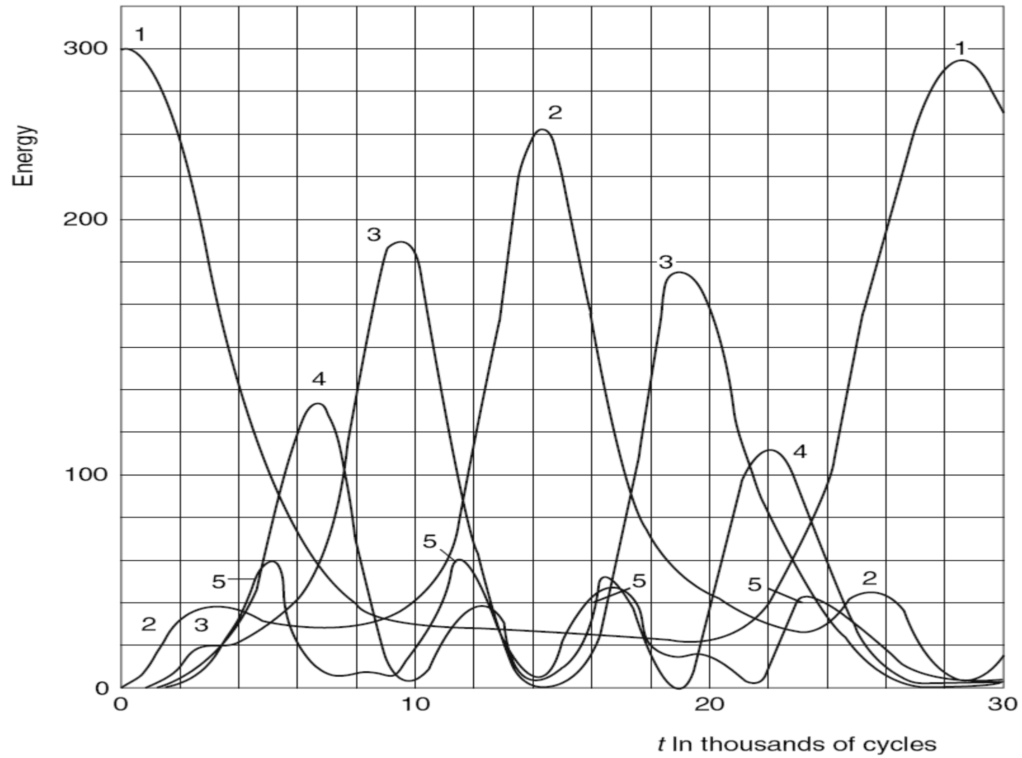
One would expect that $\tau = \tau(\alpha, \beta, E)$ and also $\tau \xrightarrow[\alpha,\beta\to 0]{} \infty$

The FPU results

- What are the relaxation times for the time averages $\overline{E}_k(t,x)$ for initial data far from equilibrium?

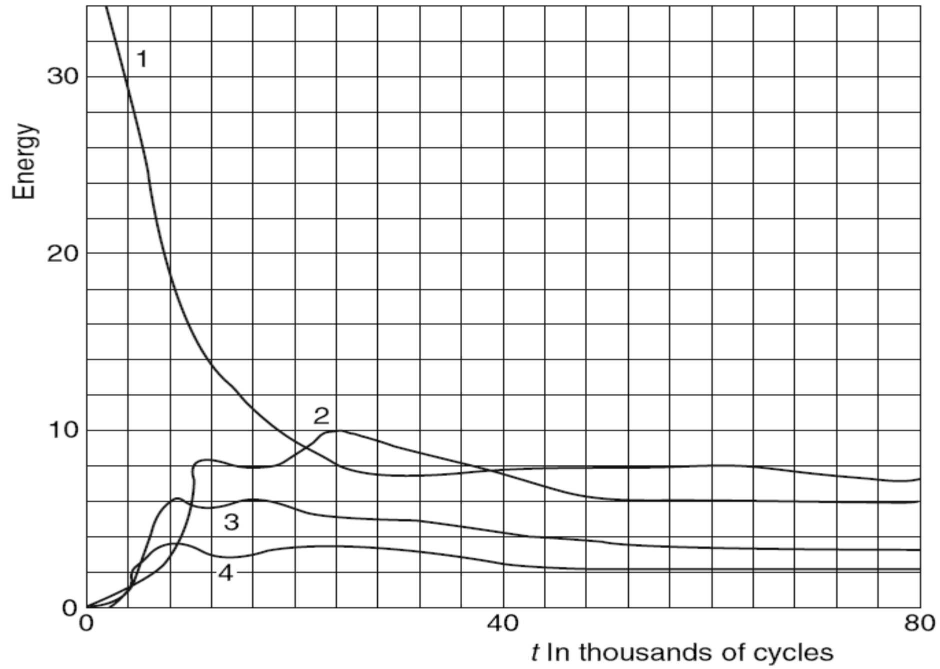
FPU considered the datum $E_1 = E,\ E_k = 0$ for $k = 2, \cdots, N$

Expected result: the energy would soon spread over all other modes. Instead....



$N = 32$ (with $\alpha = 1/4,\ \beta = 0$) the energy, instead of flowing to all the 32 modes,

of low-frequency modes, namely modes 1 up to 5



Time-averaged harmonic energies $\overline{E}_k$ versus time.

FPU paradox: instead of a **slow relaxation** to the final equilibrium state, there is a rather quick relaxation to some "nonstandard" state, in which the energy is shared within a packet of Low-frequency modes (**partial thermalization**).

Ulam wrote: "The results of the calculations...were interesting and quite surprising to Fermi. He expressed to me the opinion that they really constituted a **little discovery** in providing intimations that the precalent beliefs in the universality of mixing and thermalization in nonlinear systems **may not be always justified**"

For fixed initial conditions: $x_0(t) = x_{N+1}(t) = 0, \quad \forall t$

Flach et al (PRL 2005-), q-breathers, Giorgilli and Muraro (Boll. UMI, 2006)

Bountis et al, low q-dimensional tori (PRE, 2010)

Zabusky and Kruskal (1965)

ZK, Phys. Rew. Lett. **15**, 240 (1965)

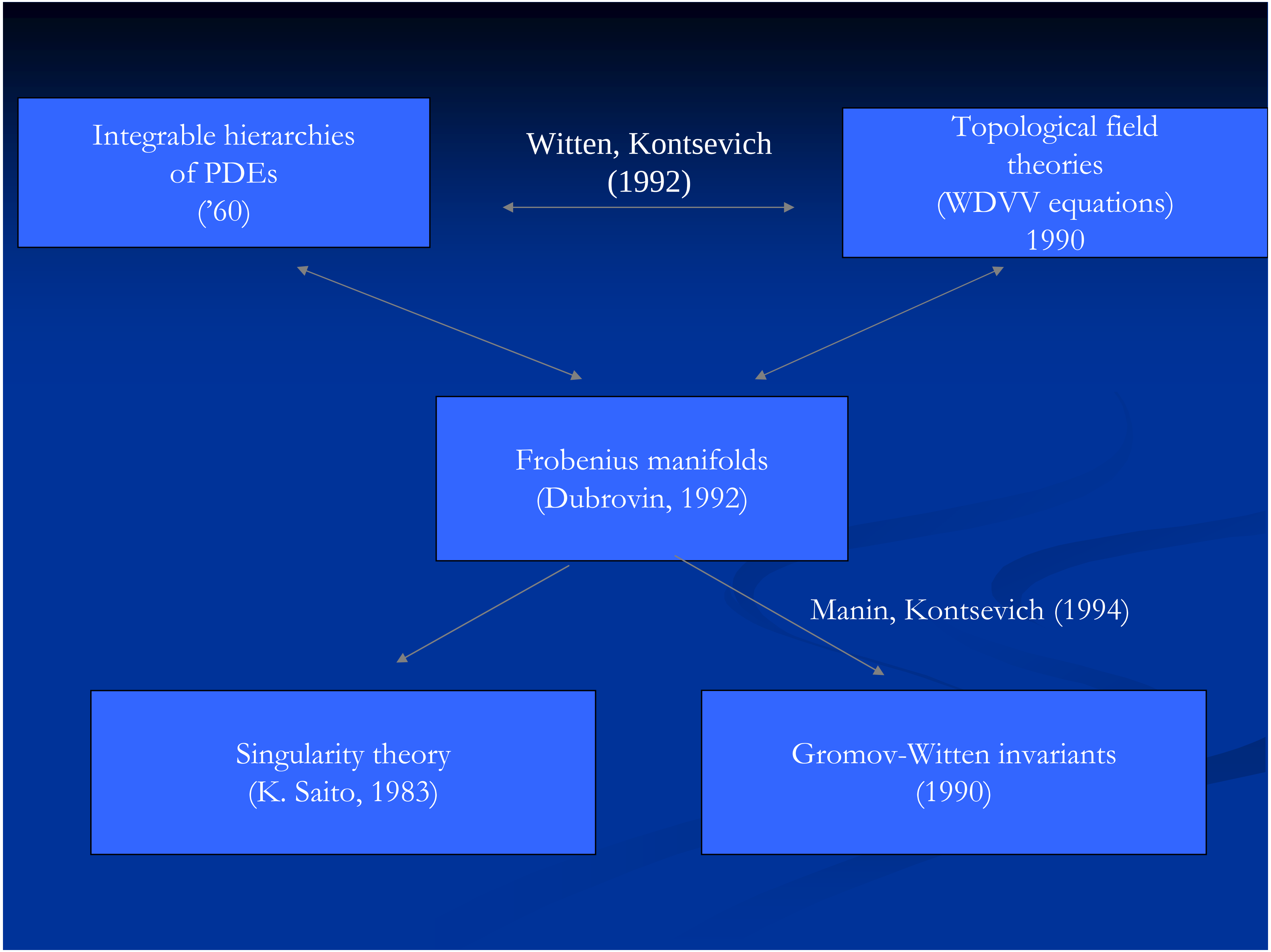
- **The Korteweg-de Vries equation:** $u_t + uu_x + u_{xxx} = 0 \qquad u = u(x,t)$

  Model of a continuous nonlinear string interpolating the FPU chain.

- **Discovery of the theory of Solitons**

- **Theory of infinite-dimensional integrable systems**

  (inverse scattering transform for the nonlinear Cauchy problem, hierarchies of infinitely many integrable equations, Lie symmetries, Wahlquist-Estabrook structures, bi-Hamiltonian geometry, topological quantum field theories, Frobenius manifolds, Gromov-Witten invartiants, connections with Random Matrix theory, solitons in optical fibres, etc.)


Integrable hierarchies
of PDEs
('60)
Witten, Kontsevich
(1992)
Topological field
theories
(WDVV equations)
1990
Frobenius manifolds
(Dubrovin, 1992)
Manin, Kontsevich (1994)
Singularity theory
(K. Saito, 1983)
Gromov-Witten invariants
(1990)

The stochasticity threshold (ST)

- Izrailev-Chirikov (1966): the FPU paradox disappears if the initial energy is sufficiently large. There exists a critical energy $E_c = E_c(N)$ such that one has quick equipartition if $E > E_c$

- What is the theoretical explanation of the ST?

KAM theorem: persistence of quasiperiodic motion under small perturbations

- There exist invariant tori that survive the nonlinear perturbation, other ones that are destroyed.Those that survive have "sufficiently irrational" frequencies (non-resonance condition) over them the motion continues to be quasiperiodic. The KAM tori that are not destroyed by the perturbation form invariant Cantor sets.
- The relative measure of the set of the perturbed invariant tori tends to 1 as the perturbation tends to zero.
- Weak KAM approach (Giorgilli et al, Bountis et al.): the resonant motion is confined in tori of dimension less than N

Other outstanding contributions:

- **The metastability scenario (1982):** the FPU state is a **metastable state**. (E. Fucito, M. Marchesoni, E. Marinari, G. Parisi, L. Peliti, S. Ruffo and A. Vulpiani, J. Phys. 43, 707 (1982).
- This state remains undisturbed for extremely long times.
- It precipitates towards a catastrophic mechanism" to the "final" equilibrium state.
- Analogy with the theory of Spin glasses (Parisi et al)
- Connections with Nekhoroshev theory, etc.
- Existence of **exact solutions** (one-mode solutions) of the full Hamiltonian (Budinsky and Bountis, Physica D 1983, Poggi and Ruffo, Physica D, 1997)

Reviews: **The Fermi-Pasta-Ulam Problem: a status report**, G. Gallavotti ed., Lect. Notes in Physics 728 (2008)
The FPU problem: the first fifty years, Chaos 15 (2005)

Nonextensive statistical mechanics

- Nonextensive statistical mechanics: a generalization of the Boltzmann-Gibbs statistics particularly suitable for the treatment of **weakly chaotic systems**.

- Tsallis entropy (1988)

C. Tsallis, *Possible generalization of the Boltzmann–Gibbs statistics* 1988 J. Stat. Phys. **52**, Nos. 1/2, 479–487

$$S_q = k\frac{1 - \sum_{i=1}^{W} p_i^q}{q-1}$$

- 2965 papers http://tsallis.cat.cbpf.br/TEMUCO.pdf

The nonextensive scenario

- Sq generalizes the Boltzmann-Gibbs entropy

$$S_1 = \lim_{q \to 1} S_q \equiv S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i$$

- q-exponential $\quad e_q^x := [1 + (1-q)x]^{1/(1-q)}$

$$S_q = -k \sum_{i=1}^{W} p_i \ln_q p_i$$

- Nonadditivity

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q)\frac{S_q(A)}{k}\frac{S_q(B)}{k}$$

- Extensivity

$$0 < \lim_{N \to \infty} \frac{S(N)}{N} < \infty$$

SYSTEMS	ENTROPY S_{BG} (additive)	ENTROPY S_q (q<1) (nonadditive)
Short-range interactions, weakly entangled blocks, etc	EXTENSIVE	NONEXTENSIVE
Long-range interactions (QSS), strongly entangled blocks, etc	NONEXTENSIVE	EXTENSIVE

(Tsallis, Tirnakli, 2010)

From weak to strong chaos

- **Perturbation of exact solutions** of the FPU system: an alternative way of thinking!

FPU β system $$H = \frac{1}{2}\sum_{i=1}^{N} {p_i}^2 + \frac{1}{2}\sum_{i=1}^{N} (x_{i+1} - x_i)^2 + \frac{\beta}{4}\sum_{i=1}^{N} (x_{i+1} - x_i)^4$$

with periodic conditions $x_{N+1} = x_1$ *and* $\beta > 0.$

Normal coordinates

$$Q_i = \sum_{j=1}^{N} S_{ij} x_j \qquad P_i = \sum_{j=1}^{N} S_{ij} p_j \qquad \text{with} \qquad S_{ij} = \frac{1}{\sqrt{N}}\left(\sin\frac{2\pi ij}{N} + \cos\frac{2\pi ij}{N}\right)$$

the harmonic energy of the mode i is

$$E_i = \frac{1}{2}\left(P_i^2 + \omega_i^2 Q_i^2\right) \qquad \omega_i^2 = 4\sin^2\frac{\pi i}{N}.$$

For $\beta = 0$, all normal modes oscillate independently and their energies E_i are constant of the motion. In the anharmonic case ($\beta \neq 0$), the normal modes are instead coupled, and the variables Q have no longer simple sinusoidal oscillations.

Strong stochasticity threshold

M. Pettini and M. Landolfi, *Relaxation properties and ergodicity breaking in nonlinear Hamiltonian dynamics* 1990 Phys. Rev. A **41**, 768–783
M. Pettini and M. Cerruti–Sola, *Strong stochasticity threshold in nonlinear large Hamiltonian systems: Effect on mixing times* 1991 Phys. Rev. A **44**, 975–987
H. Kantz, *Vanishing stability thresholds in the thermodynamic limit of nonintegrable conservative systems* 1989 Physica D **39**, 322–335

Strong stochasticity threshold (SST): the energy density threshold that characterizes the transition of the dynamics from weak to strong chaos during the relaxation of the system towards ergodicity and equipartition.

There exist nonlinear one-mode exact solutions of the FPU beta system

$$n = \frac{N}{4},\ \frac{N}{3},\ \frac{N}{2},\ \frac{2}{3}N,\ \frac{3}{4}N$$

Idea: to study the transition from weak to strong chaos (SST) by performing a numerical analysis of a suitable observable evolving according to an exact solution (N/2)

Exact solutions

In the anharmonic case the normal modes are coupled. The differential equation for the k-mode is

$$\ddot{Q}_k = -\omega_k^2 Q_k - \frac{\mu\omega_k}{2N}\sum_{i,j,l}^{N-1}\omega_i\omega_j\omega_l C_{kijl} Q_i Q_j Q_l \qquad (k=1,\ldots,N-1)$$

where $\quad C_{ijkl} = -\Delta_{i+j+k+l} + \Delta_{i+j-k-l} + \Delta_{i-j+k-l} + \Delta_{i-j-k+l},$

being $\Delta_k = (-1)^m$ for $k = mN$, if m is a positive integer, and $\Delta_k = 0$ otherwise.

the equation of motion for the excited mode amplitude Q_n is

$$\ddot{Q}_n = -\omega_n^2 Q_n - \frac{\mu\omega_n^4 C_{nnnn}}{2N} Q_n^3 .$$

If we assume that at time $t=0$ $Q_n \neq 0$ and $P_n = 0$, the solution of Eq.

$$Q_n(t) = A\,\mathrm{cn}(\Omega_n t, k)$$

$$\Omega_n = \omega_n\sqrt{1+\delta_n A^2}, \qquad k = \sqrt{\frac{\delta_n A^2}{2(1+\delta_n A^2)}} \qquad \text{with } \delta_n = \mu\omega_n^2 C_{nnnn}/2N.$$

This solution is periodic with period $T_n = 4K(k)/\Omega_n$

The energy of the mode is $\quad E_n = \frac{1}{2}\left(P_n^2 + \omega_n^2 Q_n^2 + \mu\frac{\omega_n^4 Q_n^4 C_{nnnn}}{4N}\right)$

Dynamical observables

Let us introduce the observables $\eta_i = x_i + x_{i-1}$

the variable x_i is related to the modal variable $Q_{N/2}$ by $x_i(t) = \frac{1}{\sqrt{N}}(-1)^i Q_{N/2}(t)$

Introduce an universal indicator of stochasticity

$$\rho = \frac{\sigma}{\theta}$$

i.e. **the ratio between the second and the first moment** of a given probability distribution (when they are defined and the first moment is different from zero).

a) The distribution is normal, i.e. described by the Gauss function

$$f(\xi) = \frac{a}{\sqrt{\pi}} \exp\left(-a^2\xi^2\right)$$

theoretical value $\rho = \frac{\sigma}{\theta} = \sqrt{\frac{\pi}{2}}$.

b) The distribution is a Tsallis distribution: $f(\xi) = a\left(1-(1-q)b^2\xi^2\right)^{\frac{1}{1-q}}$

with a and q dependent on ϵ,

$$b = a\sqrt{\pi}\,\frac{\Gamma\left(\frac{3-q}{2(q-1)}\right)}{\sqrt{q-1}\,\Gamma\left(\frac{1}{q-1}\right)} \qquad 1 < q < 3$$

In this case we have proved that, for $1 < q < 5/3$, $\rho(q) = \sqrt{\pi}\,\frac{\sqrt{\frac{q-1}{5-3q}}\,\Gamma\left(\frac{3-q}{2(q-1)}\right)}{\Gamma\left(\frac{2-q}{q-1}\right)}$

In the specific example of the FPU β system, θ is the mean value of the moduli

$$\xi_i = \eta_i - \langle \eta_i \rangle$$

numerically obtained and σ the standard deviation:

$$\theta = \frac{\sum |\xi_i|}{M}, \qquad \sigma = \sqrt{\frac{\sum \xi_i^2}{M}}$$

Stability threshold for the N/2 solution: $\varepsilon_t = \frac{\pi^2}{3N^2} + O(N^{-4})$

where M is the number of values of ξ_i. What one expects is that for $\epsilon < \epsilon_t$, when the system is stable, $\rho(\epsilon)$ should remain approximately constant. Instead it should change abruptly for $\epsilon > \epsilon_t$, when the π–mode starts to exchange energy with the others modes. For larger and larger values of ϵ, when an equipartition state has been reasonably reached, the parameter ρ should assume again a constant value, characteristic of the distribution of the ξ_i. For intermediate values of ϵ, a transition between weak and strong chaos should be observed.

Numerical results

- We have used a bilateral symplectic algorithm
- Initial conditions:

$$Q(0) = Q_0 \neq 0, \qquad \dot{Q}(0) = P_0 = 0.$$

- We integrate the Hamilton equations and compute the observables

$$\eta_i = x_i(t) + x_{i-1}(t), \qquad i = 1, \ldots, N$$

- We follow the system for 1 million periods of the corresponding linear mode.

The N/2 – mode exact solution

The solution for the modal variable we are studying is

$$Q(t) = Q_0 \; cn(\Omega t; k^2)$$

where cn is the periodic Jacobi elliptic function with period $T = aK(k)/\Omega$, $K(k)$ is the complete elliptic integral of the first kind and, for $\beta = 1$:

$$k^2 = \frac{1}{2}\frac{\sqrt{1+4\epsilon}-1}{\sqrt{1+4\epsilon}}, \qquad \Omega^2 = \frac{4}{1-2k^2}.$$

One has resonance if the harmonic frequencies $\vec{\omega} = (\omega_1, \omega_2, \ldots, \omega_{N/2})$, concerning the harmonic term of the Hamiltonian, satisfy the relation

$$\vec{m}\cdot\vec{\omega} = \sum_i^{N/2} m_i \omega_i \approx 0$$

where $\vec{m}$ is an array of integers and the ω_i are given by the formula $\omega_i^2 = 4\sin^2\frac{\pi i}{N}$.

Since we excite the π–mode, we have resonance, in particular, when $\Omega = m\omega_i$ with integer $m > 1$ and for some ω_i. From previous relations one obtains for the resonance energy density ϵ_r:

$$\epsilon_r = \frac{1}{4}\left(m^4 \sin^4\frac{\pi i}{N} - 1\right)$$

Stability analysis: Poggi and Ruffo, Physica D 1997,
Cafarella, M. Leo and R. A. Leo, PRE, 2006
M. Leo and R. A. Leo, PRE 2007

The edge of chaos: Liapunov approach

- The maximum Liapunov exponent plays a crucial role in the theory of chaos.

$$\xi(t) \equiv \lim_{\Delta x(0)\to 0} \Delta x(t)/\Delta x(0)$$

If the system has a positive Liapunov exponent, then ξ diverges as $\xi = e^{\lambda_1 t}$

When the maximal Liapunov exponent vanishes, we get the differential equation

$$dy/dx = a_q y^q \quad [y(0)=1;\ q \in \mathcal{R}],$$

Its solution is

$$y = e_q^{a_q x} \qquad e_q^x \equiv [1+(1-q)x]^{1/(1-q)}$$

- Conjecture: the vanishing of the maximal Liapunov exponent is a necessary condition for the Tsallis distribution to be the correct PDF for a Hamiltonian system possessing a weakly chaotic regime.
- Is it also sufficient?

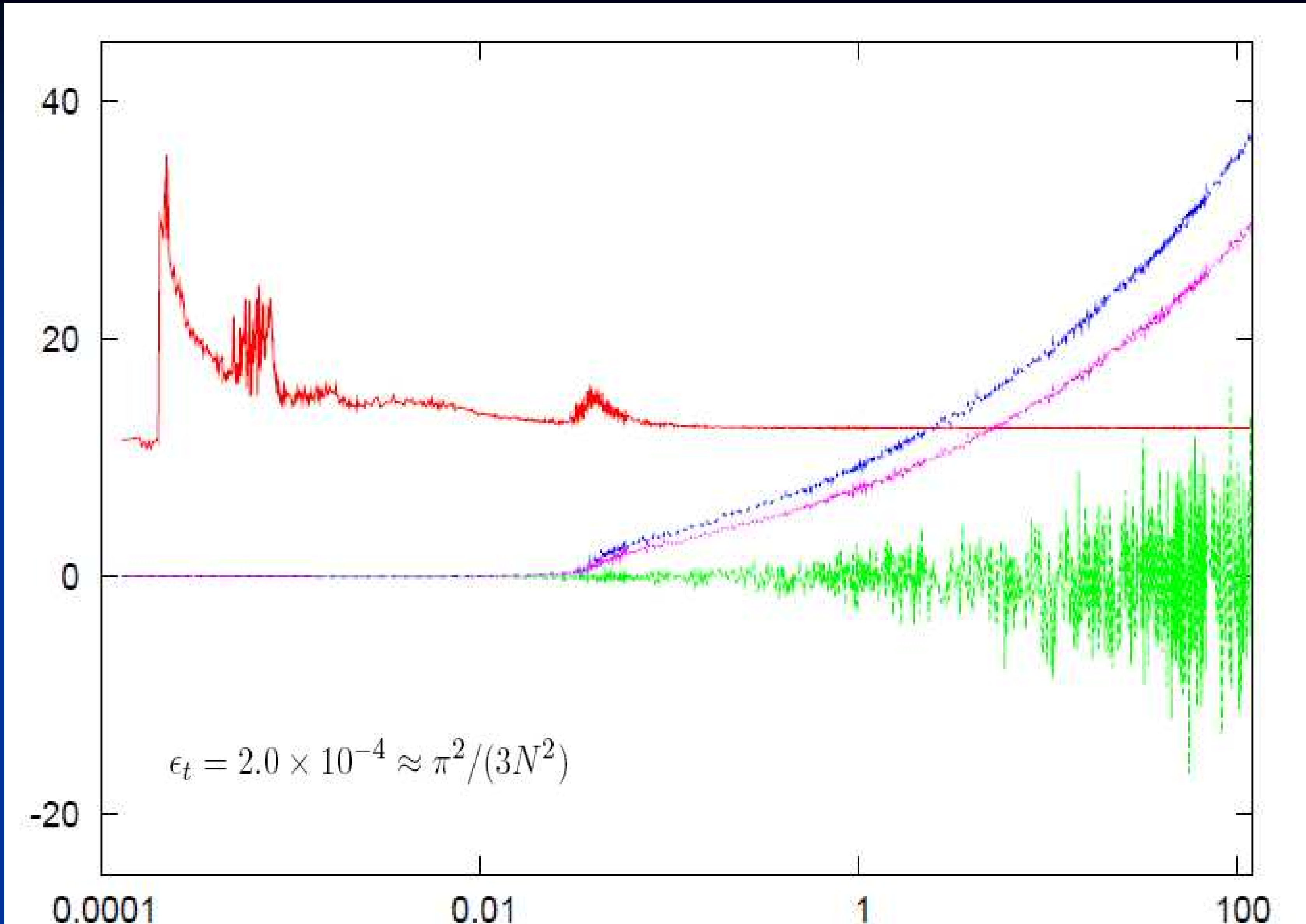


FIGURE 1. (Color on line). $N = 128$: $\rho \times 10$ (red), $\sigma \times 2$ (blue), $\theta \times 2$ (purple) and $< \eta_{64} > \times 500$ (green) vs the energy density ϵ.

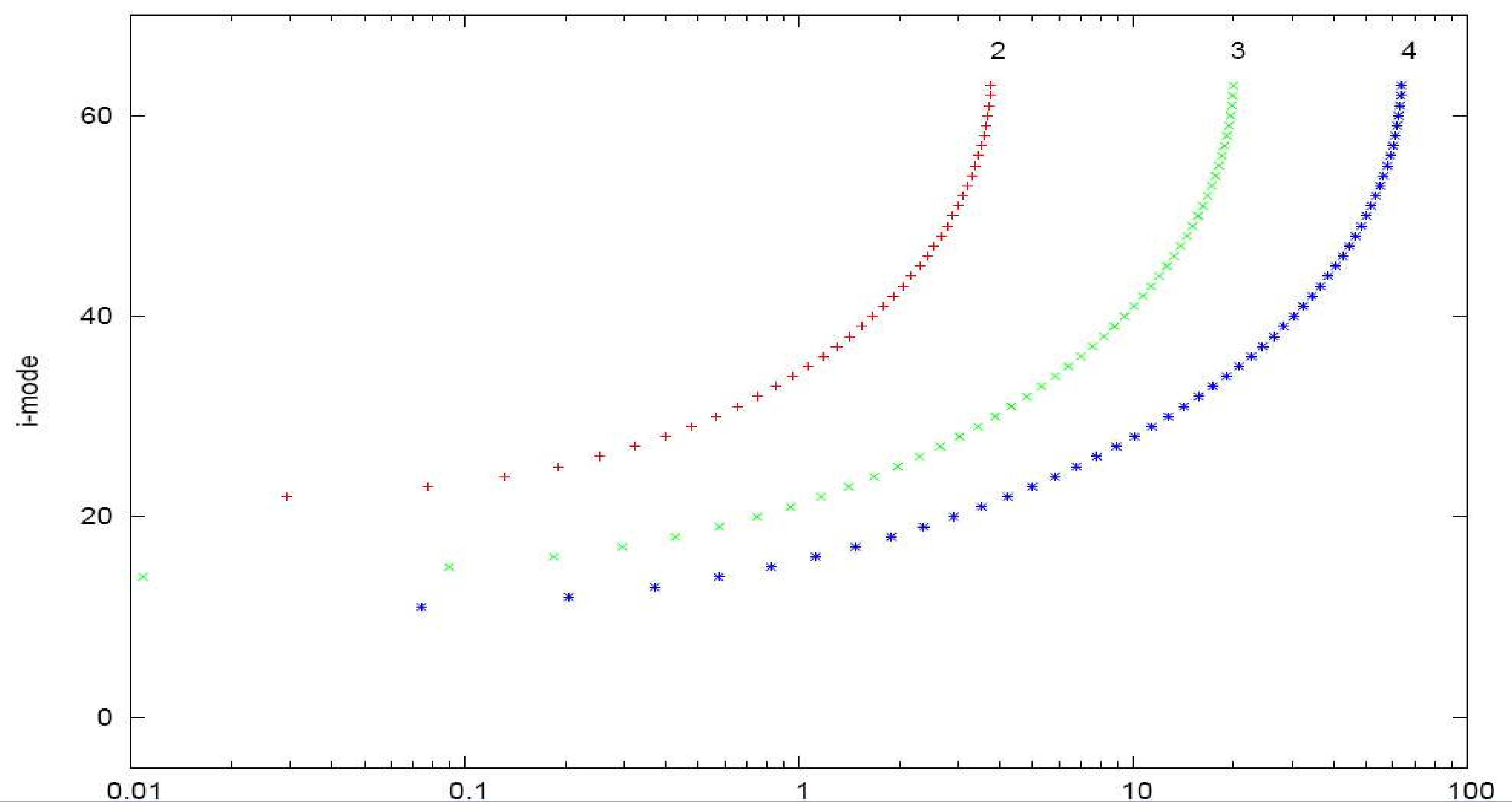


FIGURE 2. (Color on line). $N = 128$: mode number i as a function of the corresponding resonance energy density for $m = 2$ (red), 3 (green) and 4 (blue).

$$\epsilon_r = \frac{1}{4}\left(m^4 \sin^4 \frac{\pi i}{N} - 1\right)$$

The resonance is possible for values of i such that $\epsilon_r > 0$. For example, for $m = 2$ one has $i = \begin{cases} N/6 \\ [N/6]+1 \end{cases}$

The first linear mode that goes in resonance with the N/2 mode corresponds to

$i = 22$, for $\epsilon = 0.0282$

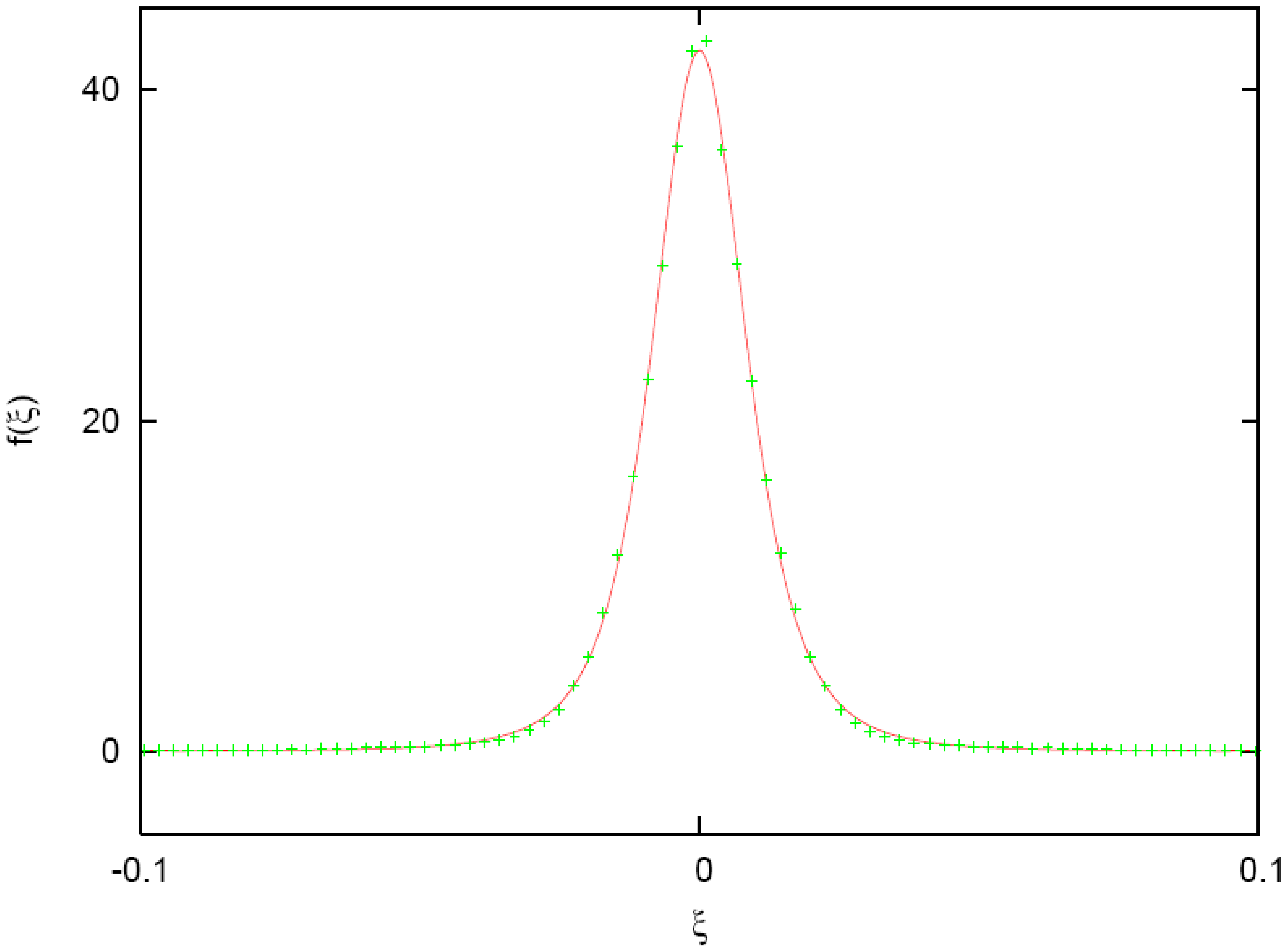


FIGURE 3. (Color on line). Numerical (green points) and Tsallis distribution (red curve) for $N = 128$ and $\epsilon = 0.006$.

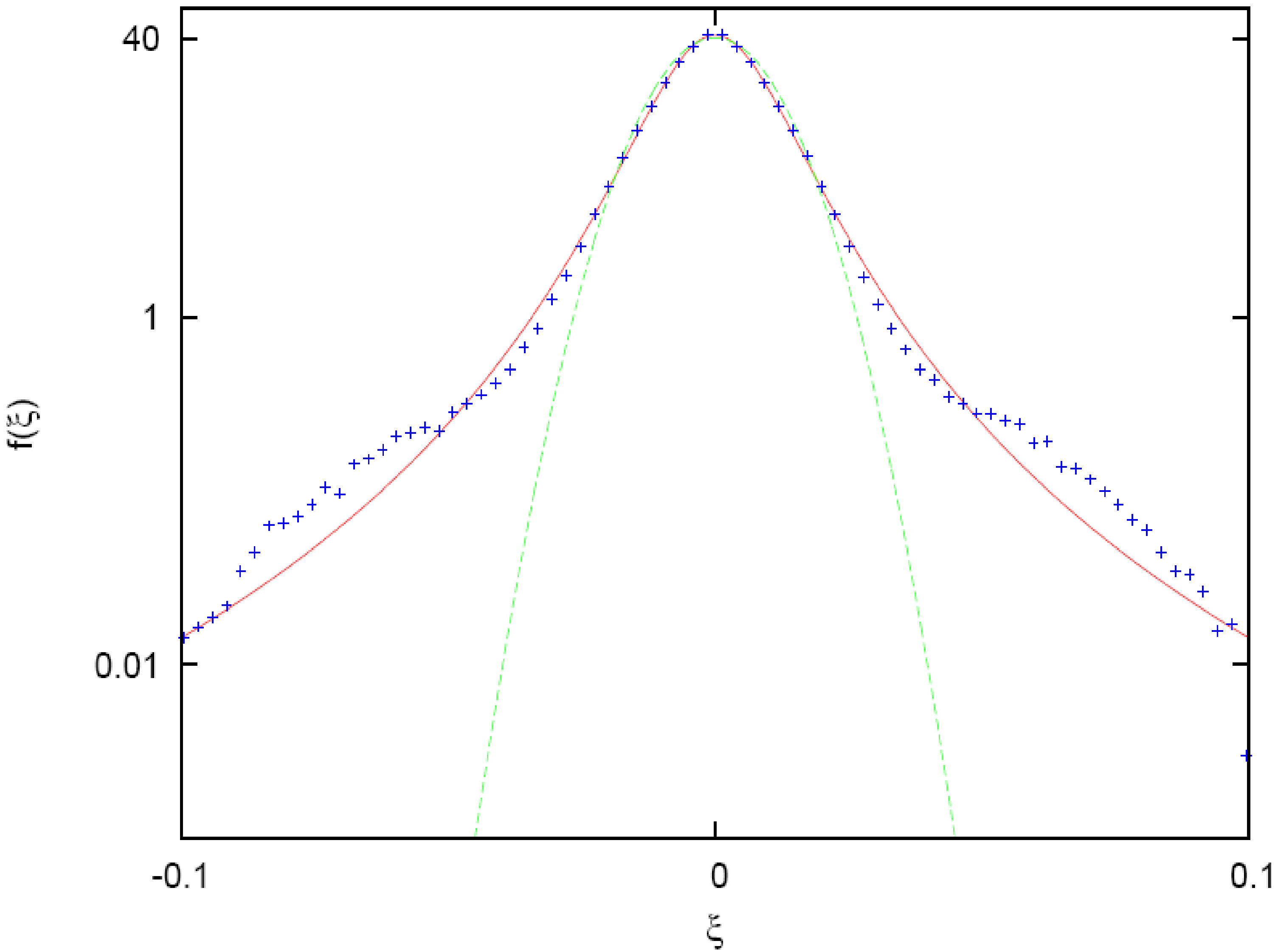


FIGURE 4. (Color on line). Plot in linear–log scale of Tsallis (red), Gauss (green) and numerical distributions (blue) for $N = 128$ and $\epsilon = 0.006$.

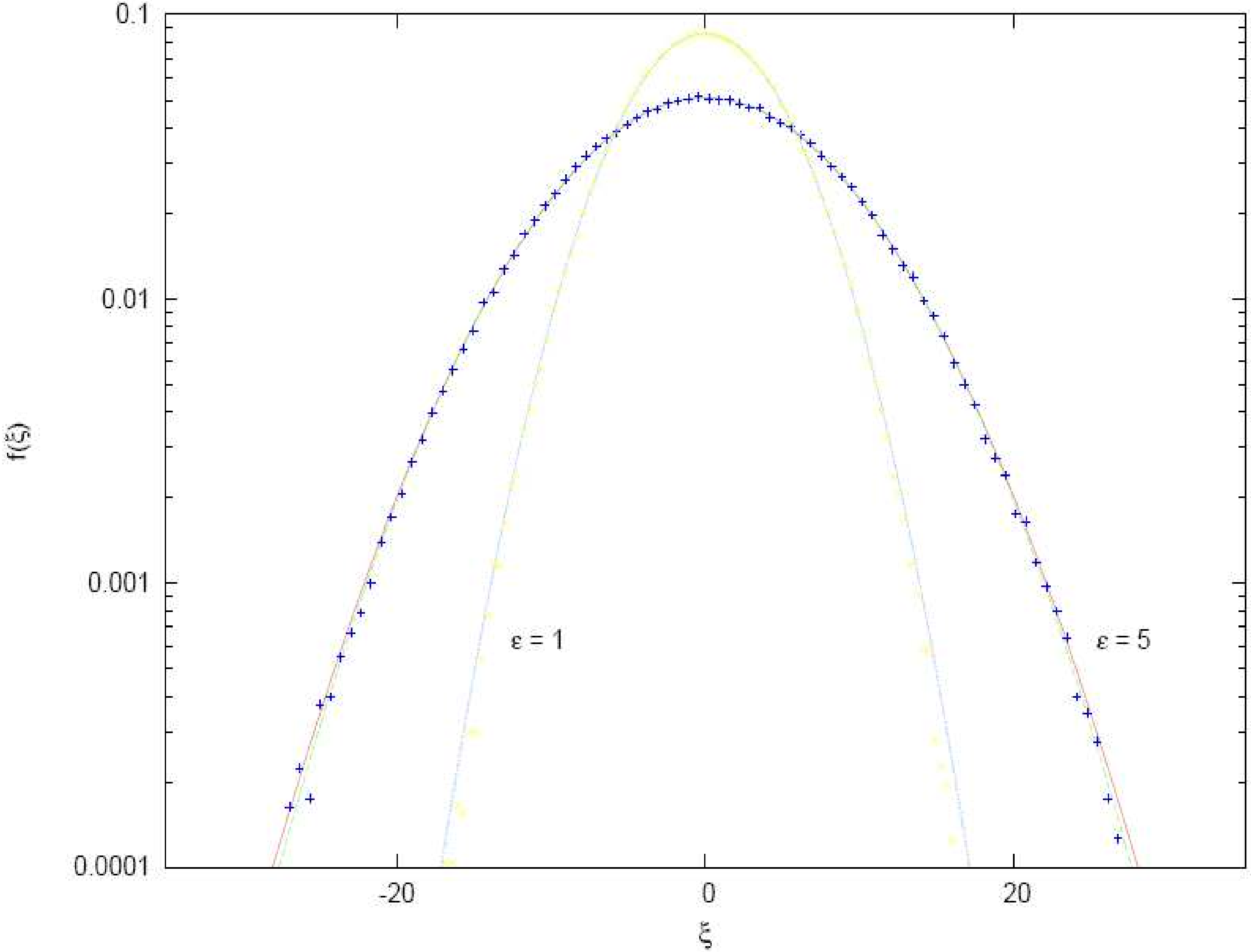


FIGURE 5. (Color on line). Plot in linear–log scale of Tsallis, Gaussian and numerical distribution for $N = 128$, $\epsilon = 1$ and $\epsilon = 5$. In both cases the Tsallis and Gaussian distributions essentially overlap.

Conclusions and future perspectives

- There are three regimes in the evolution of the system, under periodic conditions.

  i) a KAM-like one (regular and recurrent behaviour)

  ii) weak chaos

  iii) strong chaos and full symmetry breaking

- In the weakly chaotic regime, there is strong numerical evidence that Tsallis distribution describes the distribution of data. This is perfectly coherent with the fact that in this region **the maximal Liapunov exponent vanishes**. **We may conjecture that this is actually an universal behaviour of Hamiltonian dynamical systems.**

- **What happens in the case of fixed initial conditions?**

- An interesting problem concerns the metastability scenario for the FPU problem : after a sufficiently long time, is it true that this picture would collapse into a fully chaotic scenario, dominated by the Boltzmann distribution?

...e qui finisce la commedia!
Grazie!