From weak to strong chaos in the Fermi–Pasta–Ulam β system

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The key words that have characterized for more than fifty years the study of the Fermi–Pasta–Ulam (FPU) system [1] are recurrences, stability, relaxation time, weak and strong chaos and, more recently, breathers and q–breathers. These concepts apply both to non exact solutions and to exact solutions (π–mode, $\pi/2$–mode, etc.) of the system.

When a generic linear mode of wave number k is initially excited, energy is exchanged with the other modes that start to gain energy. If the coupling nonlinear parameter and the energy of the excited mode is small, then the energies exchanged remain small and change periodically. When the nonlinear effects become larger, some of the normal modes gain considerable energy, and induce the decay of the excited initial mode as well as a conspicuous exchange of energy among normal modes. This phenomenon is called the *induction phenomenon* and is observed mostly in the small energy density regime.

We recall that the Hamiltonian of the FPU–β system reads

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

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

It is well known that, for a periodic FPU–β chain with N oscillators and periodic conditions, there are nonlinear one–mode exact solutions (OMSs) [5] (π–mode, $\pi/2$–mode, etc.) corresponding to the values of the mode number n with n natiral number

$$n = \frac{N}{4}, \quad \frac{N}{3}, \quad \frac{N}{2}, \quad \frac{2}{3}N, \quad \frac{3}{4}N. \qquad (2)$$

Some years ago, the concept of strong stochasticity threshold (SST) has been introduced [3,4]. It is defined as the energy density threshold that characterizes the transition of the system dynamics between weak and strong chaos, after the induction phenomenon and during the relaxation of the system towards ergodicity and equipartition. This transition between the two chaoticity regimes, in the the FPU–β model, is numerically characterized by a change of energy density dependence of the largest Lyapunov exponent and of the relaxation time.

The aim of our recent research is to perform an analysis of the thermodynamics of the FPU–β system [6–8]. We have shown that this system possesses qualitatively two regimes, of *weak* and *strong chaos* respectively. In the weakly chaotic regime, the ergodicity hypothesis is no longer valid, the behaviour of the emerging distributions is not Gaussian and consequently the standard Boltzmann–Gibbs statistical mechanics fails to be correct. Instead, in this context, generalized thermostatistics should be considered [2]. In order to perform quantitatively our analysis, we introduce a *new universal indicator* $\rho(q)$, that measures the deviation of a generic assigned distribution from the Gaussian behaviour. This deviation is explicitly expressed in terms of a statistical parameter q. When $q \to 1$, the statistics is Boltzmannian. The function $\rho(q)$ is *model–independent* and can be used as an indicator of the behaviour at the edge of chaos of any complex physical system. This indicator is particularly suitable for the analysis of the FPU-β system. Indeed, consider the quantities $\eta_i = x_i + x_{i-1}$, where x_i denotes the deviation of the i–the particle with respect to its equilibrium position. If one excites the mode $N/2$, the relation

$$x_i(t) = \frac{1}{\sqrt{N}}(-1)^i Q_{N/2}(t) \qquad (3)$$

holds. The quantity η_i is then zero during the time evolution of the system, if it is stable. When the energy density is greater than the instability threshold value, η_i is no more equal to zero. The distribution of the values of η_i is characteristic of the dynamics of the system, namely of the exchange of energy among the mode $N/2$ and the other modes. Taking into account these considerations, we study the evolution of the system, as a function of the energy density ϵ, by means of the variation of the quantity

$$\rho = \frac{\sigma}{\theta}. \qquad (4)$$

Here σ is the standard deviation associated to the values of η_i and θ is the mean value of the moduli of differences between the values of η_i and the mean value $< \eta_i >$. The function ρ is the global indicator of our analysis. Now, observe that for $\epsilon < \epsilon_t$, the energy of the mode $N/2$ remains constant, and one has $\eta_i = x_i + x_{i-1} = 0$. For $\epsilon > \epsilon_t$, there is an energy exchange with the $N/2 - 1$ mode and subsequently with the other modes. Therefore, η_i is no more constant and the distribution of its values is determined essentially by the dynamics of energy exchange rather than the statistic of the numerical integration errors. Let ξ_i be the difference between the value of η_i at time t_i and the mean value $< \eta_i >$, evaluated in a time interval sufficiently large.

In our analysis, we distinguish two possibilities.

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

$$f(\xi) = \frac{a}{\sqrt{\pi}} \exp(-a^2\xi^2) \tag{5}$$

where a is a parameter. One has for the theoretical value of ρ:

$$\rho = \frac{\sigma}{\theta} = \sqrt{\frac{\pi}{2}} = 1.2533... \tag{6}$$

Eq. (6) is characteristic of normal distributions and can be utilized to verify roughly if a series of measures satisfies or not the Gauss distribution.

b) The distribution is a q–Gaussian:

$$\left(1 - (1-q)b^2x^2\right)^{\frac{1}{1-q}}. \tag{7}$$

In this case, one can prove that the function ρ has the following exact expression for $q < 1$:

$$\rho(q) = \frac{\frac{\sqrt{\pi}}{2}\Gamma\left(2 + \frac{1}{1-q}\right)}{\left(\sqrt{\frac{3}{2} + \frac{1}{1-q}}\Gamma\left(\frac{3}{2} + \frac{1}{1-q}\right)\right)}. \tag{8}$$

What one expects is that for $\epsilon < \epsilon_t$, when the distribution of the energy values is determined by the statistics of the errors due the numerical integration, the value of the parameter $\rho(\epsilon)$ should remain approximately constant. Also, it should change abruptly for $\epsilon > \epsilon_t$, when the $N/2$ mode starts to exchange energy with the other modes. For large values of ϵ, when an equipartition state has been reached, the parameter ρ should assume a constant value by increasing ϵ.

Another quantity that remains constant during the time evolution of the system, if the mode $N/2$ is stable, is the energy of each particle. Let the value of the nonlinearity parameter β be fixed to one. For the energy E_i of the i–th particle of the chain, one has:

$$E_i = \frac{1}{2}p_i^2 + \frac{1}{2}\{\frac{1}{2}(x_{i+1} - x_i)^2 + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{4}(x_{i+1} - x_i)^4 + \frac{1}{4}(x_i - x_{i-1})^4\} = \frac{E}{N} = \epsilon,$$

where E is the energy of the π–mode. If this mode is stable, the excitation energy remains fairly distributed among all particles of the chain. For $\epsilon > \epsilon_t$,the energy of the mode is no more constant and the previous relations are not valid. We associate to the energy E_i the global indicator $\rho = \sigma/\theta$, where now σ is the square root of the mean value of E_i^2, calculated over a time interval sufficiently long, and θ is the mean value of E_i, calculated over the same time.

The study of the function $\rho(\epsilon)$ associated to the observables η_i or E_i is then another method to explore the route of the system towards the chaos, when a one mode solution is initially excited.

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