

FPU phenomenon for generic initial data

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The well known FPU phenomenon (lack of attainment of equipartition of the mode-energies at low energies, for some exceptional initial data) suggests that the FPU model does not have the mixing property at low energies. We give numerical indications that this is actually the case. This we show by computing orbits for sets of initial data of full measure, sampled out from the microcanonical ensemble by standard Montecarlo techniques. Mixing is tested by looking at the decay of the autocorrelations of the mode-energies, and it is found that the high-frequency modes have autocorrelations that tend instead to positive values. Indications are given that such a nonmixing property survives in the thermodynamic limit. It is left as an open problem whether mixing obtains within time-scales much longer than the presently available ones.

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By the “standard” FPU phenomenon we mean the celebrated one observed for the first time in the year 1955 [1]. Namely, in numerical integrations of the equations of motion for a chain of particles coupled by weakly nonlinear springs, equilibrium is not attained within the available computational time, and a kind of anomalous pseudo-equilibrium does instead show up. This is observed at low energies, for initial data very far from equilibrium. The quantities studied were the energies $E_j(t)$ of the normal modes of the linearized system, and their time-averages $\bar{E}_j(t)$ were found to relax each to a different value rather than to a common one, against the equipartition principle (see especially the last figure of the original FPU report).

It was later found by Izrailev and Chirikov [2] that the phenomenon disappears, i.e., energy equipartition is quickly attained, if energy is large enough. A long debate then followed [3–7] concerning the questions (still unanswered) whether the phenomenon persists in the “thermodynamic limit” (i.e., when the number N of particles and the energy E both grow to infinity with a finite value of the specific energy $\epsilon = E/N$), and whether it can be interpreted in a metastability perspective [8, 9]. Another still open problem is whether the phenomenon persists when the dimensions are increased, passing from a chain of particles to a 2- or a 3-dimensional lattice [10].

In the present letter we address a further problem, namely whether some analog of the FPU phenomenon occurs if generic initial data are taken rather than some very special ones (see also [11–13]). More generally, we would like to look at the problem of the approach to equilibrium from the viewpoint of ergodic theory, in which one considers in principle all initial data, weighted with an invariant measure such as the microcanonical one. Now,

in ergodic theory it is well known that an approach to equilibrium is guaranteed if a system is proven to be mixing. Let us recall this. For a function f on phase space, define $f(t) = f \circ \Phi^t$, where Φ^t is the flow induced by a given Hamiltonian. Denote also by $\langle \cdot \rangle$ expectation with respect to the microcanonical measure. Then, mixing amounts to requiring (see [14], theorem 9.8) that for all (square-integrable) functions f and g the correlation

$$C(t) = \langle f(t)g(0) \rangle - \langle f(t) \rangle \langle g(0) \rangle$$

tends to zero as $t \rightarrow \infty$. So, equilibrium occurs if the correlations between all pairs of functions are proven to decay to zero with increasing time.

The original FPU results, although expressed in terms of time-averages and observed only for a very special class of initial data, suggests that, at low energies, the 1-dimensional FPU system “does not have mixing properties up the considered time”. In the present letter we give strong numerical indications that this is actually the case, even in the thermodynamic limit. This is obtained by computing the correlations of suitable functions, the averaging being performed over initial data sampled out from the microcanonical ensemble through a suitable Montecarlo method. According to the computations, for low enough energies the correlations appear to relax to some positive values. This we call an FPU-like phenomenon. Such a phenomenon seems to suggest a positive property, namely that the system did actually relax to some well defined anomalous state. We leave for further studies the questions whether such a result should be interpreted in a metastability perspective, and whether it persists for 2 and 3-dimensional lattices.

For what concerns the functions to be investigated, we started up by following FPU, and restricted our attention to the normal-mode energies $E_j(t)$, i.e. we studied the autocorrelations

$$C_j(t) = \langle E_j(t)E_j(0) \rangle - \langle E_j(t) \rangle \langle E_j(0) \rangle .$$

It will be shown later, however, that a major role is played by other related quantities, i.e., the energies \mathcal{E}_j of “pack-

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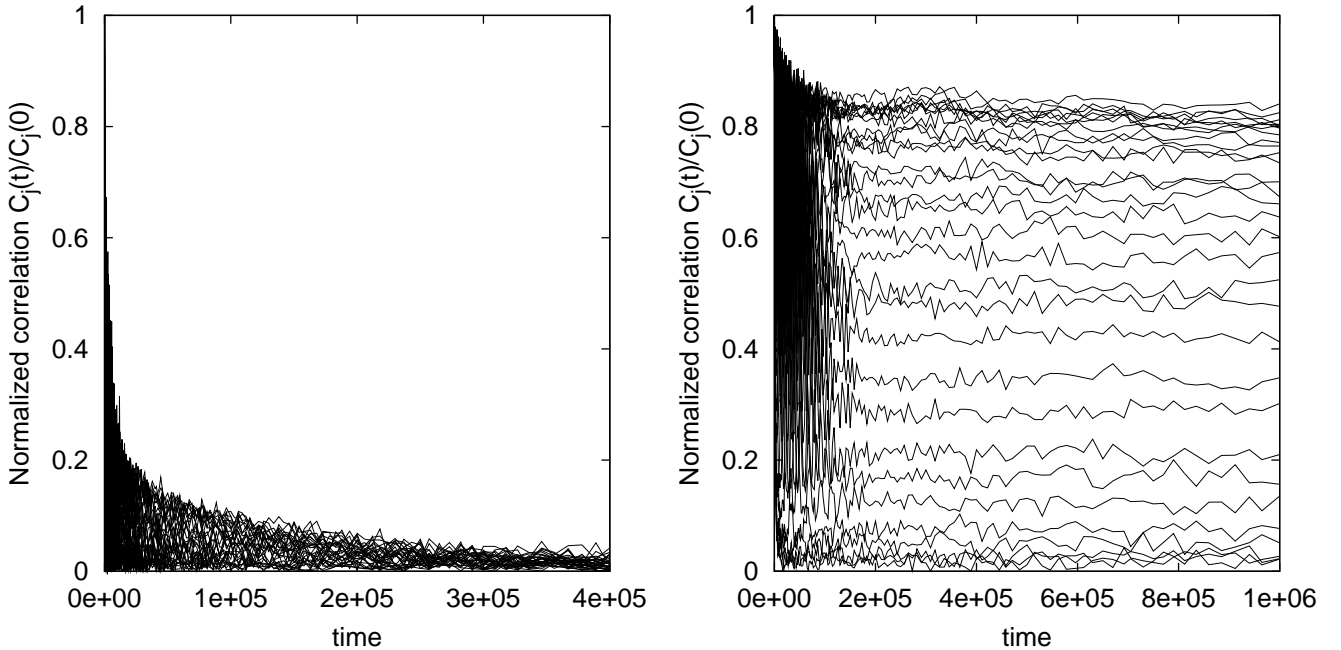


FIG. 1: The normalized autocorrelation function $C_j(t)/C_j(0)$ of the mode-energies E_j versus time, for some selected values of j ($j = 16k$, $k = 0, \dots, 32$) and $N = 511$ at two values of the specific energy ϵ . Left panel, $\epsilon = 3.16 \cdot 10^{-2}$, right panel $\epsilon = 3.16 \cdot 10^{-3}$.

ets” of nearby modes, whose relevance was pointed out in [15] (see also [12]).

The autocorrelations $C_j(t)$ of the mode-energies E_j were numerically estimated by integrating a sufficiently large number K of orbits (actually, $K = 10000$, apart from two cases which are mentioned later), and computing at any time the arithmetic mean of the values corresponding to the single orbits. The single initial data were sampled out from a microcanonical ensemble at specific energy ϵ . This was actually implemented as follows. Each initial datum was extracted from a Gibbs ensemble (with the quadratic part only of the total Hamiltonian) at temperature ϵ , and was then rescaled to let it fit the constraint $H = N\epsilon$ (H being now the total Hamiltonian).

We took the standard α -FPU Hamiltonian, namely,

$$H(p_1, \dots, p_N, x_1, \dots, x_N) = \sum_{k=1}^N \frac{p_k^2}{2m} + \sum_{k=0}^N V(x_{k+1} - x_k),$$

with $x_0 = x_{N+1} = 0$, where p_k is the momentum conjugated to the particle’s position x_k , and the interparticle potential is $V(r) = r^2/2 + \alpha r^3/3$. Units were so chosen that $m = 1$, and $\alpha = 1/4$. The integrations were performed with the standard leap-frog (or Verlet) method, with typical step 0.05.

The analog of the FPU phenomenon (together with its disappearing at high energies) is exhibited in Fig. 1, where the normalized autocorrelation functions $C_j(t)/C_j(0)$ of the mode-energies E_j are plotted versus time, for some selected values of j , with $N = 511$ and

a sample of 10000 initial data. The left and the right panels correspond to a case of a “high” specific energy and to a case of a “low” specific energy respectively, precisely, $\epsilon = 3.16 \cdot 10^{-2}$ and $\epsilon = 3.16 \cdot 10^{-3}$. It is seen that in the case of a high energy all autocorrelations decay to zero essentially within the same characteristic time, of the order of 10^5 . In the case of a low energy, instead, the decay to zero occurs only for some modes (with a characteristic time of the same order of magnitude as in the previous case), whereas for the remaining modes the autocorrelations appear to have relaxed within that time to some asymptotic nonvanishing values $c^*(j)$.

The natural question then arises of understanding whether there is any regularity in the distribution of the asymptotic values among the modes. We found the interesting result that the relevant parameter is the mode-number j/N (which is a monotonic increasing function of the corresponding frequency ω_j). This is illustrated in Fig. 2, where the asymptotic values c^* of the normalized autocorrelations are plotted versus j/N . The figure refers to the same values of ϵ , N and K (number of initial data) as in the right panel of Fig. 1. The first interesting feature is that the data appear to lie on some smooth curve. Moreover, the shape of the curve shows that the low- j modes (i.e., the low-frequency ones) are the ones that exhibit a quick relaxation to the “final” expected value 0, while the high-frequency modes remain “frozen” near the initial value 1. One should notice that it is precisely by looking at the correlations that the frequency can be found to play any role, because the microcanonical ex-

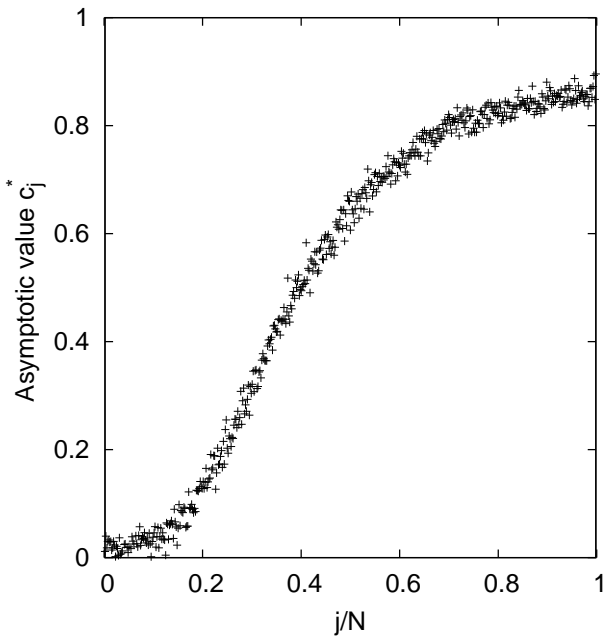


FIG. 2: The “asymptotic values” $c^*(j)$ of the normalized autocorrelation functions $C_j(t)/C_j(0)$ versus j/N , for the same parameters of Fig. 1, namely, $N = 511$ and $\epsilon = 3.16 \cdot 10^{-3}$.

pectations of the energies are instead all equal (equipartition). On the other hand, as the correlations are well known to play a major role in thermodynamics according to the fluctuation–dissipation theorem, one may conjecture that the anomalous behaviour discussed here might be of physical interest, for example for some phenomena of anomalous decay observed in recent experiments (see [16]).

We come now to the dependence of the function $c^*(j)$ on the specific energy ϵ . The curve is expected to reduce to the straight lines $c^* = 0$ and $c^* = 1$ for large and small values of ϵ respectively. We found the interesting result that, for a fixed N , the curve is a function of only one variable, precisely, one has $c^*(j, \epsilon) = f(j/\sqrt{\epsilon})$. This is illustrated in Fig. 3, where, still for $N = 511$, c^* is plotted versus $(j/N)/\sqrt{\epsilon}$ for three values of ϵ , namely, $\epsilon = 3.16 \cdot 10^{-3}$, $1.0 \cdot 10^{-3}$, $3.16 \cdot 10^{-4}$. A rather good superposition of the curves seems to be observed. In particular notice that, with increasing ϵ , the domain of the curve shrinks to the left, so that c^* is found to approach the value zero. Thus for large ϵ one has a complete decay to zero of the correlations, i.e., an analog of the Izrailev–Chirikov phenomenon. Notice that for each ϵ the asymptotic values $c^*(j)$ had to be evaluated at a suitable time, namely that at which stabilization just started occurring, in the sense of Fig.1. Such a relaxation time was found to increase as $1/\epsilon$ with decreasing ϵ .

The last point we address concerns the dependence of the results on the number N of particles. This is a quite delicate matter, on which we feel we got an interesting result. To begin with we point out that, if one

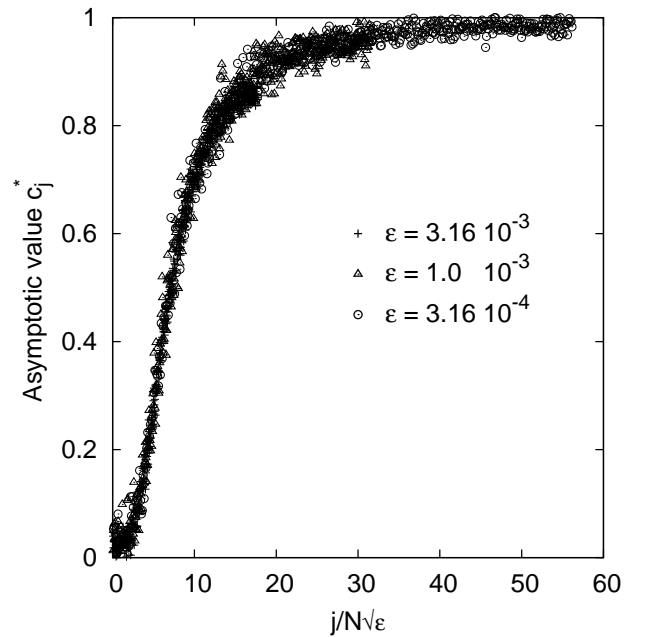


FIG. 3: The “asymptotic values” $c^*(j)$ of the normalized autocorrelation functions $C_j(t)/C_j(0)$, versus $\frac{j}{N}/\sqrt{\epsilon}$, for $N = 511$ and $\epsilon = 3.16 \cdot 10^{-3}$, $1.0 \cdot 10^{-3}$, $3.16 \cdot 10^{-4}$.

takes a naive approach and plots the curves analogous to that of Fig.2 for increasing values of N , the curves are found to collapse towards the trivial one $c^* = 0$. This is shown in Fig.4, left panel, where the curves for $N = 511, 1023, 2047, 4095$ are reported, for the same ϵ as in Fig. 2. Concerning the number K of initial data, this had forcedly to be diminished with increasing N , and we had to pass from $K = 10000$ for $N = 511$ and 1023 to $K = 5000$ and 2000 for $N = 2047$ and 4095 respectively. This, by the way, explains the broadening of the “curves” for the two large values of N .

It would however be incorrect to infer from such a collapse that mixing occurs in the thermodynamic limit, because mixing requires the decaying to zero of the correlations for all pairs of functions. Instead, a decay to positive values is observed if a suitable choice is made for the functions to be tested for autocorrelation. Actually, instead of considering the energies E_j of the single modes, we considered the energies of packets of n nearby modes, with n proportional to N , precisely, the N_0 quantities

$$\mathcal{E}_j = \sum_{k=nj+1}^{n(j+1)} E_k, \quad \text{where } n = \frac{N+1}{N_0+1}, \quad N_0 = 511,$$

for $j = 0, 1, \dots, N_0 - 1$. In Fig. 4, right panel, the analog of c^* for the quantities \mathcal{E}_j is plotted versus j/N_0 , for the same numbers N and K as in the left panel. It is true that the different curves do not superpose, and that a certain decreasing is observed, especially in passing from $N = 511$ to $N = 1023$. But for larger values

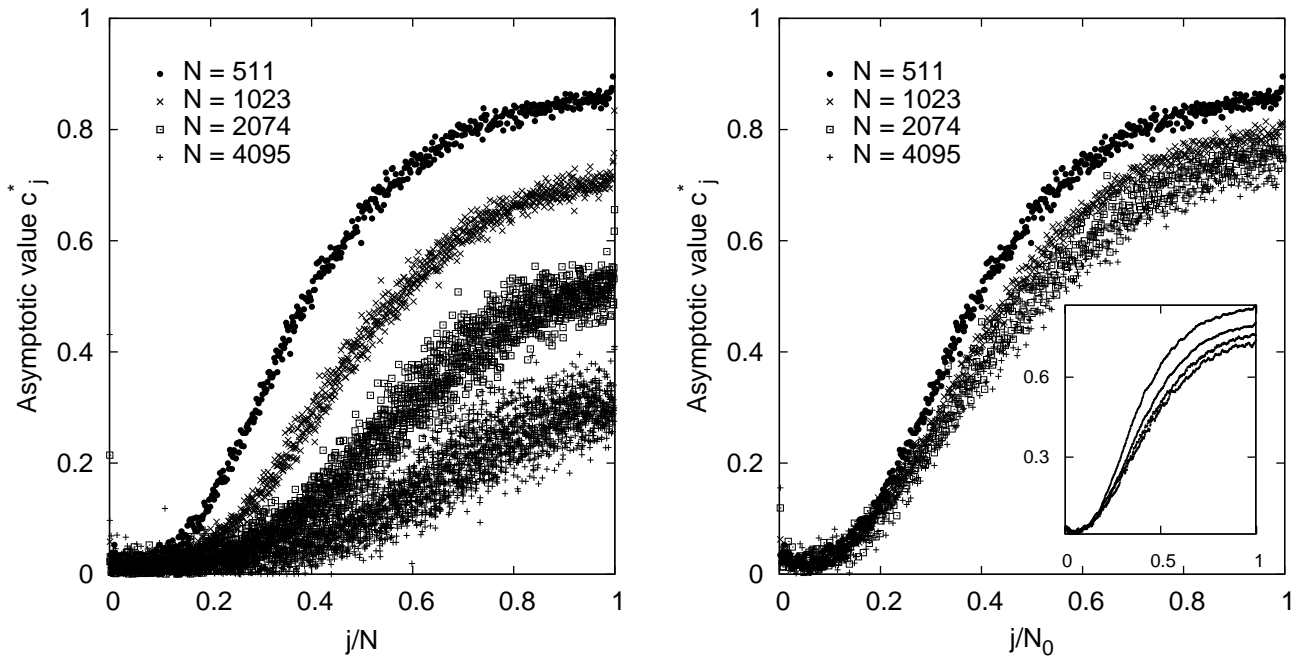


FIG. 4: The “asymptotic values” $c^*(j)$ of the normalized autocorrelation functions for the mode-energies E_j (left panel), and for the energies \mathcal{E}_j of packets of n nearby modes with n proportional to N (right panel), for an increasing number N of particles. The value of ϵ is the same as in Fig. 2. The asymptotic value $c^*(j)$ is plotted in the left panel versus j/N for $j = 1, \dots, N$, and in the right panel versus j/N_0 for $j = 0, \dots, N_0 - 1$, with $N_0 = 511$. In the inset of the right panel, for each of the four series of data the corresponding “moving averages” (over eleven points) are plotted.

of N the results seem to indicate that a nontrivial limit curve is being approached. This is better illustrated in the inset, where, in order to improve the readability of the graphs, the data were smoothed out by a standard “moving averaging” with eleven points. In our opinion, the results suggest that the FPU-type phenomenon discussed here may persist in the thermodynamic limit, for a one-dimensional chain. And this, not for very special

initial data, but in a global sense involving an averaging over all initial data, in a microcanonical setting.

It may be of interest in this connection to recall that analytical perturbative estimates for a “freezing” in the thermodynamic limit, much in the same spirit of the present paper, i.e. by averaging initial data over an invariant measure, were obtained very recently (see [17]).

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