Fermi-Pasta-Ulam phenomenon for generic initial data

A. Carati,* L. Galgani,† A. Giorgilli,‡ and S. Paleari§

Department of Mathematics, University of Milano, Via Saldini 50, I-20133 Milano, Italy

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The well-known Fermi-Pasta-Ulam (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 Monte Carlo 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 actually occurs, i.e., whether the autocorrelations vanish as time tends to infinity.

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By the "standard" Fermi-Pasta-Ulam (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 pseudoequilibrium 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 (as defined in [1]), and their time averages $\overline{E_j}(t)$ 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 the 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 two or a three-dimensional lattice [10].

In the present Brief Report we address a further problem: namely whether some analog of the FPU phenomenon occurs if, instead of taking some very special initial data, one looks 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 the microcanonical measure (see also [11–13]). 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 $t \to \infty$ 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 one-dimensional FPU system "does not have mixing properties up the considered time." In the present paper 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 Monte Carlo 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 of whether such a result should be interpreted in a metastability perspective and whether it persists for two- and three-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 "packets" of nearby modes, whose relevance was pointed out in [15] (see also [12]).

The aurocorrelations $C_j(t)$ of the mode energies E_j were numerically estimated by integrating a sufficiently large

*carati@mat.unimi.it

†galgani@mat.unimi.it

‡giorgilli@mat.unimi.it

§paleari@mat.unimi.it

number K of orbits (actually, $K=10\,000$, 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). The approximation of considering just the quadratic part in performing the sampling is due to the Gibbs distribution itself being not defined for the full Hamiltonian (as the energy surfaces are non compact when the cubic term is taken into account). On the other hand, such an approximation is expected to be adequate for the case of low energies, which is the one we are mainly concerned with.

We took the standard α-FPU Hamiltonian: namely,

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

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 leapfrog (or Verlet) method, with tipical 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 10 000 initial data. The left and bottom panels correspond to a case of a "high" specific energy and to a case of a "low" specific energy, respectively, precisely, $\epsilon = 3.16 \times 10^{-2}$ and $\epsilon = 3.16 \times 10^{-3}$. 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 $c^*(j)$. Quantitatively, the value of $c^*(j)$ is defined as a value ot the autocorrelation that remains roughly constant over a factor of the order of 10 in time.

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 bottom 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. The phenomenon of a freezing of the high-frequency modes is rather well understood in the frame of Hamiltonian perturbation theory, even in the thermodynamic limit (see [16]). However, the applicability of the known theorems to the present case is not straightforward, due to the present choice of initial conditions, so that the problem deserves further theoretical consideration. For a review concerning excitations of low-frequency modes, see [5].

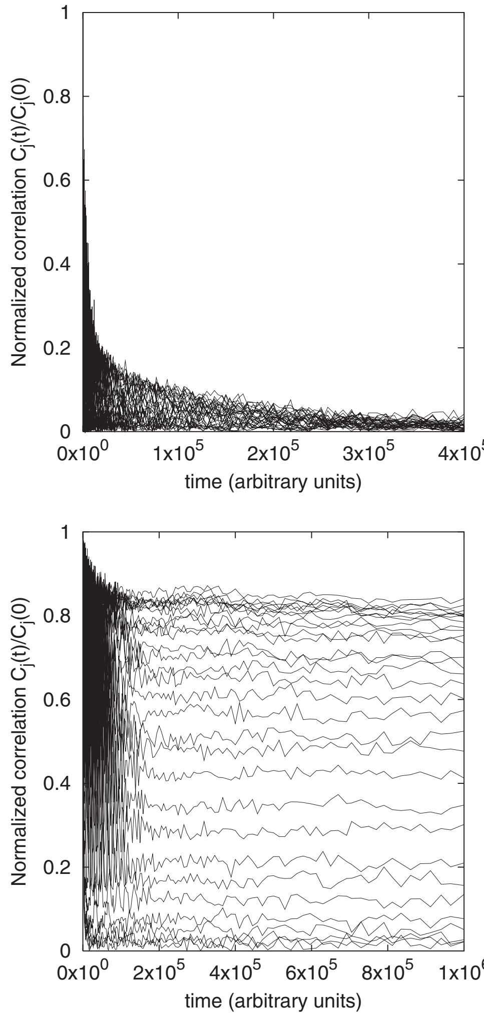

FIG. 1. The normalized autocorrelation function $C_j(t)/C_j(0)$ of the mode energies E_j versus time for some selected values of j ($j = 16k$, $k=0, \ldots, 32$) and $N=511$ at two values of the specific energy ϵ. Top panel $\epsilon = 3.16 \times 10^{-2}$, bottom panel $\epsilon = 3.16 \times 10^{-3}$.

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 expectations 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 behavior discussed here might be of physical interest—for example, for some phenomena of anomalous decay observed in recent experiments (see [17]).

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

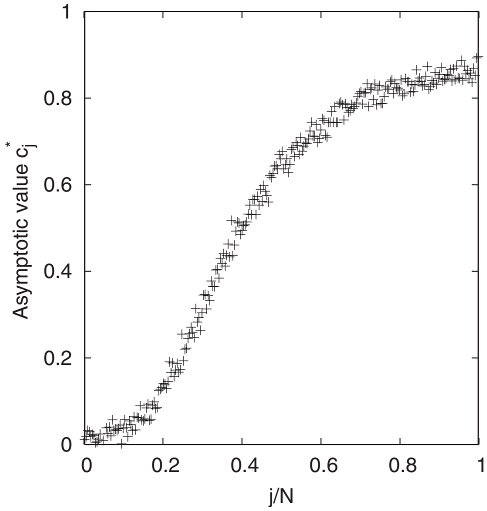

FIG. 2. The "asymptotic values" $c^*(j)$ of the normalized autocorrelation functions $C_j(t)/C_j(0)$ versus j/N for the same parameters of Fig. 1: namely $N=511$ and $\epsilon=3.16\times10^{-3}$.

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, $\epsilon=3.16\times10^{-3}$, 1.0×10^{-3}, and 3.16×10^{-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, as explained previously. 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

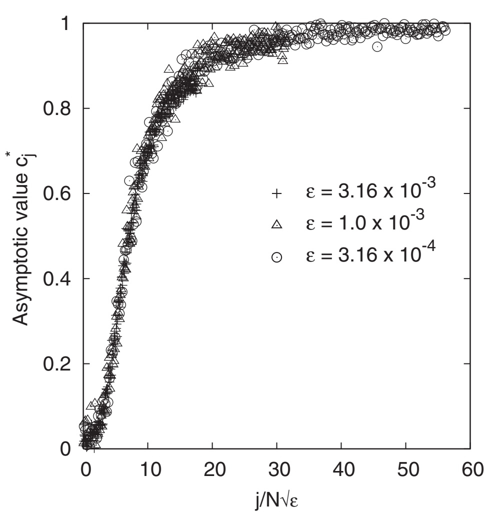

FIG. 3. The "asymptotic values" $c^*(j)$ of the normalized autocorrelation functions $C_j(t)/C_j(0)$, versus $\frac{j}{N}/\sqrt{\epsilon}$, for $N=511$ and $\epsilon=3.16\times10^{-3}$, 1.0×10^{-3}, and 3.16×10^{-4}.

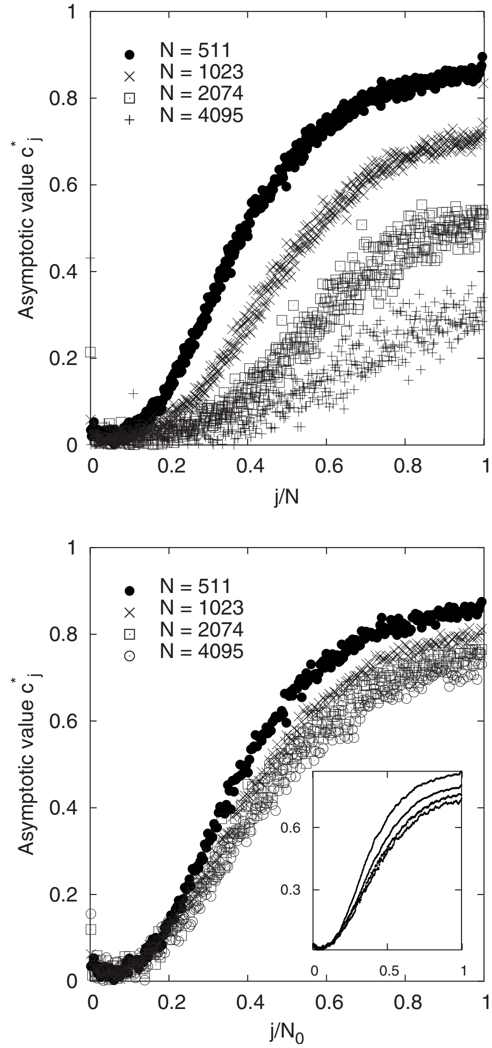

FIG. 4. The "asymptotic values" $c^*(j)$ of the normalized autocorrelation functions for the mode energies E_j (top panel) and for the energies $\mathcal{E}_j$ of packets of n nearby modes with n proportional to N (bottom panel) for an increasing number N of particles. The value of ϵ is the same as in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

begin with we point out that, if one 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, top 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 $K=10\,000$ 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 $j=0,1,\ldots,N_0-1$. In Fig. 4, bottom 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 top 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 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 11 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.

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