Weak and strong chaos in Fermi-Pasta-Ulam models and beyond

Weak and strong chaos in FPU models and beyond

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(Dated: October 29, 2018)

We briefly review some of the most relevant results that our group obtained in the past, while investigating the dynamics of the Fermi-Pasta-Ulam (FPU) models. A first result is the numerical evidence of the existence of two different kinds of transitions in the dynamics of the FPU models: *i)* a Stochasticity Threshold (ST), characterized by a value of the energy per degree of freedom below which the overwhelming majority of the phase space trajectories are regular (vanishing Lyapunov exponents). It tends to vanish as the number N of degrees of freedom is increased. *ii)* a Strong Stochasticity Threshold (SST), characterized by a value of the energy per degree of freedom at which a crossover appears between two different power laws of the energy dependence of the largest Lyapunov exponent, which phenomenologically corresponds to the transition between *weakly* and *strongly* chaotic regimes. It is stable with N. A second result is the development of a Riemannian geometric theory to explain the origin of Hamiltonian chaos. The starting of this theory has been motivated by the inadequacy of the approach based on homoclinic intersections to explain the origin of chaos in systems of arbitrarily large N, or arbitrarily far from quasi-integrability, or displaying a transition between weak and strong chaos. Finally, a third result stems from the search for the transition between weak and strong chaos in systems other than FPU. Actually, we found that a very sharp SST appears as the dynamical counterpart of a thermodynamic phase transition, which in turn has led, in the light of the Riemannian theory of chaos, to the development of a topological theory of phase transitions.

PACS numbers: 05.45.+b; 05.20.-y

In a foreword to their co-authored work reprinted in the Fermi Collected Papers [1], S. Ulam wrote: "...Fermi expressed often the belief that future fundamental theories in physics may involve non-linear operators and equations, and that it would be useful to attempt practice in the mathematics needed for the understanding of nonlinear systems. The plan was then to start with the possibly simplest such physical model and to study the results of the calculation of its long-time behavior.... The motivation then was to observe the rates of mixing and thermalization with the hope that the computational results would provide hints for a future theory. One could venture a guess that one motive in the selection of problems could be traced to Fermi's early interest in the ergodic theory..."

Actually, Fermi's early interest in ergodic theory is witnessed by his contribution to a theorem due to Poincaré and thenceforth known as the Poincaré-Fermi theorem. This asserts that neither analytic (Poincaré) nor smooth (Fermi) integrals of motion besides the energy can survive a generic perturbation of an integrable system with three or more degrees of freedom, thus, in the absence of other isolating integrals of motion, any constant energy surface of these generic systems is expected to be everywhere accessible to the phase space trajectory. At this level, no hindrance to ergodicity seems to be possible. Whence the surprise of Fermi, Pasta and Ulam (FPU) when no apparent tendency to equipartition was observed in their numerical experiment whose 50th anniversary we are celebrating. Fermi himself considered what they found a "little discovery". The almost contemporary announcement by Kolmogorov of the starting of what would later become the celebrated KAM theorem, seemed to provide an explanation to the unexpected FPU's results. But later developments

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of KAM theory, including optimal estimates of the N-dependence of the perturbation thresholds and the Nekhoroshev theorem, revealed that this is not really an adequate framework to explain the FPU problem. The rich variety of the numerical phenomenology accumulated over time seemed to keep off "the hope that the computational results would provide hints for a future theory". In fact, "rates of mixing and thermalization" have a startling and complicated dependence on energy, number of degrees of freedom and initial conditions. Actually, any dynamical evolution of the system depends on the starting point in phase space and on the "landscape" of its surroundings. Thus, there can be a huge variety of dynamical behavior entailed by the preparation of the system in an initial condition out of equilibrium. As a consequence, in order to get some global information on the phase space structure, independently of the initial conditions, one has to look at the chaotic component of phase space. This way of tackling the FPU problem is very illuminating and leads to the conclusion that the FPU problem does not threaten the validity of statistical mechanics. Moreover, this has stimulated the starting of a new theory of Hamiltonian chaos.

I. INTRODUCTION

Few problems have been studied so extensively over the last decades as the one devised originally by E. Fermi, J. Pasta and S. Ulam (FPU) in 1954 [1]. Their purpose was to check numerically that a generic but very simple non-linear many particle dynamical system would indeed behave for large times as a statistical mechanical system, that is it would approach equilibrium if initially not in equilibrium. In particular their purpose was to obtain the usual equipartition of energy over all the degrees of freedom of a system, for generic initial conditions. To their surprise, for the system FPU considered – a one dimensional anharmonic chain of 32 or 64 particles with fixed ends and in addition to harmonic, cubic (α-model) or quartic (β-model) anharmonic forces between nearest neighbors – this was not observed. A variety of manifestly non-equilibrium and non-equipartition behaviors was seen, including quasiperiodic recurrences to the initial state. In fact, a behavior reminiscent of that of a dynamical system with few degrees of freedom was found, rather than the expected statistical mechanical behavior. The duration of their calculations varied between 10000 and 82500 computation steps. These results raised the fundamental question about the validity or at least the generally assumed applicability of statistical mechanics to non-linear systems of which the system considered by FPU seemed to be a typical example. Most of the attempts to clarify this difficulty have approached the problem as one in dynamical systems theory. These analyses have revealed many very interesting properties of the FPU system and uncovered a number of possible explanations for the resolution of the observed conflict with statistical mechanics. The classical explanations are: *i)* the survival of invariant tori in the phase space of a quasi-integrable system (KAM theory) [2], *ii)* the existence of Zabusky and Kruskal's solitons in a special continuum limit leading to the integrable Korteweg de Vries equation [3, 4], *iii)* the existence of an order-to-chaos transition [5].

In this paper we will first try to exhibit the reasons why this apparently bona fide statistical mechanical system did not behave as such and, in particular, what in our opinion the significance of this apparent failure is for the general validity of statistical mechanics; then, we will review a number of results that we obtained studying the dynamics of the FPU models or being directly inspired by it.

There are a number of obvious questions related to the unstatistical mechanical behavior observed by FPU, which all address the generic nature of the results of Fermi and collaborators:

a) Was their time of integration long enough?

b) Was their dynamical system of $N = 32$ or 64 particles in one dimension large enough, i.e. possessing a sufficient number of degrees of freedom, to qualify as a statistical mechanical system?

c) Were the recurrence phenomena (to within 3%) observed by FPU, transient or generic, i.e., possibly related to a Poincaré recurrence time?

The search for answers to these questions made the work of FPU very seminal, spawning many new developments and connections in the theory of nonlinear dynamical systems, such as the connection with continuum models based on the Korteweg – de Vries equation, leading to solitons [3], heavy breathers etc., or with few degrees of freedom models like the Hénon-Heiles [6] and the Toda lattice [7].

Thus, the effort to resolve the so-called FPU problem has led to enormous advances in our understanding of non linear dynamical systems; for a review we refer to [8]. Although in our opinion the FPU problem has possibly not yet exhausted its power of inspiration, we believe that the FPU paradox, i.e., FPU's original question, can nowadays be reasonably answered along the lines we are going to describe hereafter.

II. STOCHASTICITY THRESHOLDS IN FPU MODELS

For some time, it has been a commonly accepted idea [8] that the KAM theorem provides the essential answer to FPU's observations, i.e., for sufficiently small nonlinearities and a class of initial conditions living on non-resonant tori, the FPU system behaves like an integrable system and is represented by deformed tori in phase space. With increasing strength of the non-linearities, a progressive chaotic behavior appears, which would ultimately lead to the expected approach to equilibrium and equipartition. Even though we found regular regions in phase space, the existing typical KAM estimates of the N-dependence of the perturbation threshold (below which a positive measure of KAM tori survive), are qualitatively different from our results, indicating that the physics of the FPU model is quite different from what is contained in these estimates.

Thanks to the power of modern computers, we have considerably extended the calculations performed in the past by various authors and we have been able to reconcile different, and sometimes contradictory, aspects of the FPU dynamics.

A. FPU-α model

Very interesting results have been obtained revisiting the FPU-α model [9] by focusing on the development of chaoticity in the time evolution of the system rather than on the attainment of equipartition. For these numerical experiments, the chosen initial conditions – single mode excitations – were the same as chosen by Fermi and collaborators in their original experiment.

The model is described by the Hamiltonian [1]

$$H(p,q) = \sum_{k=1}^{N} \left[\frac{1}{2} p_k^2 + \frac{1}{2}(q_{k+1} - q_k)^2 + \frac{\alpha}{3}(q_{k+1} - q_k)^3 \right], \tag{1}$$

where the particles have unit mass and unit harmonic coupling constant and the end-points are fixed ($q_1 = q_{N+1} = 0$).

Comparing the behaviour in time of the largest Lyapunov exponent in the FPU system with that of the same quantity in a suitable integrable system, it has been possible to define clearly what a trapping time in a regular region of phase space is and to determine numerically and unambiguously its value. The integrable system we chose for this comparison is the Toda lattice, from which the FPU-α model can be obtained as a third order truncation of the power series expansion of its potential. The Toda lattice is defined by the Hamiltonian

$$H(p,q) = \sum_{k=1}^{N} \frac{1}{2} p_k^2 + \frac{a}{b} \sum_{k=1}^{N} \left[e^{-b(q_{k+1} - q_k)} + b(q_{k+1} - q_k) - 1 \right] . \tag{2}$$

The decay pattern toward zero of $\lambda^{Toda}(t)$ is undistinguishable from the decay pattern of $\lambda^{FPU}(t)$ up to some time τ_T, after which $\lambda^{FPU}(t)$ separates from $\lambda^{Toda}(t)$ and converges to a finite value while $\lambda^{Toda}(t)$ goes to zero. This suggests that non-integrable motions of the FPU lattice, originated by one-mode initial excitations, enter their chaotic component after a transient and possibly long trapping in a regular region of phase space (some kind of "Nekhoroshev-like" trapping) and that equipartition is eventually attained on a finite, albeit possibly very long, time scale.

Fig. 1 shows that the trapping times $\tau_T(\varepsilon, N)$ – so defined – for the FPU-α model at different values of both the energy density ε and of the number of degrees of freedom N, with decreasing ε first tend to increase monotonically, then, abruptly, display an apparently divergent behavior.

This very steep increase of τ_T with decreasing ε suggests the existence of, at least, a very narrow bottleneck in phase space, through which the system can only escape with great difficulty or, perhaps, it might not escape at all. The sharp variation with ε of the shape of $\tau_T(\varepsilon)$ brings about a natural definition of a threshold value of ε below which τ_T seems to diverge.

For what concerns the behavior of the largest Lyapunov exponents, when ε is smaller than the threshold value, $\lambda^{Toda}(t)$ and $\lambda^{FPU}(t)$ do not show any separation, even after a very long integration time. That τ_T is really a trapping time and not, for example, a trivial effect of the numerical statistics is suggested by the fact that $\tau_T(\varepsilon) \sim \varepsilon^{-2}$ whereas $\lambda(\varepsilon) \sim \varepsilon^{3/2}$, that is $\lambda \neq \tau_T^{-1}$. In Fig. 2, $\lambda^{FPU}(\varepsilon, N)$ is reported.

The shapes of both $\lambda^{FPU}(\varepsilon, N)$ and $\tau_T(\varepsilon, N)$ strongly suggest the existence of a threshold value – *which depends on* N – of the energy density, above which the motion is chaotic and below which the trajectories appear to belong to a regular region of phase space. This threshold is referred to as stochasticity threshold (ST). To our knowledge, its *direct* evidence in a non-linear Hamiltonian system at $N \gg 2$ has been found for the first time in [9].

Fermi and coworkers chose an initial condition well below this ST (the energy density corresponding to their initial condition is shown by the vertical dotted line in Fig. 2); had they taken a ten times larger amplitude of the initial

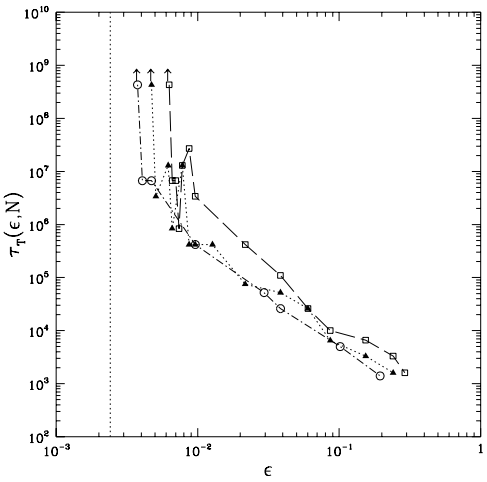

FIG. 1: FPU-α model. The trapping times $\tau_T(\varepsilon, N)$ at different values of energy density ε (i.e. at different values of the initial excitation amplitudes), are reported. Open squares refer to the case $N = 32$, solid triangles refer to $N = 64$, open circles refer to $N = 128$, respectively. The endpoints of the broken lines are lower bounds for the trapping time (the cut-off of the integration time is at $t = 4.3 \times 10^8$). The dotted vertical line at $\varepsilon = 0.00241$ corresponds to the initial excitation amplitude of the FPU's original paper. From Ref. [9].

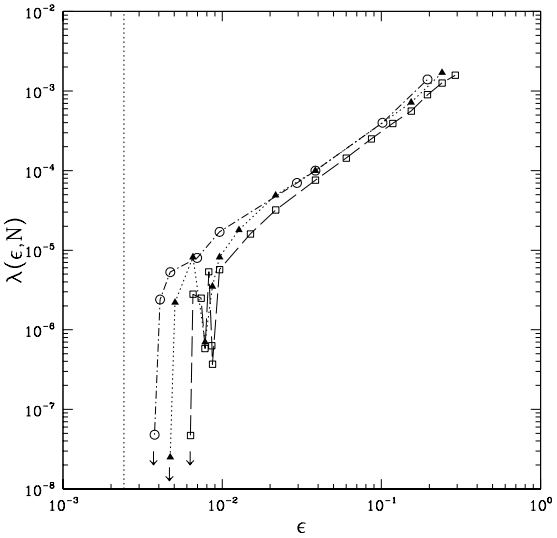

FIG. 2: FPU-α model. The largest Lyapunov exponents $\lambda(\varepsilon, N)$ are shown for different values of the energy density ε and a sine wave initially excited. Symbols as in Fig. 1; here the arrows are upper bounds for λ. From Ref. [9].

excitation, they would have observed equipartition during the integration time they used. This appears to be the simple but non-trivial explanation of the lack of statistical mechanical behavior observed in the original FPU numerical experiment.

In order to understand whether the ST refers to a global property of the constant energy surface Σ_E or is rather a local property of Σ_E, sensitive to the initial condition, two other choices of more physically generic initial conditions, i.e., random positions and momenta, were considered.

In each case a threshold energy (or equivalently energy density, since N is fixed) was found. This fact suggests

that the phase space undergoes some important structural change as the energy is varied: we can find regions of the phase space where ordered trajectories are observed, regions where there is coexistence of order and chaos and regions where chaos is fully developed.

An important question is whether the stochasticity threshold is stable or unstable with respect to N. Unambiguous information about this point is provided by the Lyapunov exponents $\lambda(\varepsilon, N)$ computed at different N, always starting with random initial conditions (Fig. 3).

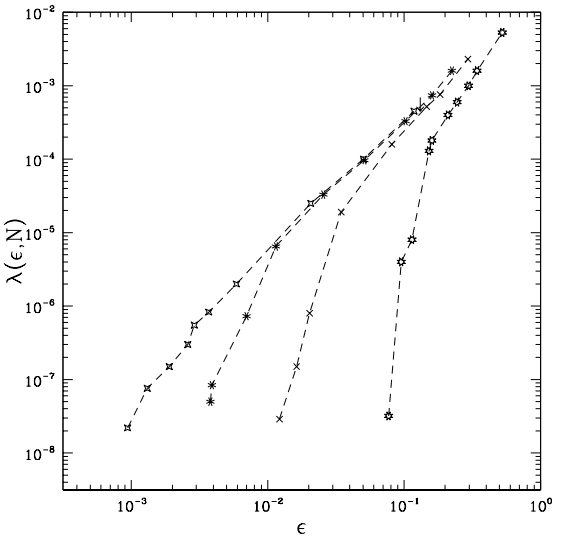

FIG. 3: FPU-α model. The largest Lyapunov exponents $\lambda(\varepsilon, N)$ are plotted *vs.* the energy density ε, for different values of N. Random initial conditions are chosen. Star-like polygons refer to $N = 8$, crosses to $N = 16$, asterisks to $N = 32$ and star-like squares to $N = 64$, respectively. The arrows have the same meaning as in Fig. 2. From Ref. [9].

At large ε, there is a tendency of all the sets of points to join, while they tend to separate at small ε: the larger N, the smaller the energy density at which the separation occurs. The "critical" energy density ε_c at which the separation occurs shows the N-dependence $\varepsilon_c(N) \propto 1/N^2$.

A qualitative agreement about the vanishing with N of the critical energy to get chaos is reported in a recent paper on the FPU-α model [10]. The question of how to explain the existence and the $1/N^2$ dependence of the stochasticity threshold remains open.

We thus see that revisiting the FPU-α model led to the observation of some very interesting phenomena: the apparent existence of regular regions in the phase space of a non-integrable Hamiltonian system with many degrees of freedom at large values of the anharmonic energy (even very large if compared with what they should be according to the KAM theory), and the existence of almost regular regions of phase space where the trajectories are trapped during long but finite times. The behavior of the largest Lyapunov exponent suggests that the sudden escape from the regular region might occur as if the trajectory would eventually find a 'hole' in its boundary.

Moreover, the coexistence of regular regions of the phase space and of a large chaotic "sea" reconciles different and sometimes apparently contradictory aspects of the FPU dynamics found in the past. The lack of equipartition in the original FPU experiment is not representative of a global property of phase space: apparently regular, soliton-like structures, similar to those of Zabusky and Kruskal, have a very long, possibly infinite, life-time below the stochasticity threshold, whereas, above the same threshold, they have only a finite life-time[9].

The threshold energy density for the onset of chaos shows a clear tendency to vanish at an increasing number of degrees of freedom ($\sim 1/N^2$), so that strong evidence has been found in support of the point of view that the so-called "FPU-problem" does not invalidate the (generic) approach to equilibrium and the validity of equilibrium statistical mechanics. On the other hand the existence of long living initial states far from equilibrium, may well have interesting, non trivial physical applications.

B. FPU-β model

The FPU-β model is described by the Hamiltonian [1]

$$H(p,q) = \sum_{k=1}^{N} \left[\frac{1}{2} p_k^2 + \frac{1}{2}(q_{k+1} - q_k)^2 + \frac{\beta}{4}(q_{k+1} - q_k)^4 \right], \tag{3}$$

where the particles have unit mass and unit harmonic coupling constant and the end-points are fixed ($q_1 = q_{N+1} = 0$); for this model also periodic boundary conditions have been considered ($q_1 = q_{N+1}$).

The approach to equilibrium of the FPU-β model was studied extensively for various classes of initial conditions by Kantz *et al.* [11] and recently by De Luca *et al.* [12] who extended and improved earlier computations of ours [13, 14].

A very detailed picture has emerged from these works, as to the behavior of the FPU-β model in its dependence on non-equilibrium initial conditions as well as in the role played by low frequency and high frequency mode-mode couplings [15] during its time evolution.

Several years ago, we introduced [14] a time dependent spectral entropy $S(t) = -\sum_i w_i(t) \log w_i(t)$, where $w_i(t) = E_i(t)/\sum_k E_k(t)$ is the normalized energy content of the i-th harmonic normal mode, defined so as to detect energy equipartition (when it attains its maximum value) and to measure the time needed to reach it. By means of this spectral entropy, we investigated in Refs. [16, 17] the relationship between equipartition times, measured through the time relaxation patterns of this spectral entropy, and the chaotic properties of the dynamics in nonlinear large Hamiltonian systems. For the FPU-β model, we have put in evidence that, at different initial conditions and at long times, the spectral entropy always relaxes toward its maximum value signaling equipartition, however, depending on the value of the total energy density, the relaxation occurs with quite different modalities. The relaxation time is approximately constant for energy densities greater than some threshold value ε_c, but it steeply grows by decreasing the energy density below this threshold. Moreover, the largest Lyapunov exponent shows a crossover in its ε-dependence corresponding to this threshold value. We interpret this phenomenological result as the (smooth) transition – at ε_c – between two different regimes of chaoticity, weak chaos and strong chaos, thus we called this transition the Strong Stochasticity Threshold (SST) [16]. Weak and strong chaos are qualitative terms to denote slow and fast phase space mixing respectively. In Refs. [16, 17] we resorted to a random matrix model for the tangent dynamics to try to make more precise and quantitative the definitions of weak and strong chaos. At least in a limited high energy range of values, the random matrix model predicts the numerically observed scaling $\lambda(\varepsilon) \sim \varepsilon^{2/3}$ (this law changes to $\lambda(\varepsilon) \sim \varepsilon^{1/4}$ at very high energy density, however this is not explained by the random matrix model, the reason is that a free parameter, a time-scale of unknown ε dependence, enters the random matrix model. This time-scale is arbitrarily assumed constant). Thus we say that *chaos is strong* in the energy density range where $\lambda(\varepsilon) \sim \varepsilon^{2/3}$, because the random matrix model assumes that the dynamics looks as a random uncorrelated process (if sampled with the just mentioned unknown time scale). At low energy density, the ε-scaling of λ is found to be steeper, $\lambda(\varepsilon) \sim \varepsilon^2$, so that λ fastly decreases as ε is lowered and is much smaller than it should be if the high energy random matrix prediction could be extrapolated down to low energy values. For this reason we say that here *chaos is weak*. Figure 4 shows $\lambda(\varepsilon, N)$.

The SST is independent of the initial conditions so it has to be ascribed to some change in the global properties of the phase space, for this reason it has to have major consequences on the dynamics. An interesting explanation based on a model for phase space diffusion is given in Ref. [18].

The SST has been found to be correlated with changes in the *transient non-equilibrium* behavior (e.g., relaxation to equipartition) [16, 17, 19], and has been found to be also correlated with *stationary non-equilibrium* phenomena like heat conduction[20]. The SST is found to be independent of the number of degrees of freedom, which makes it of prospective relevance for *equilibrium statistical mechanics*. Among the model dependent consequences of the existence of the SST, it is worth mentioning that in the FPU-β model, at $\varepsilon < \varepsilon_c^{SST}$ high-frequency excitations yield longer relaxation times with respect to low frequencies. This is in agreement with the common belief that high-frequencies have the tendency to freeze; at $\varepsilon > \varepsilon_c^{SST}$ the situation is reversed. High frequency excitations yield a quicker relaxation than low frequencies [16].

It is remarkable that the existence of the SST is not only a characteristic of the FPU-β model. In fact, it has been detected in the following one dimensional lattices: with diatomic Toda interactions (i.e., with alternating masses that break integrability) [21]; with single-well ϕ^4 interactions [17]; with smoothed Coulomb interactions [21]; with Lennard-Jones interactions [21]; in an isotropic Heisenberg spin chain [22]; in a coupled rotators chain which displays two thresholds separating two regions of weak chaos (occurring at low and high energies) from an intermediate region of strong chaos [23, 24]; in a "mean-field" XY chain [25] and in homopolymeric chains [26]. It has been also detected in two and three dimensional lattices, with two-wells φ^4 interactions [27, 28], with XY Heisenberg interactions [29, 30]. Therefore the SST seems to be a generic property of Hamiltonian systems with many degrees of freedom.

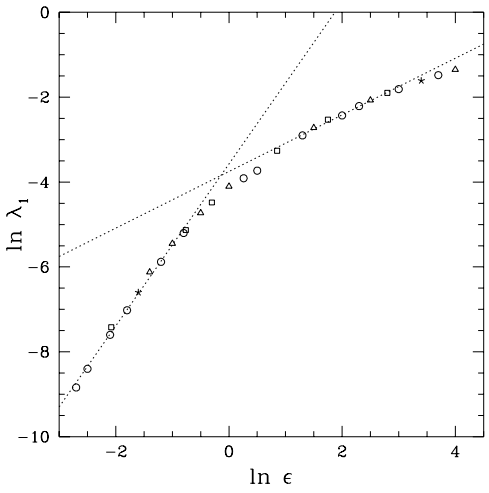

FIG. 4: FPU-β model. Largest Lyapunov exponents λ_1 vs. energy density ε at $N = 128$ and at different initial conditions: random at equipartition (circles), wave packets at different average wave numbers (squares, triangles and asterisks). From Ref. [16].

C. FPU-($\alpha + \beta$) model

In the FPU-α model, the existence of a stochasticity threshold (ST) at an energy density below which the dynamics is regular has been observed. In the FPU-β model, a strong stochasticity threshold (SST) above which the dynamics is strongly chaotic has been found. By combining these two models into the FPU-($\alpha + \beta$) model, it is possible to observe the coexistence of both the ST and the SST. This model has been studied recently in [31]. It is described by the Hamiltonian

$$H(p,q) \;=\; \sum_{k=1}^{N} \left[\frac{1}{2} p_k^2 + \frac{1}{2}(q_{k+1} - q_k)^2 + \frac{\alpha}{3}(q_{k+1} - q_k)^3 + \frac{\beta}{4}(q_{k+1} - q_k)^4 \right] \;, \tag{4}$$

where the particles have unit mass and a unit harmonic coupling constant and the end-points are fixed ($q_1 = q_{N+1} = 0$). This model Hamiltonian, with the choice of $\alpha = 0.25$ and $\beta = \frac{2}{3}\alpha^2$, is a fourth-order expansion of the Toda model (2). Consequently, its potential function is very close to interatomic potentials of the Morse or Lennard-Jones type in solids, provided that a suitably restricted energy density range is considered. Random initial conditions have been chosen. The results of the computation of the largest Lyapunov exponents at different energy densities and for different values of N are shown in Fig. 5. The patterns of $\lambda(\varepsilon, N)$, therein reported, display some remarkable features. For small values of the energy density, there is a sudden drop of λ which, in close analogy with Ref. [9], allows us to define an ST below which we can assume that the overwhelming majority of the trajectories in phase space are regular. This ST moves to smaller and smaller values of ε as N is increased.

Around $\varepsilon \simeq 0.8$, a "knee" is observed in the pattern $\lambda(\varepsilon, N)$ (Fig. 5), due to a crossover between two power law behaviors, $\sim \varepsilon^2$ at small ε and $\sim \varepsilon^{\frac{1}{4}}$ at large ε, where the latter has been attributed to the existence of an SST [16, 17]. This crossover is the signature of the transition from weak to strong chaos, as already discussed in [16, 17].

III. RIEMANNIAN GEOMETRY OF CHAOS IN THE FPU-β MODEL

In this Section we sketch how we have analytically computed, in the limit of arbitrarily large N, the largest Lyapunov exponent λ as a function of the energy density ε for the FPU-β model. The excellent agreement of the analytic outcome with the numerical results for $\lambda(\varepsilon)$ provides a preliminary understanding of the transition between weak and strong chaos (SST), and strongly supports the general validity of the proposed explanation of the origin of Hamiltonian chaos.

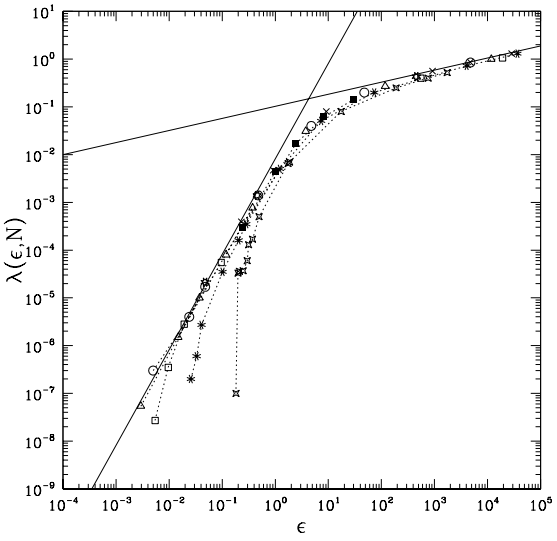

FIG. 5: FPU-$(\alpha+\beta)$ model. The largest Lyapunov exponents $\lambda(\varepsilon, N)$ are shown for different values of the energy density ε for various values of N. Starlike squares refer to $N = 8$, asterisks to $N = 16$, open squares to $N = 32$, open triangles to $N = 64$, open circles to $N = 128$, starlike polygons to $N = 512$ and crosses to $N = 1024$, respectively. Full squares refer to $N = 32$ and excitation amplitudes A ranging from 5 to 50. Solid lines are the asymptotic scalings ε^2 and $\varepsilon^{\frac{1}{4}}$ at low and high energy density, respectively. From Ref. [31].

For generic non-integrable Hamiltonian systems, when the number of degrees of freedom is large, which in practice means already a few hundred, the whole phase space is filled by chaotic trajectories, at least at physically meaningful values of the energy density. Therefore, any framework of analytic description of the dynamics has to cope with chaos. However, even the basic question about the origin of chaos itself, in many degrees of freedom Hamiltonian systems seems to lack an answer. For example, all the theoretical machinery of Classical Perturbation Theory (CPT) is of little use if we want to deal with chaos, and so does the traditional explanation of its origin based on *homoclinic intersections* [24].

Until a few years ago, the "only game in town", which seemed of potential interest to treat chaos at large N, was an attempt by Krylov [32] at explaining the origin of phase space mixing as a consequence of negative scalar curvature of suitable Riemannian manifolds whose geodesics coincide with the solutions of Newton equations of motion. Krylov's idea was to take advantage of some mathematical results about the stability properties of geodesics on negatively curved Riemannian manifolds. These results are associated with the names of Hadamard [33], Hedlund [34] and Hopf [35]. Since Krylov's, other attempts have been done along the same line of thought (see e.g. the discussion in [36]), but none of them appeared very useful.

More recently, we have reconsidered the Riemannian geometric approach and, with the aid of numerical simulations on the FPU-β model, we have discovered why the previous attempts failed: the dominant mechanism for chaotic instability in physically relevant geodesics flows is *parametric instability* due to curvature variations along the geodesics, and *not necessarily geodesic flows on negatively curved manifolds* [24, 36, 37, 38, 39, 40]. On this basis, we have started the formulation of a Riemannian theory of Hamiltonian chaos which applies to dynamical systems described by a standard Lagrangian function

$$L(q, \dot{q}) = \frac{1}{2} a_{ik} \dot{q}^i \dot{q}^k - V(q) \ , \tag{5}$$

where a_{ik} is the kinetic energy matrix ($a_{ik} = \delta_{ik}$ for the usual form of the kinetic energy) or, equivalently, by the Hamiltonian $H(p, q) = \frac{1}{2} a^{ik} p_i p_k + V(q)$, where the momenta are given by $p_i = a_{ik} \dot{q}^k$. From Maupertuis' least action principle for asynchronous isoenergetic varied paths $\gamma(t)$ with fixed endpoints

$$\delta \int_\gamma 2W(q, \dot{q}) dt = \delta \int_\gamma \{2[E - V(q)] a_{ik} \dot{q}^i \dot{q}^k\}^{1/2} dt = 0 \ , \tag{6}$$

where W is the kinetic energy, the equations of motion follow. Equation (6) is equivalent to the extremization of the length-integral $\int_\gamma ds$ where ds is $ds^2 = g_{ik}(q) dq^i dq^k = 2[E - V(q)] a_{ik} dq^i dq^k$. In other words, mechanical trajectories

are geodesics of the configuration space endowed with a proper Riemannian manifold structure described by the metric tensor

$$g_{ik}(q) = 2[E - V(q)]a_{ik} \ . \tag{7}$$

This is known as Jacobi metric and is defined in the region of the configuration space where $V(q)$. In local coordinates, the geodesic equations on a Riemannian manifold are given by

$$\frac{d^2q^i}{ds^2} + \Gamma^i_{jk}\frac{dq^j}{ds}\frac{dq^k}{ds} = 0 \ , \tag{8}$$

where s is the proper time and Γ^i_{jk} are the Christoffel coefficients of the Levi-Civita connection associated with g_{ik}. By direct computation, using $g_{ik} = (E - V(q))\delta_{ik}$, $\Gamma^i_{jk} = \frac{1}{2W}\delta^{im}(\partial_j W\delta_{km} + \partial_k W\delta_{mj} - \partial_m W\delta_{jk})$ and $ds^2 = 2W^2dt^2$, it can be easily verified that the geodesic equations yield

$$\frac{d^2q^i}{dt^2} = -\frac{\partial V}{\partial q^i} \ , \tag{9}$$

i.e. Newton's equations associated to the Lagrangian (5).

Among other Riemannian geometrizations of Newtonian dynamics, a very interesting one is defined in an enlarged configuration spacetime $M \times \mathbb{R}^2$, with local coordinates $(q^0, q^1, \ldots, q^i, \ldots, q^N, q^{N+1})$, endowed with a non-degenerate pseudo-Riemannian metric whose arc-length is [42]

$$ds^2 = g_{\mu\nu}\, dq^\mu dq^\nu = a_{ij}\, dq^i dq^j - 2V(q)(dq^0)^2 + 2\, dq^0 dq^{N+1} \ , \tag{10}$$

called *Eisenhart metric*. The natural motions are obtained as the canonical projection on the configuration space-time of those geodesics for which the arclength is positive-definite and given by $ds^2 = (\text{const})^2dt^2$. A way of measuring of how much a Riemannian manifold deviates from being a Euclidean manifold is provided by the degree of non-commutativity of the covariant derivatives which is properly defined by the Riemann-Christoffel curvature tensor $R(X,Y) = \nabla_X\nabla_Y - \nabla_Y\nabla_X$, where ∇ is the Levi-Civita connection, and X, Y are tangent vectors [41]. There are two relevant curvature scalars: the *Ricci curvature* K_R in a given direction v, and the *scalar curvature* $\mathcal{R}$ (see [36]).

There is an important relation between the curvature of a manifold and the stability of its geodesics. In fact, the evolution of a vector field J, called geodesic separation vector, is completely determined by the curvature tensor according to the equation

$$\nabla^2_{\dot\gamma}J(s) \ + \ R[J(s), \dot\gamma(s)]\dot\gamma(s) \ = \ 0. \tag{11}$$

This is the *Jacobi – Levi-Civita equation*, where $\nabla_{\dot\gamma}$ is the covariant derivative in the direction of the velocity vector $\dot\gamma = v$. J contains the whole information on the stability – or instability – of any given reference geodesic $\gamma(s)$ because it locally measures the distance from $\gamma(s)$ of any given geodesic close to $\gamma(s)$.

Since the Jacobi equation (11) relates the stability of the geodesics of a manifold to its curvature, the Jacobi equation links stability and instability (chaos) of the dynamics with the curvature of the "mechanical" manifold [43], if the metric is associated with a physical system.

In the particular case of *isotropic* – or *constant curvature* – manifolds, Eq. (11) becomes very simple: choosing a geodesic frame, i.e., a reference frame transported parallel along a reference geodesic, the Jacobi equation is written as

$$\frac{d^2J}{ds^2} + K\, J = 0 \ , \tag{12}$$

where $K = K_R/(N-1) \equiv \mathcal{R}/N(N-1)$, which has either bounded oscillating solutions $\|J\| \propto \cos(\sqrt{K}\, s)$ or exponentially unstable solutions $\|J\| \propto \exp(\sqrt{-K}\, s)$ according to the sign of the curvature and thus of the constant K.

As long as the curvatures are negative, the geodesic flow is unstable even if the manifold is no longer isotropic, and the instability exponent is greater than or equal to $(-\max_M(K))^{1/2}$. Geodesic flows on compact manifolds with everywhere negative curvature were studied for the first time in the classic works by Hadamard, Hedlund and Hopf [33, 34, 35] and many results were then established by Anosov [44], among them the fact that such systems are ergodic and mixing.

Equation (12) is valid only when K is constant. Nevertheless in the case in which $\dim M = 2$ (surfaces), the Jacobi equation – again written in a geodesic reference frame for the sake of simplicity – takes a form very close to that of isotropic manifolds,

$$\frac{d^2J}{ds^2} + \frac{1}{2}\mathcal{R}(s)\, J = 0 \ , \tag{13}$$

where $\mathcal{R}(s)$ denotes the scalar curvature of the manifold along the geodesic $\gamma(s)$. The solutions of Eq. (13) may exhibit an exponentially growing envelope even if the curvature $\mathcal{R}(s)$ is everywhere positive but non constant. For example, in the case of the celebrated Hénon-Heiles model [6], the scalar curvature $\mathcal{R}$, computed with the Jacobi metric, is always positive despite the existence of fully developed chaos above some threshold energy [39]. As a matter of fact, the generic condition of physically relevant systems (like coupled anharmonic oscillators on d-dimensional lattices) is that Ricci and scalar curvatures of the mechanical manifolds are neither constant nor everywhere negative, and the straightforward approach based on Eq. (12) does not apply.

The key point is to realize that negative curvatures are not necessary to generate chaos, while the generic non constancy of the curvature of mechanical manifolds (in the absence of very "exotic" hidden symmetries [45]), triggers *parametric instability* of the geodesics. Thus the exponential growth of the solutions of the stability equation (13), that is chaos, even if no negative curvature is "felt" by the geodesics.

A. A geometric formula for the Lyapunov exponent

In the large N case, with some simplifying assumptions, mainly that the mechanical manifolds are *quasi-isotropic* [24, 36], it is possible to derive an effective scalar stability equation resembling Eq. (13), where the role of $\mathcal{R}(s)$ is played by a random process, so that an analytic estimate of the largest Lyapunov exponent can be worked out. This effective equation is *independent of the knowledge of the dynamics* and has the form

$$\frac{d^2\psi}{ds^2} + \Omega(s)\,\psi = 0 \tag{14}$$

where ψ denotes any of the components of J because now all of them obey the same effective equation of motion, and the squared frequency $\Omega(s)$ is a gaussian random process

$$\Omega(s) = \langle k_R \rangle_\mu \ + \langle \delta^2 k_R \rangle_\mu^{1/2}\, \eta(s)\ , \tag{15}$$

where $k_R = K_R/(N-1)$ and $\langle \delta^2 k_R \rangle_\mu$ is a shorthand for $\frac{1}{N-1}\langle \delta^2 K_R \rangle_\mu$; the averages $\langle\cdot\rangle_\mu$ are microcanonical averages; $\eta(s)$ is a gaussian random process with zero mean and unit variance. Our estimate for the (largest) Lyapunov exponent λ is then given by the growth-rate of $\|(\psi,\dot\psi)(t)\|^2$ according to the definition

$$\lambda = \lim_{t\to\infty} \frac{1}{2t} \log \frac{\psi^2(t) + \dot\psi^2(t)}{\psi^2(0) + \dot\psi^2(0)}\ . \tag{16}$$

The ratio $(\psi^2(t) + \dot\psi^2(t))/(\psi^2(0) + \dot\psi^2(0))$ is computed by means of a technique developed by Van Kampen, summarized in Ref. [24], where the following expression for λ has been derived

$$\begin{aligned} \lambda(\Omega_0, \sigma_\Omega, \tau) \ &= \ \frac{1}{2}\left(\Lambda - \frac{4\Omega_0}{3\Lambda}\right), \\ \Lambda \ &= \ \left(2\sigma_\Omega^2\tau + \sqrt{\left(\frac{4\Omega_0}{3}\right)^3 + (2\sigma_\Omega^2\tau)^2}\right)^{1/3}, \end{aligned} \tag{17}$$

where $\Omega_0 = \langle k_R\rangle_\mu$, $\sigma_\Omega = \langle \delta^2 k_R\rangle_\mu = \frac{1}{N}[\langle K_R^2\rangle_\mu - \langle K_R\rangle_\mu^2]$ and τ is a time scale expressed in terms of Ω_0 and σ_Ω. The quantities Ω_0, σ_Ω and τ can be computed as static, i.e. *microcanonical* averages. Therefore Eq. (17) gives an analytic, though approximate, formula for the largest Lyapunov exponent *independently* of the numerical integration of the dynamics and of the tangent dynamics.

A completely analytical computation of $\lambda(\varepsilon)$ has been performed – in the thermodynamic limit – for the FPU-β model (such a result first appeared in [46], then it was refined in [24, 36]) and for other models. We report in Fig. 6 the result for the FPU case: the agreement is strikingly good. The analytic values of λ agree with the numerical ones with errors of a few percent in a range of six orders of magnitude both in $\varepsilon = E/N$ and λ, and no use of adjustable parameters has been made. A preliminary explanation of the existence of the SST proceeds as follows. At low ε, the amplitude of the curvature fluctuations σ_Ω is much smaller than the average curvature Ω_0, thus the mechanical manifolds are not very different from constant curvature manifolds, so that the geodesic flow has many of the features that it would have if it lived on a strictly constant curvature (equal to the average curvature) manifold, and, loosely speaking, a slow phase space filling through tortuous paths will take place: chaos is weak. Conversely, when $\sigma_\Omega \sim \Omega_0$,

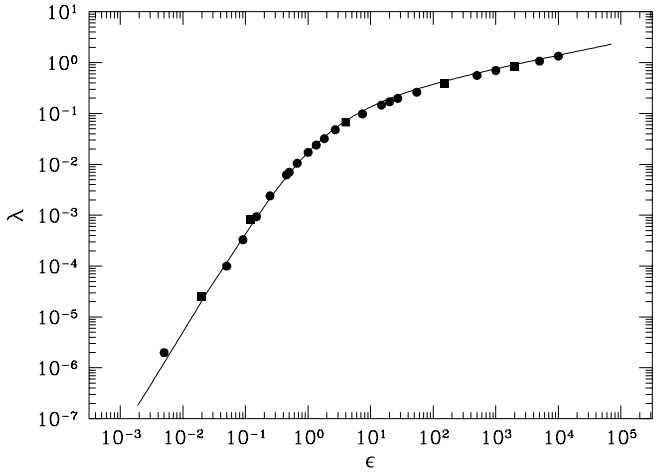

FIG. 6: FPU-β model. Lyapunov exponent λ *vs.* energy density ε with $\beta = 0.1$. The continuous line is the theoretical computation according to Eq. (17), while the circles and squares are the results of numerical simulations with N respectively equal to 256 and 2000. From Ref. [24].

we can imagine that no similarity at all will exist between the chaotic geodesic flow and its integrable counterpart living on a constant curvature (equal to the average curvature) manifold. As a consequence the geodesic flow can quickly diffuse in any direction in phase space: chaos is strong.

Other systems for which good results have been obtained are: a one-dimensional chain of coupled rotators [24], two and three dimensional classical XY Heisenberg models [30], two and three dimensional classical lattice φ^4 models [27, 28], "mean-field" XY model [25], though some adjustments are necessary in these cases.

An important remark is in order. The geometrical theory of chaos aims at explaining what is the origin of chaos in Hamiltonian systems, and not at providing a recipe for the computation of Lyapunov exponents. The impressive success of the theory in analytically computing Lyapunov exponents for the FPU model, means that we have actually found the right conceptual framework and the right explanation for the existence of Hamiltonian chaos and warrants that any effort to further develop the theory is worthwhile.

One has to keep in mind that the above given analytic formula for the largest Lyapunov exponent has a limited validity domain: that of the fundamental assumption of quasi-isotropy of the mechanical manifolds. The next step will be that of relaxing the assumption of quasi-isotropy by letting in nontrivial topology of configuration space.

IV. HAMILTONIAN DYNAMICS, PHASE TRANSITIONS AND TOPOLOGY

Though the content of this Section could appear to be somewhat far from the initial FPU problem, we have nonetheless sketched it in order to remark how fertile, inspiring and far reaching a systematic investigation of the (once) surprising behavior of the FPU dynamics has been.

The macroscopic properties of large-N Hamiltonian systems can be understood by means of the traditional methods of statistical mechanics. The origin of the possibility of describing Hamiltonian systems via equilibrium statistical mechanics are the chaotic properties underlying the dynamics.

Above, we have observed that the crossover in the ε-dependence of λ phenomenologically corresponds to a transition between weak and strong chaos (SST), or slow and fast mixing respectively. Thus we have surmised that this transition has to be the consequence of some "structural" change occurring in configuration space, and thus also in phase space. This dynamical (mild) transition has been observed, we said above, in many other systems besides FPU. Then, some natural questions arise: could some kind of dynamical transition between weak and strong chaos (possibly sharper than the SST found in FPU models) be the microscopic counterpart of a thermodynamic phase transition? and if this was the case, what kind of difference in the $\lambda(\varepsilon)$ pattern would discriminate between the presence or absence of a phase transition? and could we make a more precise statement about the kind of "structural" change to occur in configuration space when the SST corresponds to a phase transition and when it does not?

During the last years, after an earlier attempt in Ref. [29] where the classical XY model in two dimensions was considered, and its largest Lyapunov exponent was found to display some indication of the transition temperature of the Kosterlitz-Thouless phase transition, there has been a renewed interest in the study of the behaviour of Lyapunov exponents in systems undergoing phase transitions, and a number of papers have appeared: see [27, 28, 30] and [25, 47, 48, 49, 50, 51, 52, 53, 54, 55].

Two systems have received considerable attention in this framework: the so-called lattice φ^4 model, and the mean-field XY model. The lattice φ^4 model is described by the Hamiltonian

$$H = \sum_i \frac{1}{2} p_i^2 + \frac{J}{2} \sum_{\langle i,j \rangle} (\varphi_i - \varphi_j)^2 + \sum_i \left[-\frac{m^2}{2} \varphi_i^2 + \frac{u}{4!} \varphi_i^4 \right], \tag{18}$$

where the p_i are momenta conjugated to the φ_i, real valued scalar variables defined on the sites of a d-dimensional lattice; m^2 and u are positive parameters, and the brackets $\langle i, j \rangle$ stand for nearest-neighbors. This model has a phase transition at a finite temperature provided that $d > 1$.

The mean-field XY model [56] describes a system of N equally coupled planar classical rotators. It is defined by the Hamiltonian

$$H = \sum_i \frac{1}{2} p_i^2 + \frac{J}{2N} \sum_{i,j=1}^{N} [1 - \cos(\varphi_i - \varphi_j)] - h \sum_{i=1}^{N} \cos \varphi_i \ . \tag{19}$$

Here $\varphi_i \in [0, 2\pi]$ is the rotation angle of the i-th rotator. Defining at each site i a classical spin vector $\mathbf{s}_i = (\cos \varphi_i, \sin \varphi_i)$ the model describes a planar (XY) Heisenberg system with interactions of equal strength among all the spins. The equilibrium statistical mechanics of this system is exactly described, in the thermodynamic limit, by mean-field theory [56]. In the limit $h \to 0$, this system has a continuous phase transition.

Through standard methods of molecular dynamics, thermodynamical observables have been computed and found to be in agreement with statistical mechanical predictions. The energy density ($\varepsilon = E/N$) dependence of the largest Lyapunov exponent numerically found in the φ^4 model – reported in Fig. 7 – shows a pattern similar to that found in the FPU model but now the mild transition between weak and strong chaos is replaced by an abrupt transition, a sharp SST: a "cuspy" point in $\lambda(\varepsilon)$ shows up which corresponds to the critical energy locating the phase transition. Also the Lyapunov exponent of the mean field XY model, obtained through an analytic estimate worked out in the limit $N \to \infty$ [25] by means of the above discussed geometrical theory of chaos, sharply signals the phase transition (see Fig. 8).

In both cases, it is evident that the ε-pattern of the largest Lyapunov exponent clearly signals the presence of a phase transition; the same happens for all the other models studied in the above mentioned references.

Then, coming to the other questions, as Lyapunov exponents are tightly related with the geometry of the mechanical manifolds in configuration space (as well as in phase space), we have been led to conjecture that in presence of a phase transition we have to go to the deeper level of *topology* of these manifolds to find an adequate explanation [57]. If this is actually the case, we are confronted with a possible – at least conceptual – deepening of our understanding of the origin of phase transitions. In fact, the topological properties of configuration space submanifolds, mainly equipotential hypersurfaces $\Sigma_v = V^{-1}(v) = \{q \in \mathbb{R}^N | V(q) = v\}$ or the regions bounded by them $M_v = \{q \in \mathbb{R}^N | V(q) \leq v\}$, are already determined when the microscopic potential V is assigned and are completely independent of the statistical measures. The appearance of singularities in the thermodynamic observables could then be the *effect* of a suitable topological transition in configuration space. Several results strongly support this *Topological Hypothesis* and suggest that a phase transition might well be the consequence of an abrupt transition between different rates of change in the topology above and below the critical point. More details can be found in the review paper [36] and in the subsequent papers: [58] where the topology of the M_v is analytically studied for the mean-field XY model; [59, 60] where the topology of the M_v is analytically studied for a trigonometric model undergoing also a first-order phase transition; [60, 61] where an analytic relationship between topology and thermodynamic entropy is given among other results; [62, 63] where a preliminary account of a general theorem on topology and phase transitions is given.

V. CONCLUDING REMARKS

By chance, Fermi, Pasta and Ulam chose the initial condition, in their numerical experiment on the α-model, below the threshold energy of a transition between regular and chaotic motions. With a stronger initial excitation, no "FPU problem" would have arisen because equipartition of energy could have been observed even with the rather short integration time that the authors could afford 50 years ago. Apparently the observed phenomenology cannot be explained by the existing formulations of the KAM theory, both because of the large degree of anharmonicity

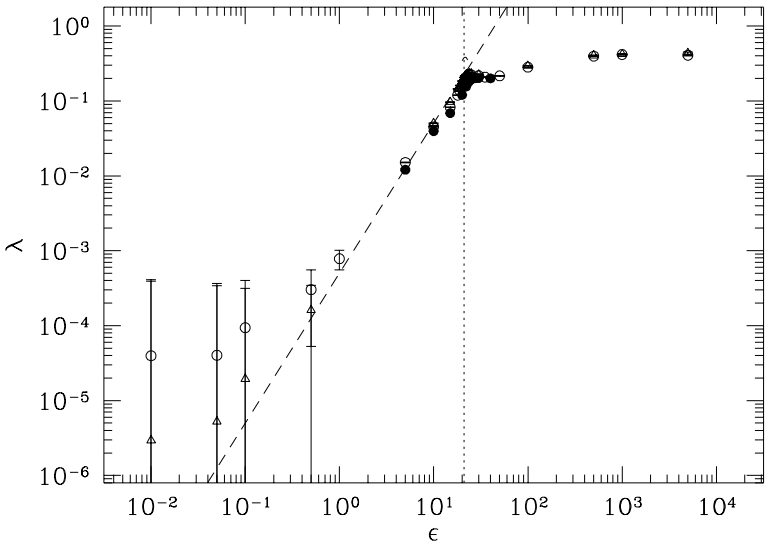

FIG. 7: Lyapunov exponent λ *vs.* the energy per particle ε, numerically computed for the two-dimensional $O(1)$ φ^4 model, with $N = 100$ (solid circles), $N = 400$ (open circles), $N = 900$ (solid triangles), and $N = 2500$ (open triangles). The critical energy is marked by a vertical dotted line; the dashed line is the power law ε^2. From Ref. [27].

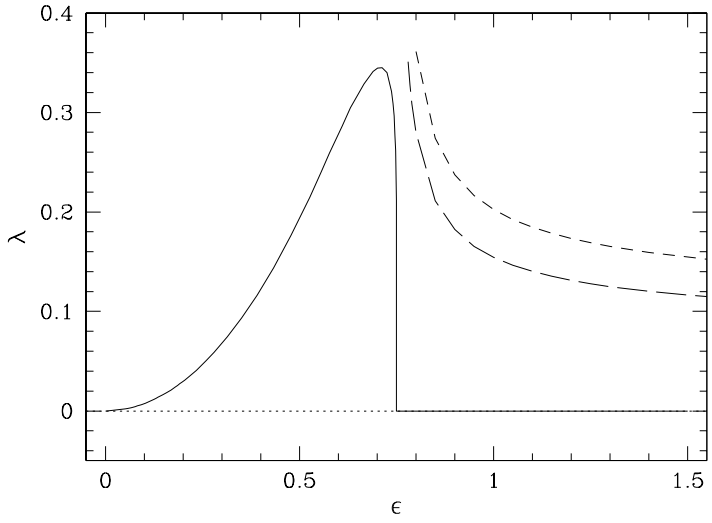

FIG. 8: Mean field XY model: analytic expression for the Lyapunov exponent (solid curve). The curves above the transition are finite-N results for $N = 80$ (upper dashed line) and $N = 200$ (lower dashed line): here $\lambda \propto N^{-1/3}$. From Ref. [25].

(nonintegrability) at which the ST occurs, and because of its slow vanishing at increasing N. Since this threshold energy goes to zero as the number of degrees of freedom is increased, the FPU problem is not a true problem for equilibrium statistical mechanics. Nevertheless, the existence of possibly long-living transient nonequilibrium phenomena draws attention to the relevance of dynamics, initial conditions and observational time scales in order to assess whether dynamics can be replaced by statistics or not. Because of the cubic potential, the α-model is unstable above an upper bound in energy density, so FPU considered also the so-called β-model which is well defined at any energy. However, in the β-model it is hard to detect the ST because it seems to occur at a very low energy density, where the convergence of the largest Lypaunov exponent requires huge computational times. On the other hand, the β-model displays another and much more interesting chaotic transition, that we called SST, which is a transition

between weak and strong chaos. Strong chaos is related with fast phase mixing and fast thermalization of an out of equilibrium initial condition. Weak chaos is associated with a sudden increase of relaxation times of nonequilibrium initial conditions when the energy density is smaller than a threshold value (which corresponds to the SST). At sufficiently low energy density the thermalization can be so slow that the system can give the wrong impression to recur *ad infinitum*, if the observational time is not long enough. The study of the $\alpha + \beta$–model, which provides a good approximation of interatomic interaction potentials of the Morse or Lennard-Jones type, displays both the ST and the SST. However, only the SST is stable with N and can thus be relevant for equilibrium and nonequilibrium statistical properties of a large class of classical many-body systems. In fact, this kind of transition seems a common property of many degrees of freedom Hamiltonian systems.

The systematic investigation of the chaotic properties of FPU models – being a heavy numerical task – has become possible only rather recently, with the advent of modern powerful computers. The results so obtained demanded a satisfactory and constructive explanation of the origin of Hamiltonian chaos as well as for the reason of the transition between weak and strong chaos. Motivated by the need of understanding chaos in FPU models, we have started a new and successful theory of Hamiltonian chaos which resorts to basic concepts and methods of Riemannian geometry. Later on, all these findings have suggested to look at phase transition phenomena from a new point of view which, eventually, has inspired the development of a new theoretical approach to them, based on topological concepts.

Acknowledgments: We thank D. K. Campbell, P. Rosenau and G. Zaslavsky for their kind invitation to contribute to this special issue commemorating the 50th anniversary of the fundamental work by E. Fermi, J. Pasta and S. Ulam.

E.G.D.C. gratefully acknowledges support from the Office of Basic Energy Sciences of the US Department of Energy under Grant DE-FG02-88-ER13847.

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