

## Enrico Fermi's *excursions* through the fields of classical physics: Watching the landscapes of phase space and the nature of dynamical paths, looking for ergodicity<sup>(\*)</sup>

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**Summary.** — The (relatively few) works of Fermi within the fields of classical physics had, and still have, a deep impact on our understanding of the structure of phase space of generic nonlinear systems, along with the relative implications on the justification of a statistical description of macroscopic systems and the approach towards equilibrium. One of those milestones along the path to reconcile microscopic dynamics with macroscopic description is the first *inverse experiment*, performed by Fermi, Pasta, Ulam and Tsingou on an one-dimensional anharmonic chain (FPU model). After a brief historical introduction whose aim is mainly to show how that revolutionary experiment frames perfectly into Fermi's personality, I discuss how this model, and particularly the *philosophy* beyond it, can be considered, still today, a valid *conceptual paradigm*. I show how to obtain analytical estimates of dynamic and geometric quantities through which it is possible to generalize the existing definitions of chaoticity indicators and of the *threshold* marking the onset of strong chaos. Nevertheless, as far as some of the most recent successful approaches to FPU problem are concerned, I outline how these cannot be generalized painlessly. Discussing in some details why they work for FPU-like models, we meet with the difficulties and troubles emerging when trying to applying them to *peculiar* Hamiltonian systems, for which these methodologies can give, at most, just some hints on their macroscopic behaviour. In particular, I review some conceptual and technical aspects of the combined use of the *geometrical transcription of dynamics* and the theory of *stochastic differential equations*, pointing out the issues preventing a direct extension to more general systems.

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Notwithstanding, this analysis gives noteworthy hints even on the much more controversial issue of a statistical description of gravitationally interacting  $N$ -body systems, furthermore allowing to understand some seemingly inconsistent results existing in the literature.

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## 1. – Introduction

Enrico Fermi, allegedly, spent most of his research activities on atomic and nuclear physics [1,2]; nevertheless his *digressions* from that main path revealed outmostly fruitful and stimulating, both because of the originality of issues addressed and the novelty of the approaches proposed. To this it must be added the usual depth and *clarity of physical reasoning* (using Feynman's words [3]) of almost all Fermi investigations.

Among his most relevant studies within the fields of classical (*i.e.* non-quantum) physics, it should be certainly mentioned the extension of the *Poincaré theorem* [4] on the non existence of analytic first integrals for (generically) perturbed Hamiltonian systems, who reinforced the belief that, from a practical point of view, a generic nonlinear system had to be ergodic, and consequently it could be successfully described by Statistical Mechanics (SM) methods. That theorem was probably one of the inspirations for the first *inverse experiment* performed with Pasta, Ulam and Tsingou devised to verify the approach towards equilibrium of *nonlinear* many degrees of freedom (mdof) systems [5].

There are, of course, many other Fermi's seminal contributions to classical dynamics, many of them with direct astrophysical implications: we just recall how his interest on the origin of high energy *cosmic rays*, led to the formulation of a very simple and elegant model for particle acceleration [6,7], which became, again, a paradigmatic example for the interpretation of a wide class of phenomena, in the fields of fluid dynamics and chaotic systems (see, *e.g.*, ref. [8]). He, young, gave also important contributions to the interpretation of some aspects of general relativity (when even that theory was almost in its infancy), strictly linked to one of its most physically pregnant concepts, *i.e.* the *Equivalence Principle* [9,10]. His *statistical* model of (heavy) nuclei [11,12], found later interesting extensions to the description of gravitationally collapsed objects [13].

Furthermore, the attraction felt by Fermi towards SM and thermodynamics is witnessed not only by his celebrated fundamental studies [14] on the distribution law of half-integer spin particles<sup>(1)</sup> (owing him their name), but also by his involvement in writing down the *Statistical Mechanics* item for the *Enciclopedia Italiana* [16] and several monographies and textbooks on the same subject, on thermodynamics and even on

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<sup>(1)</sup> And it is worth mentioning that, contrary to what usually reported, Fermi was led to this very important result by his aim at obtaining a satisfactory derivation of the Sackur-Tetrode formula for the entropy of an ideal monoatomic gas, rather than by its (presumed) interests in the conduction in metals [15]. This confirms the persistent attention maintained by Fermi towards the basic concepts of thermodynamics.

fluid dynamics [17].

Nowadays, however, the work of Fermi, referred to as the most thought-provoking for modern studies on the links between classical dynamics and SM foundations, is certainly the *pioneering inverse experiment*<sup>(2)</sup> mentioned above [5], whose goal was to find a dynamical (microscopic) justification of the occurrence and effectiveness of thermodynamic (macroscopic) relaxation processes in generic non-integrable dynamical systems<sup>(3)</sup>.

Very good discussions about the implications of the FPU experiment on SM foundations can be found in this volume (see, *e.g.*, ref. [18]), also in connection with the issue of relaxation in stellar systems [19].

Therefore, in the following, rather than again commenting on the outcomes of that *experiment* and of its *technologically improved* successive repetitions, I will put more emphasis on the interpretations and generalization of those approaches which can be relevant for the long-standing issue of a *rigorous* justification of the statistical approach for mechanical systems [20].

More specifically, I deal with the *signatures* accompanying the onset of chaos in mdof Hamiltonian systems, using *alternative* tools to characterize and quantify the degree of instability. Within the phenomenology of the FPU model, it is possible to introduce a (rather elementary) generalization of Lyapunov exponent (or LCN), which, despite its simplicity, allows to overcome the ambiguities raising in some settings, mainly of astrophysical or cosmological interest. On its grounds, the implications of the onset of chaos in general mdof Hamiltonian systems are discussed, with some emphasis on the gravitationally bound  $N$ -body problem, where important *caveats* have to be kept in mind. On this light, I review critically the approaches which revealed very fruitful for the study of FPU-like models, and discuss the points which deserve a critical reconsideration, when trying to extend the above frames to more *critical* Hamiltonians. I derive some analytical (or semi-analytical) expressions for relevant quantities related to *dynamical*, *geometrical* and *statistical* scales of time and energy for the FPU model, and outline why similarly reliable estimates cannot be obtained so easily for the much more complex gravitational  $N$ -body system, discussing analogies and differences.

In a sense, the key ingredient of the analyses that follow has its foundation in the belief that the relevant, macroscopic (*i.e.* thermodynamic) properties of mdof systems can be obtained, in the generic case, by relatively simple and general physical considerations, supported by rather elementary mathematical computations. Obviously, *peculiar* systems and/or further investigations on detailed aspects can instead require articulated physical argumentations, and perhaps also (more) sophisticated mathematical treatment.

The approach just outlined is an (arduous and humble) attempt to follow what was

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<sup>(2)</sup> I prefer to term the *numerical integrations* of the equations of motion of model systems as *inverse experiments*. Without going into detailed (and here inopportune) discussions, a loose rationale is that there, instead of starting from observations, from where trying to formulate a tentative general law, open to successive refinements and improvements through *laboratory experiments*, one starts from a *certain* hypothetical law to obtain *experimental* data, to be compared (hopefully!) with observations of the real physical system whose modellization is sought.

<sup>(3)</sup> The depth of Fermi insights into the issue of relaxation and the foundations of the statistical description of mdof systems earned him a very deep esteem even by one of the *founding fathers* of SM, *i.e.* Ehrenfest, who manifested repeatedly his interest in a collaboration with Fermi, which however has never been finalized [15].

Fermi's initial attack to complicated problems. As universally recognized<sup>(4)</sup>, Fermi researches, and teaching as well, were characterized by the already mentioned *clarity of physical reasoning* [3], which is undoubtedly connected with his ability to keep explanations simple, emphasizing conceptual understanding rather than calculations [22]. He was firmly convinced that, exposing physics in simple terms, forces the clarification of his own comprehension, and taught, even in his informal lectures, that knowledge of physics is achieved gradually, insisting that a deep understanding profits mostly by *intuitive and geometric, rather than analytic* arguments (see ref. [1], p. 673). Fermi repeated often that a first attack to solve a new and difficult problem must proceed through simplifications and analogies with known situations, and that every logical step had to be made with due reflection, even at the cost to proceed slowly.

There are a lot of appealing aspects in Fermi's trait: the preference he showed towards problems whose solutions can be guessed by simple calculations, based mainly on order of magnitude estimates [23]; his deep and active involvement in the experimental setup and his genial intuitions about the possibility to project and realize completely new kind of *experiments*, using tools which were appointed before for different tasks (see [24], p. 19). Also it must be mentioned his enthusiasm which led him to actively participate even in the *practical implementation* of his projects; *e.g.*, he was so much involved in the task of testing the validity of the ergodic hypothesis that, in a few weeks, he was able to effectively contribute in *programming electronic machines*.

The above repeatedly mentioned preference for heuristic and qualitative approaches should not be interpreted absolutely as a lack of rigor; as Ulam wrote (see ref. [24] p. 15), *Strangely enough, [Fermi] started as a mathematician. [...] When he wanted to, he could do any kind of mathematics.*"

To further exemplify the innate Fermi attitude towards a *deep, conceptual*, and, at the same time, *physical and intuitively understandable* comprehension of *real* phenomena, it suffices to remember his opinion (after his period in Göttingen, around 1925) against the *operational and formal* foundations of the rising Quantum Mechanics, especially in the form of a *Mechanics of Matrices*: "*according to my taste, I feel that they are going too far along the tendency to renounce to understand the things*" (cited in ref. [25]). Coherently with this dislike for methods and approaches *that work, though it is not well understood why*; Fermi's projects for his, unfortunately never arrived, "*old age*" included the writing of a Physics book addressing all those difficult points usually concealed behind phrases like "*it is well known that...*" [21].

Fermi's *genius* was always moderated by a serious, systematic preparation, that led Feynman to feel himself affected by *confusion*, facing with "*the clarity of the exposition and the perfection [...] to make everything look so obvious and beatifully simple*", whenever Fermi gave a lecture "*about any subject whatever he had thought before*" [3].

When necessary, after the first heuristic and qualitative attack, Fermi was always able to go beyond this initial framing of the problem, completing all the detailed physical arguments and mathematical steps to arrive at a comprehension of the phenomena at hand as complete as possible. Thus, presenting, six months before the submission of Dirac article on the same subject, his quantum theory of the ideal gas, "*Fermi worked out its consequences in more detail [and], [...], showed that at low temperatures the equation of*

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<sup>(4)</sup> See the tribute to Fermi [21], from where I have extracted some of the memoirs that follow.

state of the Fermi-Dirac gas has the form (from ref. [26], pp. 160-1)

$$(1) \quad p = \frac{ah^2n^{5/3}}{m} + \frac{bmn^{1/3}k_B^2T^2}{h^2} + \dots$$

All the above is an attempt to outline Fermi's way to physics, starting from heuristics and simple approaches, arriving at an almost complete solution, through all the necessary steps.

In what follows the reader will not find, instead, a definite answer to (perhaps none of) the issues addressed. Nevertheless, I will present a general, though quantitative enough, critical reconsideration of some allegedly established beliefs and, for the issues left open, are indicated the directions along which the *right* answers could be possibly obtained.

## 2. – The Fermi-Pasta-Ulam experiment

The results of the FPU experiment are usually alleged to disprove the validity of the ergodic hypothesis and, consequently, of the Poincaré-Fermi theorem [25], as numerical integrations of the equations of motion showed an *almost periodic* behaviour of the instantaneous energy distribution among the modes of different wave numbers, “*To our surprise, the string started playing a game of musical chairs, only between several low notes, [...], afterwhat would have been several hundred ordinary up and down vibrations, it came back almost exactly to its original shape*” (from [24], p. 19).

Subsequent numerical works showed instead that this almost astonishing result (“*a little discovery*”, Fermi said<sup>(5)</sup>) was mainly due to the small energy given to the system and to the too short integration time.

By now it is largely agreed that there are some *thresholds* separating different regimes in the dynamics of FPU chains. From a thermodynamical viewpoint, the lower threshold, related to the KAM behaviour, is of negligible relevance, as it tends to zero (quickly, *i.e.* almost exponentially) as the number of degrees of freedom increases. It is more interesting to investigate the applicability of the *Nekhoroshev theory*, which deals with the finite time conservation of the *actions*. This latter theory, of undeniable utmost relevance from the point of view of analytical mechanics, has been invoked [27] to explain the existence of a threshold in the scaling of the relaxation times for FPU (and similar) chains. However some inconsistencies survive, related mostly to the  $N$ -dependence of the predicted threshold. It is thus generally recognized, at least in the Physics community (though, admittedly, no rigorous proof exists), that a further threshold exists, whose location depends, for a given Hamiltonian, only on the energy density and which does not vanish in the Thermodynamic Limit (TL). This so-called *strong stochasticity threshold* (SST) is clearly linked to the stochastic properties of the dynamics and the *failure*, with respect to Fermi's expectations, of the *experiment* performed on the MANIAC computer can be attributed to the energy densities used, all below the *critical energy density*,  $\varepsilon_c \doteq (E/N)_c$ , characterizing the SST. Indeed it has been found [27-31], that FPU chains show a quasi regular behaviour, associated to very long relaxation times, for  $\varepsilon < \varepsilon_c$ , and a strongly chaotic dynamics, in turn leading to fast equilibration, above the threshold.

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<sup>(5)</sup> How important Fermi actually considered those results was witnessed by his intention to focus his planned *Gibbs Lecture* on them. Unfortunately, the cancer prevented him to achieve that aim.

Furthermore, it has been found that  $\varepsilon_c$  is an *intensive* quantity, *i.e.* does not depend on  $N$ . One can correctly speak about a *threshold* because of the *qualitatively different* behaviours below and above  $\varepsilon_c$ . In fact, the dynamic properties undergo a rather abrupt modification, witnessed, *e.g.*, by a change in the slope of the maximal Lyapunov exponent as a function of the energy density (see below for details), and the statistical behaviour is drastically influenced as well, as pointed out by the very different scaling of the relaxation times, changing from a strong (for  $\varepsilon < \varepsilon_c$ ) to a very weak (if any) dependence on  $\varepsilon$ , above the threshold.

### 3. – Strong stochasticity threshold and geometric properties of configuration manifold

The existence of a SST has been proposed initially on the basis of numerical simulations, and has found later some theoretical justifications. In the last decade, moreover, the geometrical transcription of dynamics<sup>(6)</sup>, revived [34] in the 80ths, helped to show that the above threshold has a clean geometrical counterpart, which allows to obtain a very convincing scenario for the onset of strong chaoticity in the FPU chains and similar  $m$  dof Hamiltonian systems [31, 35, 32, 36].

As shown in fig. 1, already the first numerical integrations of the FPU model devoted to investigate the nature of the SST gave some support to its possible relationship with Nekhoroshev theory; though the predicted  $N$ -dependence of the critical value of the energy density was not confirmed. Subsequent works (see, *e.g.*, refs. [37-40]) seem to support the interpretation that SST and Nekhoroshev theory describe two different kinds of transition, and this is confirmed also by the geometrical approach [31, 41, 32], which predicts, for the SST, a value which does not depend on  $N$ , in particular it remains finite (*i.e.* does not vanish) in the TL.

Without going into details (see, *e.g.*, the recent review [36]), we just recall the basic steps of the *Geometro-dynamical* approach (GDA), needed to illustrate the results obtained for FPU-like systems and the assumptions which have to be checked before to extend those results to more general dynamical systems (as self-gravitating  $N$ -body ones).

Within the GDA, the dynamical evolution of a Hamiltonian system with  $N$  degrees of freedom is rephrased in terms of a geodesic flow over a suitable manifold<sup>(7)</sup>, whose stability properties are determined by the Jacobi-Levi-Civita equation for geodesic spread:

$$(2) \quad \frac{\nabla}{ds} \left( \frac{\nabla z^a}{ds} \right) + \mathcal{H}_c^a z^c = 0 \quad (a = 1, \dots, N),$$

where  $\nabla/ds$  stands for the covariant derivative *along* the flow,  $\{z^a\}$  is an arbitrary perturbation to the reference geodesic, and the mixed tensor,  $\mathcal{H}$ , describe the curvature properties of the dynamical manifold. Under some rather *mild* assumptions [32], the behaviour of a generic perturbation to a *given* geodesic (and then the stability of the

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<sup>(6)</sup> Developed, among others, by Levi-Civita, Synge, Eisenhart and others (see ref. [32] for references to these historical works) before 1930, and whose relevance for the issue of relaxation in many-body systems was first realized by Krylov [33].

<sup>(7)</sup> Which can be either Riemannian [34, 41, 31, 32], pseudo-Riemannian [35, 42, 36] or Finslerian [42, 43].

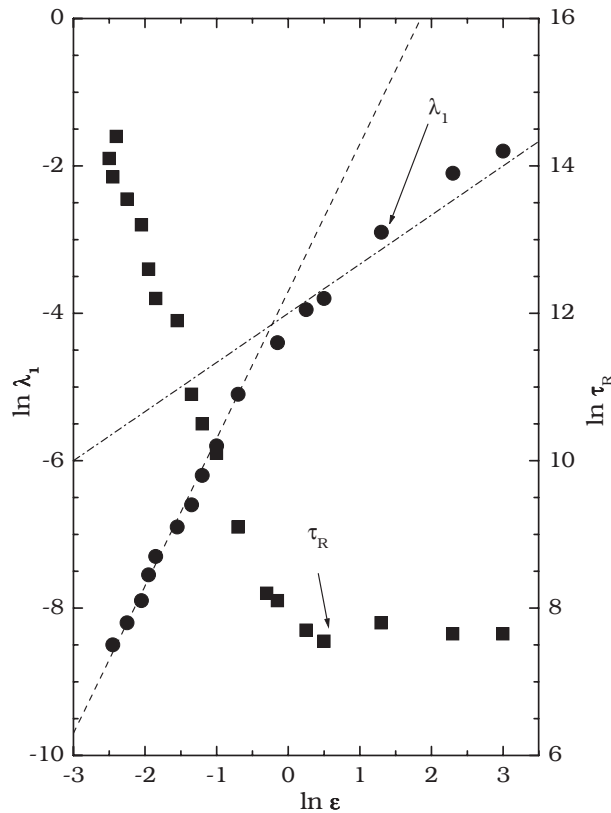


Fig. 1. – Scaling of maximal Lyapunov exponent  $\lambda_1$  (circles, scale on the left) and of relaxation time  $\tau_R$  (squares, scale on the right) with energy density. The figure has been generated from data taken from ref. [27].

flow) can be *reasonably*<sup>(8)</sup> described using a single scalar *effective* equation, instead of the  $N$  equations (2), which reads

$$(3) \quad \frac{d^2 z}{ds^2} + k_R[s]z \cong 0 ,$$

where  $z \doteq (g_{ab}z^a z^b)^{1/2}$  is the norm of the perturbation ( $g_{ab}$  being the metric over the manifold) and  $k_R[s] \doteq Ric[\mathbf{q}(s), \mathbf{u}(s)]/(N-1) \equiv \mathcal{H}_a^a/(N-1)$  is the Ricci curvature per degree of freedom in the  $(N-1)$  two-directions determined by the flow.

For non-singular dynamics (*i.e.* Hamiltonian systems whose potential energy has a finite lower bound whose absolute value increases at most linearly with  $N$ ), like FPU and similar models<sup>(9)</sup> the above effective equation (3) can be written [31, 41, 35, 32],

<sup>(8)</sup> And the crucial point is just to determine what these two words, *mild* and *reasonably*, actually mean, case by case.

<sup>(9)</sup> Many-body Hamiltonians with Lennard-Jones interactions, short-range coupled rotators,  $\lambda\Phi^4$ -models, and so on.

equivalently<sup>(10)</sup>, as an evolution equation in terms of the *Newtonian* time  $t$ , related to the affine parameter of the geodesic  $s$ , by a transformation  $ds = \mathcal{A} dt$ , where the explicit form of the conformal factor  $\mathcal{A}$  depends on the manifold used [42]:

$$(4) \quad \frac{d^2 Y}{dt^2} + Q(t)Y \cong 0 ,$$

where  $Y(t)$  and  $Q(t)$  are simply related [41, 42, 36], to  $z[s(t)]$  and  $k_R[s(t)]$ , respectively.

Having made a long story short, we arrived at eq. (4) which has been the starting point of a very elegant and effective method [45, 35] of computation of the maximal Lyapunov exponent for mdof Hamiltonian systems. This approach, which make use of the theory of stochastic differential equations [8], has been enormously successful [36].

Briefly, under suitable assumptions, analyzed below, the average growth rates of a solution  $y(t)$  of eq. (4), are determined by the equation for the moments [8, 45]:

$$(5) \quad \frac{d}{dt} \begin{pmatrix} \langle y^2 \rangle \\ \langle \dot{y}^2 \rangle \\ \langle y\dot{y} \rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 & 2 \\ \sigma_Q^2 \tau_Q & 0 & -2Q_0 \\ -Q_0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \langle y^2 \rangle \\ \langle \dot{y}^2 \rangle \\ \langle y\dot{y} \rangle \end{pmatrix} ,$$

where  $Q_0 \doteq \langle Q \rangle$ ,  $\sigma_Q^2 \doteq \langle Q^2 \rangle - Q_0^2$  and  $\tau_Q$  represent, respectively, the average, the variance and the autocorrelation time of the (hypothetically assumed Gaussian) stochastic process  $Q(t)$ . The eigenvalues of the above equations can be easily calculated [8] and, for the present purposes, can be conveniently written in the following form [41]:

$$(6) \quad \mu_1 = 2\sqrt{\frac{Q_0}{3}} \left( g^{1/3} - g^{-1/3} \right)$$

and

$$(7) \quad \mu_{2,3} = -\sqrt{\frac{Q_0}{3}} \left[ g^{1/3} - g^{-1/3} \pm i\sqrt{3} \left( g^{1/3} + g^{-1/3} \right) \right] ,$$

where, for brevity of notation, it has been introduced the quantity  $g$ , defined as

$$(8) \quad g \doteq \xi + \sqrt{1 + \xi^2} \geq 1 ,$$

and, in turn,

$$(9) \quad \xi \doteq \frac{9 \sigma_Q^2 \tau_Q}{8\sqrt{3} Q_0^{3/2}} .$$

From the formulae above a series of results follow immediately:

- A particular form of conservation of volumes in the space of moments; that is  $\sum_{i=1}^3 \mu_i \equiv 0$ .

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<sup>(10)</sup> This point is somewhat controversial, in that there can be, in principle, the possibility that the reparametrization leads to different answers as far as the stability of the flow is concerned [44]. There are however rather stringent arguments to exclude that this could happen for non singular systems, whereas the issue is open for peculiar (*e.g.*, gravitational)  $N$ -body systems.



- As it is always  $g \geq 1$ , it follows that  $\text{Re}(\mu_1) \geq 0 \geq \text{Re}(\mu_{2,3})$ , with equality if and only if  $g = 1 \iff \xi = 0$ .
- From the previous point it follows that, in the space of moments, there are always two *contracting* and one *expanding* (or three *neutral* in the case  $\xi = 0$ ) *eigendirections*.
- This means that, under the assumptions adopted to derive eq. (5), the average asymptotic growth rate of  $|y(t)|$ , *i.e.* the maximal Lyapunov exponent, is

$$(10) \quad \lambda_1 \equiv \mu_1/2 \equiv \sqrt{\frac{Q_0}{3}} \left( g^{1/3} - g^{-1/3} \right) .$$

- Thus, the instability exponent increases from zero, for constant, positive *effective frequency*,  $Q(t)$ , monotonously as the amplitude of fluctuations grows.

Before to discuss the limits of validity of this approach, let us showing how well it works *within* these limits. The reliability of the GDA is witnessed by fig. 2, where, in the upper panel, the maximal Lyapunov exponent is computed according to the Van Kampen-Pettini formula, eq.(10), using the time averages of the geometrical observables [41,32]. As it follows immediately from a comparison with fig. 1, where the Lyapunov exponents are computed using the standard BGS algorithm [46], in the  $\beta\varepsilon$  region of overlap, the agreement is very good<sup>(11)</sup> and the GDA give a much faster and perturbation independent method, which allows to extend the energy and  $N$  ranges of the simulations. However, the simulations performed up to very high energy densities [41] allow to correct the first claims about a scaling of the  $\lambda_1(\beta\varepsilon) \propto (\beta\varepsilon)^{2/3}$ . Indeed, figure 2 shows clearly that, while the scaling  $\lambda_1 \propto \varepsilon^2$  for  $\varepsilon \ll \varepsilon_c$  is confirmed, above the threshold, it is instead  $\lambda_1 \propto \varepsilon^{1/4}$ . This results has very deep implications on the nature of chaos of FPU model; firstly because it raises some questions against the *explanations* of the nature of stochasticity based on *Random Matrices Approximation*. Moreover, the scaling above the SST suggests that the dynamics is in a regime of fully developed stochasticity, in which the diffusion of orbits in phase space proceeds at the maximal rate allowed by the dynamics. The bottom panel of fig. 2 shows indeed the same data of the plot above, where the Lyapunov exponent  $\lambda_1(\beta\varepsilon)$  is multiplied by the *dynamical time*,  $t_D(\beta\varepsilon)$ , of the system, which has been introduced in ref. [32] and whose precise meaning is described below. Furthermore, the extension of numerical simulations to larger  $N$ , confirms the  $N$ -independence of the threshold, thus giving further support to the idea that the SST marks a different transition to chaos with respect to the one predicted on the basis of Nekhoroshev theory.

The above interpretation of a strong chaotic regime above the SST is further confirmed by the comparison of the  $\lambda_1$  values reported in fig. 2, in which the parameters entering eqs. (6), (10) are computed as time average along numerically integrated trajectories, with the analogous results obtained by Pettini and coworkers [45,35], who used the same formula<sup>(12)</sup>, using instead the phase space averages of the same parameters. The results

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<sup>(11)</sup> Notice that data in fig. 1 are expressed in *natural* logarithms.

<sup>(12)</sup> And the Eisenhart geometrization, rather than the Jacobi one. However, for FPU-like systems and for  $N \gg 1$  they are equivalent, as discussed in detail below.

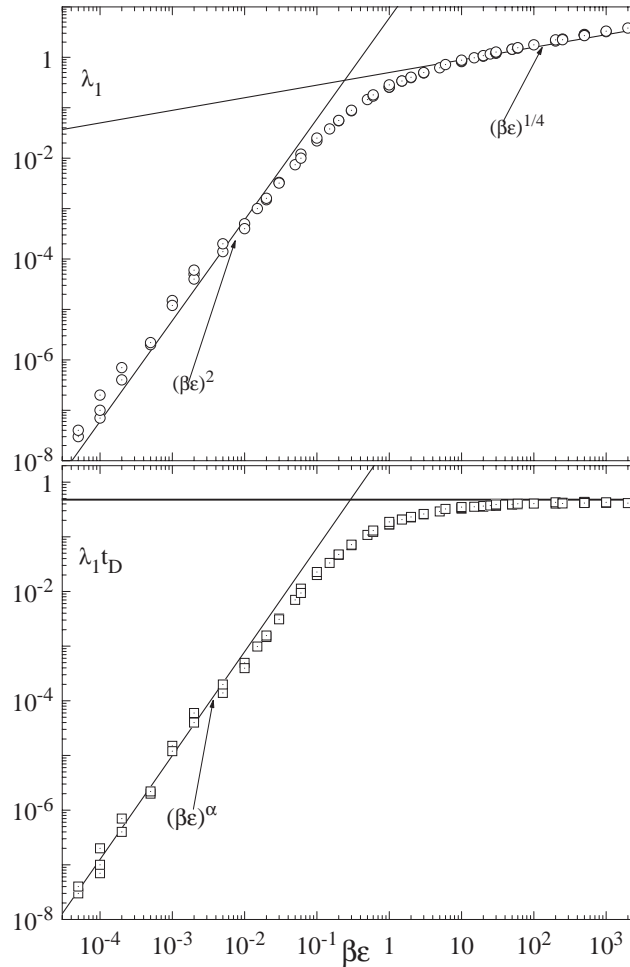


Fig. 2. – The upper plot shows the energy density dependence of the maximal Lyapunov exponent for different FPU- $\beta$  chains. For a given  $\beta\varepsilon$ , are reported the values of  $\lambda_1$  computed according to equation (10), for  $N$  ranging from 50 to 450 and anharmonicity parameter  $\beta$  varying in the interval  $[0.05, 0.2]$ . The significant parameter is clearly  $\beta\varepsilon$ . The lines indicate the slopes  $(\beta\varepsilon)^{-2}$  and  $(\beta\varepsilon)^{1/4}$  and cross each other (conventionally) in correspondence of the SST. In the lower plot the  $\lambda_1$  values are multiplied by the dynamical time,  $t_D(\beta\varepsilon)$ , (see text), showing that the quantity  $\lambda_1 t_D$  is virtually constant above the SST. Below the threshold the slope is  $\alpha \simeq 2$ .

agree completely<sup>(13)</sup>, thus proving that, above the threshold, strongly chaotic dynamics is accompanied by *physical ergodicity*, relaxation is fast for every  $N$  and the equilibrium values do not show any dependence on  $N$  (provided that  $N \gg 1$ ). On the contrary, at low energy densities there is a weak  $N$ -dependence, both in the values of the Lyapunov exponents and in the relaxation rates towards equilibrium.

<sup>(13)</sup> Except at very low energy density, thus confirming a lack of ergodicity in the quasi-integrable limit, or, more probably, very long ergodicity times [47], though, from a physical viewpoints, either interpretation does not make a relevant difference.

**3**1. *Geometric signature of the SST: numerical and analytical evidence.* – Up to now we have mainly reviewed and commented the emergence of the SST from dynamical and statistical viewpoints. It is obvious however that the results based on the computation of the maximal Lyapunov exponent through eq. (10) shows how the geometrical features of the manifold detect, at least indirectly, the transition.

Therefore it is natural to see whether the SST has also a more direct signature within the GDA. We will see that this is indeed the case and, moreover, this will lead also to clarify the meaning of the dynamical time introduced above.

Referring to the literature (*e.g.*, ref. [32]) for the details of the steps leading from eq. (2) to eq. (3), let us start from the explicit expression of the *effective* frequency, as it can be determined, without loss of generality<sup>(14)</sup>, within the Jacobi GDA, for a  $N$ -degrees of freedom *natural* Hamiltonian system, reads

$$(11) \quad Q(t) = \frac{\Delta U}{N} + \frac{(\nabla U)^2}{NW} + \frac{1}{N} \left[ \frac{\ddot{W}}{W} - \frac{3}{2} \left( \frac{\dot{W}}{W} \right)^2 \right],$$

where  $H = (1/2)a_{ij}\dot{q}^i\dot{q}^j + U(\mathbf{q}) \equiv E$  is the conserved Hamiltonian,  $W \doteq (E - U)$  is a shorthand for the total kinetic energy and, as usual, dots stand for (Newtonian-)time derivatives.

For the FPU- $\beta$  system, that is, for chains of  $N$  coupled anharmonic oscillators with Hamiltonian

$$(12) \quad H = \sum_{i=1}^N \left[ \frac{p_i^2}{2m} + U(q_{i+1} - q_i) \right] \quad \text{with} \quad U(x) = \frac{1}{2}x^2 + \frac{\beta}{4}x^4,$$

and, *e.g.*, periodic boundary conditions,  $q_{N+1} = q_1$  and  $q_0 = q_N$ , in the large- $N$  limit, the last two terms in the expression of  $Q(t)$  give essentially no contributions, neither to the average  $Q_0$ , not to the amplitude of fluctuations  $\sigma_Q$ . Also the (squared) gradient term, though with a comparatively weaker  $N$ -dependence, tends to disappear in the thermodynamic limit. All this is well evident from fig. 3, where the numerically computed values of the (time) averages of (rescaled) Ricci curvature (squares)  $\hat{k}_R \doteq 2W^2k_R$ , effective frequency  $Q$  (circles) and Laplacian of the potential energy per degree of freedom  $\Delta U/N$  (triangles) are shown, for FPU chains of different lengths (from  $N = 50$  to  $N = 450$ ), against the parameter  $\beta\varepsilon$ , which measures the departure from integrability. From the figure it emerges clearly that the average values of the three quantities are almost the same, unless conditions very near to integrability are considered and/or the number of

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<sup>(14)</sup> It is obviously out of place here, but it can be easily shown [42] that the different GDA's, based on Jacobi (Riemannian), Eisenhart (pseudo-Riemannian) or Finsler geometries, differ only in the ranges of applicability; and that, for *natural and non singular* Lagrangian systems, which can be *geometrized* in all the settings, all them give the same results *as long as the number of degrees of freedom is large!* The differences between the various geometrizations indeed vanish in the large  $N$  limit (at least) as  $E/N^2$ , where  $E$  is the total energy. If the governing interaction is *stable* [48], then it follows that, in the large  $N$  limit, all the results are independent from the particular geometrization adopted. This, again, is not necessarily true if the interaction potential is not stable, in which case some differences could survive.

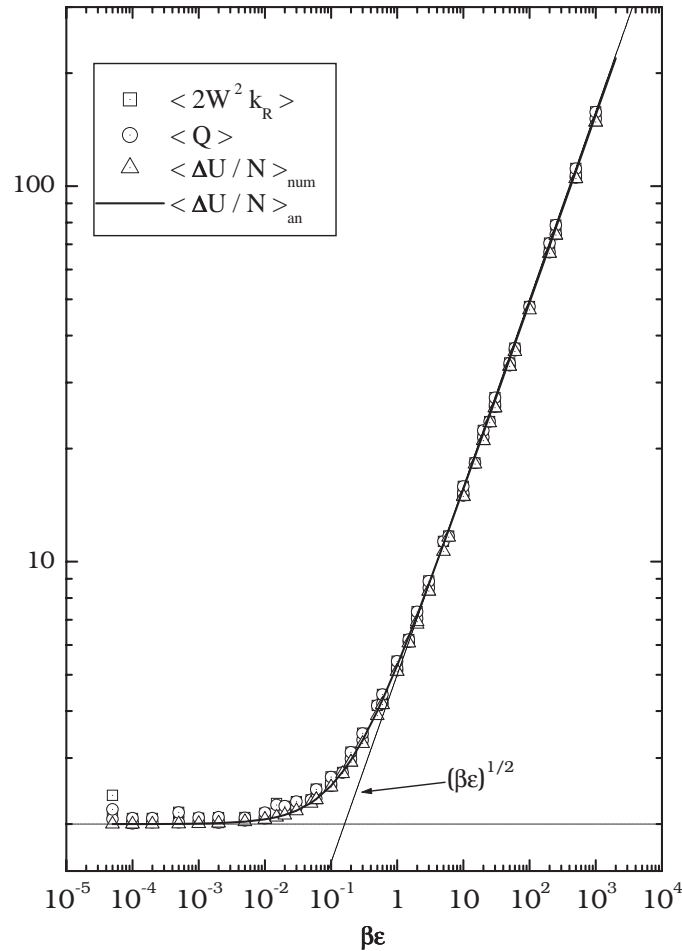


Fig. 3. – Energy density dependence of curvature related quantities. Circles, squares and triangles refer, respectively, to the averages of  $k_R$ ,  $Q$  and  $\Delta U/N$ , computed along numerically integrated trajectories of FPU chains with  $N$  ranging from 50 to 450 and anharmonicity parameter  $\beta$  varying in the interval  $[0.05, 0.2]$ . Data are taken from ref. [41]. The significant parameter is clearly  $\beta\varepsilon$ . The thick curve refers to the analytical formula described in the text, while the thin lines are simply a guide for the eyes and help to locate the geometrical (counterpart of the) threshold.

degrees of freedom is small<sup>(15)</sup>. From this and the inspection of eq. (11), it is clear that, at least for FPU chains, the terms additional to the Laplacian in the expression for  $Q(t)$  give a negligible contribution to the average. It can be verified [41] that, as far as the amplitude of fluctuations is concerned, the situation is almost the same, with some greater discrepancies for low  $N$  at very small energy densities. Thus we can conclude that, at least enough far from the quasi-integrable regime and for sufficiently large  $N$ ,

<sup>(15)</sup> For a given value of  $\beta\varepsilon$ , multiple values of dependent variables are plotted, for different values of  $N$ , though in most cases they virtually coincide.

the stability of motions depends only on the behaviour of the Laplacian term appearing in  $Q(t)$ <sup>(16)</sup>.

In the case of FPU models, for many geometric quantities it is also possible to obtain reliable (semi-)analytical estimates. Indeed, if we define  $\langle \delta q \rangle \doteq \langle q_{i+1} - q_i \rangle_i$  and put

$$(13) \quad \eta \doteq \frac{\langle \delta q^4 \rangle - \langle \delta q^2 \rangle^2}{\langle \delta q^4 \rangle} ;$$

using the virial theorem in its most general form, we find that the ratio between anharmonic and harmonic potential energies depends only on  $\beta\varepsilon$  and  $\eta$

$$(14) \quad \frac{\langle U_4 \rangle}{\langle U_2 \rangle} = \frac{1}{3} \left( \sqrt{1 + 3\beta\varepsilon(1 + \eta)} - 1 \right) .$$

Using again the virial, an analytic expression for the Laplacian is found:

$$(15) \quad \frac{\Delta U}{N} = 2 + \frac{4}{1 + \eta} \left( \sqrt{1 + 3\beta\varepsilon(1 + \eta)} - 1 \right) .$$

From numerical simulations it is easy to obtain a numerical estimate of the correlation term  $\eta$  and, finally, the closed form:

$$(16) \quad \frac{\Delta U}{N} = 2 \left[ 1 + \left( \sqrt{1 + 6\beta\varepsilon} - 1 \right) \right] ,$$

which is plotted as a continuous (thick) line in the same figure 3 and is in very good agreement with *experimental* data.

Moreover, we see that the GDA give a consistent, direct and convincing evidence of the existence and location of the SST. It can be conventionally located by the crossing of the two asymptotic behaviours of the Laplacian, and a direct comparison with the plot of the scaling of the maximal Lyapunov exponent of fig. 2 show the good agreement between the dynamical and geometrical signatures of the threshold. Along with the equally well convincing correspondence between dynamic and statistical mechanical thresholds, this completes the path from SM to GDA.

**3.2. The dynamical time scale and the adimensional instability indicator.** – The steps which allow an analytical estimate of the scaling of  $\Delta U(\beta\varepsilon)/N$ , turn out to help the explicit computation of the above introduced dynamical time scale,  $t_D(\beta\varepsilon)$ ; which, at a heuristic level, gives the overall rescaling, when the energy density changes, of any dynamical process occurring in the chain.

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<sup>(16)</sup> Nevertheless, it should be emphasized that the approach necessarily fails in the quasi-periodic regime and at small  $N$ , where, for example, negative values of the curvature  $k_R$  occur more frequently than in the high energy regime, and persist for very long transient periods. This is clearly due to the large collective oscillations accompanying the virialization process, during which the terms containing the time derivatives in eq. (11) can assume relatively large values. The combined effects of small  $N$  (these terms vanish in the TL at least as  $N^{-1/2}$ ), along with the very slow *phase mixing* due to quasi periodic behaviour [41, 32] invalidate the starting assumptions at the grounds of the approach leading to eq. (10).

It is well known, indeed, that in FPU-like models it is possible to introduce the normal modes frequencies, which describe the hierarchy of time scales associated with the dynamics of phonon-like excitations. Those frequencies do not depend however on the energy density, have always a maximum which is  $\mathcal{O}(1)$ , whereas the lowest frequencies scale as  $\mathcal{O}(1/N)$ . To the extent that the chain is near the integrable (*e.g.*, harmonic) limit, normal modes frequencies suffice to describe the dynamics of the system; however, when the departure from integrability is strong, *i.e.* when the anharmonic interaction tends to become comparable with the harmonic one, the normal modes hierarchy does not more describe correctly the internal dynamics (and even the very definition of normal modes loses partially its meaning).

There are several ways to extract an energy dependent overall time scale for anharmonic systems, many of them can be based simply on dimensional arguments and give the correct qualitative behaviour [41]. In order to obtain a more *quantitative* estimate, we proceed in complete analogy with what is done in stellar dynamics, where a proper (dynamical) time scale is defined with the *typical* time required for a star to cross the system. In that case it is assumed a sort of energy equipartition between the stars, and in this case we have to make a similar assumption, which, however, *cannot be extended to the normal modes*, just because for them it is clear that equipartition holds *only after the systems has relaxed* and the conditions for the equipartition among them is one of the main issues. The simplest and most safe assumption, rigorously verified by *inverse experiments* of any kind, is that each oscillator has, on the average, the same energy. As the FPU system is an extensive one, independently of the  $N$  and  $\varepsilon$  values, we can assume that this average energy is of the order of the energy density itself. Simple dimensional arguments indicate that the  $t_D(\beta\varepsilon)$  scaling is related to the ratio of the anharmonic to the harmonic potential energies. We write, for the maximal values of these potential contributions to the total energy, respectively,  $U_{4\text{MAX}}$  and  $U_{2\text{MAX}}$ , and the rather intuitive parametric pair of equations:

$$(17) \quad U_{2\text{MAX}}(\eta) = E \cos^2 \varphi \quad \text{and} \quad U_{4\text{MAX}}(\eta) = E \sin^2 \varphi ,$$

where  $\eta$  has been defined in eq. (13) and  $\varphi = \varphi(\eta)$  is an obvious measure of the departure from the harmonic regime.

Using the virial theorem, in complete analogy as before for the determination of the analytic formula for  $\Delta U$ , a quantitative expression for the dynamical time scale is found:

$$(18) \quad t_D(\beta\varepsilon) = 2\sqrt{2} \frac{[\sqrt{1 + 4\beta\varepsilon(1 + \eta)} - 1]^{1/2}}{[\beta\varepsilon(1 + \eta)]^{1/2}} \int_0^1 \frac{dx}{\sqrt{1 - x^2 \cos^2 \varphi - x^4 \sin^2 \varphi}} .$$

Taking into account that from numerical simulations we have a precise measure of  $\eta$ , the expression for  $t_D$  can be written in closed form as

$$(19) \quad t_D(\beta\varepsilon) = 4[\Theta(\beta\varepsilon)]^{1/2} \mathcal{E}_K \left[ [1 - \Theta(\beta\varepsilon)]^{1/2} \right] ,$$

where  $\mathcal{E}_K(x)$  is the complete elliptic integral, defined in terms of the incomplete elliptic integral,

$$\mathcal{E}_F(z, x) = \int_0^z \frac{dt}{\sqrt{1 - t^2} \sqrt{1 + x^2 t^2}} ,$$

as  $\mathcal{E}_K(x) \doteq \mathcal{E}_F(1, x)$ ; and we defined moreover,

$$\Theta(\beta\varepsilon) = \frac{\sqrt{1 + 8\beta\varepsilon} - 1}{4\beta\varepsilon} .$$

Despite its seemingly complicate expression, the essential  $\beta\varepsilon$ -dependence in the above equation is almost completely represented by the  $\Theta^{1/2}$  term. Indeed, the argument of the elliptic integral varies only in  $[0, 1]$  and the variation of  $\mathcal{E}_K(x)$  within this range is very small. In the harmonic limit,  $\beta\varepsilon \rightarrow 0$ , it is evident that  $\Theta \rightarrow 1$ , and then

$$\lim_{\beta\varepsilon \rightarrow 0} \mathcal{E}_K[(1 - \Theta)^{1/2}] = \mathcal{E}_K(0) = \frac{\pi}{2} \cong 1.5708 \dots .$$

On the other hand, when  $\beta\varepsilon \rightarrow \infty$ ,  $\Theta(\beta\varepsilon) \rightarrow (\beta\varepsilon)^{-1/2}$ , so that

$$\lim_{\beta\varepsilon \rightarrow \infty} \mathcal{E}_K[(1 - \Theta)^{1/2}] = \mathcal{E}_K(1) = \frac{\pi^{3/2}\sqrt{2}}{4 [\Gamma(\frac{3}{4})]^2} \cong 1.311 \dots .$$

Incidentally, as  $\Theta(\beta\varepsilon) \sim (\beta\varepsilon)^{-1/2}$  at high energy, eq.(19) shows that in the high energy density regime it is  $t_D \propto (\beta\varepsilon)^{-1/4}$ . Recalling the scaling of the maximal Lyapunov exponent above the SST, this result *explains* the significance of the lower panel in fig. 2, *i.e.* why  $\gamma_1 \doteq \lambda_1 t_D$  is almost exactly constant above the threshold, an observation of crucial relevance for the interpretation of the nature of the chaotic behaviour above the SST.

It must be observed that the result of the above computation differs very much *in the form* from those based on more naive approaches. For example, an estimate based on simple dimensional arguments leads to the much simpler expression

$$(20) \quad t_{D_a}(\beta\varepsilon) = \left[ 1 + \frac{2}{3} \left( \sqrt{1 + 3\beta\varepsilon} - 1 \right) \right]^{-1/2} ,$$

which, as shown in fig. 4, gives values appreciably different from those obtained from the *exact* equation (19). Nevertheless, if the dimensional arguments are complemented by numerical estimates on the degree of correlations among nearby sites, then the results obtained are in a much better agreement with the *exact* ones, though, formally, the corresponding expressions still differ from eq. (19).

To illustrate this fact, in fig. 4 we report, along with the *exact* and the *naive* curves predicted by eqs. (19) and (20), respectively, also two other semi-analytical estimates, based on the virial theorem and numerical estimates of suitable correlation functions, reading as

$$(21) \quad t_{D_b}(\beta\varepsilon) = \left[ 1 + \frac{2}{3} \left( \sqrt{1 + 6\beta\varepsilon(1 + \zeta)} - 1 \right) \right]^{-1/2}$$

and

$$(22) \quad t_{D_d}(\beta\varepsilon) = t_{D_d}(0) \left[ \frac{\sqrt{1 + 4\beta\varepsilon(1 + \eta)} - 1}{\frac{4}{3}\beta\varepsilon - \frac{2}{9(1+\eta)} \left[ \sqrt{1 + 3\beta\varepsilon(1 + \eta)} - 1 \right]} \right]^{1/2} ,$$

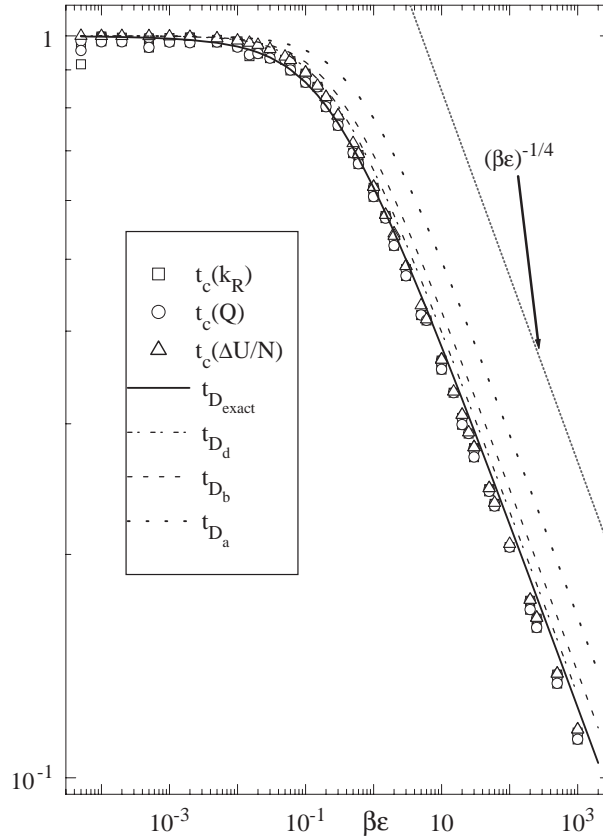


Fig. 4. – The curves show the behaviour of the analytical estimates of the dynamical time scale,  $t_D(\beta\varepsilon)$ , according to the various formulas discussed in the text. The line on the right indicates the asymptotic behaviour of all the above estimates,  $t_D(\beta\varepsilon) \propto (\beta\varepsilon)^{-1/4}$  and the symbols represent the numerical estimates of the dynamical periods associated to the *effective* frequencies governing the evolution of perturbations within the GDA.

where  $\eta$  is the same quantity defined above, eq. (13), and  $\zeta$  is related to the correlations of the form  $\langle q_i q_{i+1} \rangle$  and similar ones.

Despite that rather different look, the last two estimates are in satisfactory agreement with the exact one; and, moreover, they agree rather well even with *experimental* values, shown also in fig. 4. The different symbols represent the *experimental*, numerical determinations of the correlation times for the geometrical and dynamical quantities determining the evolution of perturbations, that is  $\hat{k}_R$ ,  $Q$  and  $\Delta U/N$ . The analytical estimates, except the one given by eq. (20), are in a complete agreement with the numerical data. The *exact* expression is only slightly better than those based on dimensional arguments alone, pointing out how the virial theorem, in its more general form [41, 32, 49], captures all the essential time-energy scaling of internal dynamics.

The previous results show that, starting from two completely separate approaches, it is found that the scaling of the instability time, as measured by the (reciprocal of the) maximal Lyapunov exponent, and the dynamical time, for the FPU- $\beta$  model, scale, in



the strong stochastic region, exactly at the same rate<sup>(17)</sup>.

This evidence, suggests a new *invariant* criterion to detect the SST, or, more precisely (and generally), the onset of the regime in which the spreading of orbits proceeds at the maximal rate allowed by the underlying dynamics. It can be defined using the adimensional chaoticity indicator  $\gamma_1 \doteq \lambda_1 t_D$ : the onset of fully developed stochasticity is detected by the constancy of the indicator  $\gamma_1$ .

This rather trivial generalization has some relevant consequences in those frameworks where the time scales of the systems under study change rapidly varying some parameters (*e.g.*, the energy, the external field, etc.), and also for systems undergoing intermittent evolution, where quiescent and irregular phases are intermingled and characterized by very different time scales. Furthermore, *the introduction of an adimensional instability measure, get rid of most of the ambiguities raising in those settings where the choice of the appropriate evolution parameter (e.g., in general relativistic dynamical systems) is an issue.*

Among the most important problems which can get some important hints from the above discussion, I mention briefly the issue of the statistical mechanical and thermodynamical description of  $N$ -body self-gravitating systems. For them the above analysis has some noteworthy consequences [50, 51]: it is found that, with all the remarks and warnings appropriate to their intrinsically peculiar nature<sup>(18)</sup>, it can be guessed that they are, at any binding energy, in a state of strong stochasticity. On the basis of a *fast mixing hypothesis* [50, 51], this allows to propose a coherent thermodynamic setting, which give a dynamical justification to many phenomenological descriptions adopted previously.

Referring to the cited bibliography for a complete account of the suggestions and results which can be obtained from the GDA in order to understand better the onset of instability in more general Hamiltonian systems than FPU-like models, I will conclude this contribution trying, as said in the Introduction, to deepen the investigation of the *dark side*: in the next section a list of concrete and practical remarks are presented which should be taken into account, *before* to carry out any direct extension of the approach.

#### 4. – Check of the hypotheses at the ground of the analytical computation of the maximal Lyapunov exponent

Already the steps illustrated in the previous section point out that a critical reconsideration of the general setting is in order if an extension of the framework to systems of different nature than FPU-like models is sought. Therefore, we recall the key hypotheses at the grounds of the method and proceed to verify their limits of validity:

- The fundamental assumption for the application of the Van Kampen formulae, is that the (squared) *frequency*,  $Q(t)$  represents a faithful realization of a stochastic process. This amounts to say that the distribution of the  $Q$  values should be reasonably well described by a gaussian and that the autocorrelation function of

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<sup>(17)</sup> This derivation, incidentally, devoids of any content the assert, sometimes reported, according to which the dynamical time is *defined* as the reciprocal of the maximal LCN: the dynamical time exists and is finite, according to the above prescription, even for completely integrable systems, when the Lyapunov time is infinite!

<sup>(18)</sup> And already pointed out by Gurzadyan and coworkers in a series of papers [52, 53].

$Q(t)$  can be approximated, on the time scales of the evolution, as a  $\delta$ -function, *e.g.*,

$$\langle Q(t+t')Q(t) \rangle \cong Q_0^2 + \sigma_Q^2 \tau_Q \delta(t').$$

- From a physical perspective, this amounts to say that the evolution of  $Q(t)$  must be fast with respect to the dynamical time scales. Geometrically, this means that the *effective* curvature is a strongly fluctuating quantity.
- To the above arguments, it must be added the following trivial consideration: in all the derivations it is assumed that  $Q(t)$  is a non-negative quantity, although it can be argued that, if the probability of occurrence of negative values is sufficiently small, then the growth rate of the solution is accurately represented by  $\lambda_1$ . Thus, it follows that, if the amplitude of fluctuations exceeds the average value,  $\sigma_Q > Q_0$ , then the frequency cannot longer be assumed as positive definite, and the approach does not work anymore.
- A further obvious breakdown of the method occurs when the dynamic evolution is quasi-periodic. In such a case, indeed, independently of the amplitude of fluctuations, the values of  $\xi$  and  $g$  can be arbitrarily large, and so  $\lambda_1$  can formally increase even if the underlying dynamics is not chaotic<sup>(19)</sup>.
- As, in practice, the  $Q(t)$  is self-consistently generated by the dynamics itself, and depends on the evolution of *state space* coordinates of the system, it is clear that a full justification of the validity of the approach must be always checked *à posteriori*. That is, if the underlying dynamics is *not enough chaotic*, then the fluctuations of  $Q(t)$  cannot be assumed as stochastic, and the instability rate predicted by the use of Van Kampen formula can be, at best, an upper limit to (twice) the true Lyapunov exponent.
- Stated otherwise, eq. (6) is hardly valid in the quasi-constant curvature limit. It could be guessed that there must exist some threshold  $\xi_+$ , below which the predicted instability exponent cannot be exact. However the estimate of this possible limiting value is not so immediate. Indeed, if it is clear that the shorter the correlation time  $\tau_Q$ , the greater must be the fluctuations, in order to keep constant the value of  $\xi$  (and, then, of  $g$ ), on physical grounds, it is instead plausible that, for very short correlation times, even small fluctuations can lead to stochasticity. Indeed, it follows from eq. (10) that, in the small fluctuation and small correlation times, that is, for  $\xi \rightarrow 0$ , it is  $\mu_1 \propto Q_0^{1/2} \xi$ .
- It is otherwise clear that in the opposite limit, that is for  $\xi \gg 1$ , the above formula is not more justified. In fact, neglecting numerical factors, we have

$$\xi \sim \left( \frac{\sigma_Q^2}{Q_0^2} \right) \frac{\tau_Q}{t_G},$$

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<sup>(19)</sup> This is indeed what is really observed for nearly integrable conditions and when the number of degrees of freedom is not large enough, so that statistic relative fluctuations, of order  $\mathcal{O}(N^{-1/2})$ , mimic true curvature fluctuations. In these cases the Van Kampen-Pettini formula, eq. (10), clearly overestimates the instability rate.

where  $t_G \doteq Q_0^{-1/2}$  sets a sort of *geometro-dynamical time scale*. Thus, values of  $\xi$  greater than a few units, immediately imply the failure of at least one of the assumptions: if  $\xi \gg 1$ , then, necessarily it must be either  $\sigma_Q \gg Q_0$  or  $\tau_Q \gg t_G$  (or both). In the first case the hypothesis of a positive *frequency* is not more verified, in the second even the very definition of  *$\delta$ -correlated stochastic process* could be questioned. Furthermore, in the limit  $\xi \gg 1$ , the expression for the instability exponent can be rewritten as

$$\lambda_1 \sim t_G^{-1} \xi^{1/3} ,$$

which, to my knowledge, has never been observed. What happens, in FPU-like models, is that, increasing the energy, and then the degree of chaos, the correlation time goes to zero (as shown in the previous section and in fig. 4) so that the limit  $\xi \gg 1$  is never reached, except when the number of degrees of freedom is so small that the existence of conserved quantities introduces quasi periodicities and spurious long time correlations, even in the presence of chaotic dynamics.

As we have seen, in the case of FPU model it is easy to test the validity of the approach against the possible sources of inconsistency listed above. Both the Gaussian distribution of the  $Q$  values can be checked and the autocorrelation time  $\tau_Q$  can be either analytically estimated and numerically computed [41]. The limits of validity of the Van Kampen-Pettini formula are easily located and the results obtained are in a comfortable agreement with those obtained with other approaches.

Figure 5 shows, for an intermediate energy density, that the gaussian distribution of *curvatures* and *frequencies* is indeed a rather well satisfied hypothesis, both for what concerns their values and (still better) for their time-derivatives as well. It must be mentioned that, while the distributions of the Laplacian and of Hill's frequency  $Q$  share common averages and widths, the  $k_R$ -distribution is much broader. This evidence hints at reconsidering the applicability of the Van Kampen-Pettini approach within the *purely* geometrical setting related to the Jacobi metric. Though this remark is not of so much relevance for the FPU models, it can have deep impact on the general applicability of the method. In particular, in the case of large fluctuations all the results appealing to the existence of an *average* curvature lose their justification.

Let us then analyze from where the most serious hindrances to the application of the method above can originate, considering that we have in mind the extension of the approach to the gravitational  $N$ -body problem.

- For systems with non smooth interactions, the curvature fluctuations are usually much bigger than for FPU-like potentials, unless there is a minimum in the interaction potential (*e.g.*, LJ or Morse systems) and the energy density is slightly above that minimum. This amounts to say that fluctuations are comparable with mean values as soon as the departure from the *integrable limit (if it exists!)* is appreciable.
- Nevertheless, non smooth potentials usually imply a very large spectrum of time scales and often also non homogeneous distributions. This partially can compensate the consequences of the previous remark, as it can lead to very fast decay of correlations, that is to very small correlation times.
- Obviously, large fluctuations imply that the assumption of an everywhere positive curvature is hardly fulfilled. In the case in which the frequency of negative values

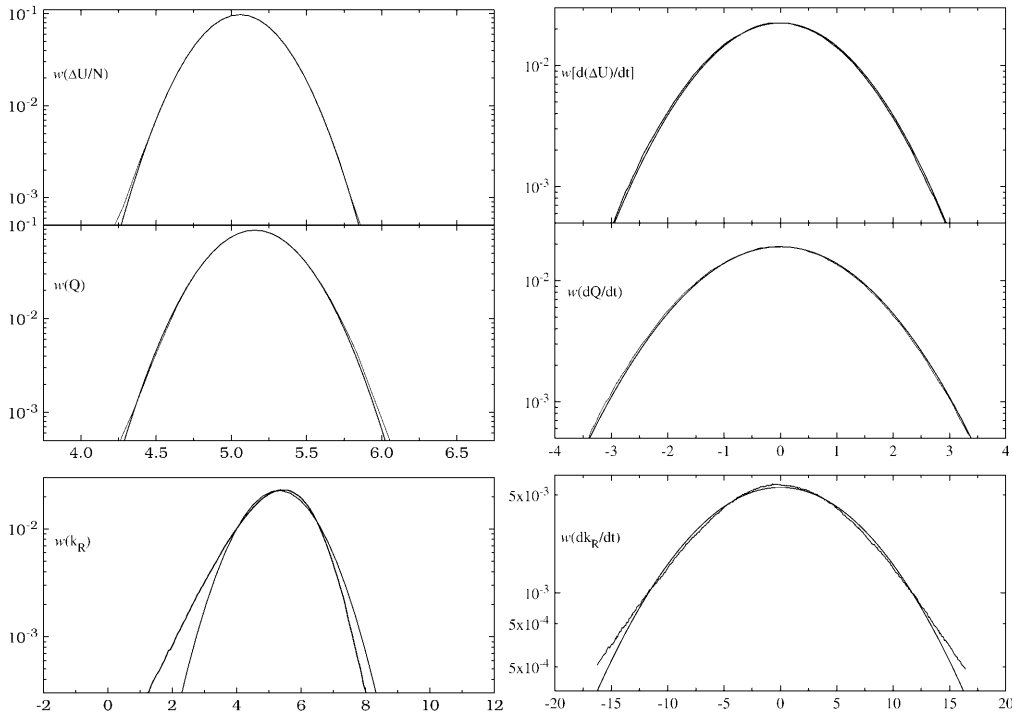


Fig. 5. – Check of the Gaussian distribution of the values of *curvature* and *frequencies*. A) In the left column, from bottom to top, are shown, respectively, the distributions of  $k_R$ ,  $Q$  and  $\Delta U/N$ . Thick curves represent the actual distributions as obtained from long time numerical integrations of dynamics (data taken from [41]), while thin curves represent the best fits with a Gaussian (N.B.: notice that vertical scales are in log-scale). B) Distributions of the time derivatives of the quantities represented in A). Except for the Ricci curvature  $k_R$ , where a clear asymmetry is evident, all other quantities are well distributed according to a Gaussian. Data refer to an intermediate value of  $\beta\varepsilon$ , near the SST.

is appreciable, instability can originate both from mechanisms like those described above, and also from the local instability related to negative curvature. Any attempt to estimate analytically the instability growth rate is in such cases hopeless. At the other extreme, if the curvature is almost everywhere negative, then the estimate of the instability time is possible, though this is not the case for almost any realistic model of physical many degrees of freedom system<sup>(20)</sup>.

- In systems with non extensive interactions (*e.g.*, self-gravitating  $N$ -body systems), a strongly unstable evolution, with fast *phase mixing* and decay of correlations, can coexist with very long time correlations of collective degrees of freedom, associated, for example, with the *Virialization* process (*e.g.*, with the *Violent Relaxation*

<sup>(20)</sup> Though there is no rigorous proof of this statement. For instance, V. Gurzadyan (private conversation, see also ref. [34]) confirmed to the author that spherical stellar systems constitute probably an example of a system for which the assumption of almost everywhere negative curvature can be verified rigorously.

phase). A signature of this phenomenon, though with much weaker consequences, is present even in the FPU model, where the probability of negative curvature values is relatively high when the system is left to evolve from initial conditions far from (global) equilibrium. After that equilibrium is attained, that probability becomes vanishingly small [32].

- Obviously, systems with singular interactions, in consequence of what stated above, support even more reliably the assumption of uncorrelated fluctuations, just because a singular two body interaction can occur almost independently from a previous one [54]. Furthermore, the hypothesis of uncorrelated fluctuations depends crucially on the dimensionality of the systems, being much more easily fulfilled in 3D-systems than in one-dimensional chains.
- Most of the results on FPU-like models, and in particular the analytical computations of  $\lambda_1$  on the basis of eq. (10), greatly profited of the possibility of canonical estimates of geometric quantities [35]. This is legitimate in systems like FPU, provided that ergodicity (and mixing) can be safely assumed. Indeed, in this case, time averages coincide with microcanonical phase averages. As the system is *tempered* and *stable*, then the *rigorous theorems* [48] assert that microcanonical and canonical averages coincide in the TL (differences being at most of order  $\mathcal{O}(1/N)$ ). Indeed the results obtained in [41, 32], through dynamical (*i.e.* microcanonical) numerical integrations of equations of motion show a very good agreement with those obtained in [45, 35, 36], using phase space averages. Clearly both the logical steps above can be questioned for systems with non compact phase space and non-extensive interactions: ergodicity and mixing cannot be rigorously defined and the equivalence between microcanonical and canonical ensembles does not hold. In refs. [50, 51] possible solutions to these issues are discussed.
- The above points can be summarized saying that, while for FPU-like models it is clear that fluctuations are responsible for the onset and development of chaos, this simple paradigm cannot be extended to *peculiar* Hamiltonians. This also because, in the most general case, the simple order of magnitude estimates which allow to claim, for FPU, that in the large- $N$  limit the fluctuations come essentially only by the first two terms in the right hand side of eq. (11), are not so easy, and the relative weight, in the fluctuations, of various terms must be checked carefully.
- Although the dynamics of singular systems can be, in a sense, strongly chaotic, it is possible that some relevant collective quantities, included those used in the GDA, can have virtually infinite ergodicity times, so that phase and time averages lead to conflicting indications.

Notwithstanding all the remarks above, it is worth to emphasize that the GDA helps to deepen the understanding of the interplay between the energy and time scales, leading naturally to operate a due distinction between *mathematical and physical ergodicities*, arguing that the latter (alone) can be relevant for a statistical mechanical description. As remarked already before, as long as the system is above the SST, that is, if the dynamics is strongly chaotic, then a complete and precise agreement exists between the time and phase averages of any geometrical and dynamical observable. However, the agreement remains very good even below that threshold if the number of degrees of freedom is large enough. The *ergodicity times*, however, increase rapidly with  $N$ . It is puzzling to observe that the same happens for, *e.g.*, self-gravitating systems, notwithstanding they seem to

be in a dynamic regime at least as chaotic as FPU chains well above the SST. This points out once more that the *analogic method* is often a good guide to guess the behaviour of more complex problems, but, if left alone, without any further rigorous investigation, can sometimes lead to dangerous conclusions.

## 5. – Epilogue

I started my Ph.D. as an astrophysicist, (at least, this is what I was believing). For a true trick of the fate, I met the FPU problem, without intention, and this problem became afterward my principal interest for two years, forming then the core of (more than half of) my Ph.D. Thesis.

I cannot say whether the crossing of my life with the FPU problem was lucky or not, what is sure is that it marked a *threshold*, and as such, I feel still today, fascinated and at the same time frightened by its immense richness of faces and traps. And this is amazing, because I was attracted by the FPU problem because of its deceptive simplicity, as, perhaps [55], many others. Yes, indeed what surely I like is the Fermi's first approach to problems, "*based on simple math*"; and I tried, in the pages above, to learn the Fermi's lesson, avoiding to take for granted what is not demonstrated, without however to give up to being guided, in the first investigations, by intuition and analogies. Probably I didn't succeed more than slightly; nevertheless I hope that the few good remarks can be useful to my own future works and, perhaps, also to other people.

People who worked with Fermi learned from him how to face physical problems; they better than others can pass to us the atmosphere around him at work.

It seems appropriate to finish with these few notes, by Stan Ulam [24], which was involved with Fermi in the project and realization of the study which has been the central point of this contribution. They point out once more how Fermi's personality reflected coherently in his work.

*"His [Fermi's] eyes, darting at times, would be fixed reflectively when he was considering some questions. He would try to elucidate other persons thoughts by asking questions in a Socratic manner, [...] . I think he had a supreme sense of the important. He did not disdain work in the so-called smaller problems; at the same time, he kept in mind the order of importance of things in physics. This quality is more vital in physics than in mathematics, which is not so uniquely tied to reality". (p. 15)<sup>(21)</sup>.*

*"As soon as the machines were finished, Fermi, with his great common sense and intuition, recognized immediately their importance for the study of problems in theoretical physics, astrophysics and classical physics". (p. 19).*

And, after a personal reflection [24] (p. 19), "*Now Banach, Fermi and von Neumann were dead—the three great men whose intellects impressed me the most.*"; another Ulam's memoir on Fermi, reported by a close friend of him [24] (p. 27): "*[Ulam] admired Fermi's genius for solving physical problems with the minimum amount of math. Since that time Fermi remained for him the ideal of a scientist. In his old age he liked to repeat that Fermi had been the last physicist*".

\* \* \*

To MARIA TERESA, for her patience and for having forced me to go a little beyond

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<sup>(21)</sup> That is, a physicist should not *be fascinated* by elegant mathematical approaches, unless they improve the physical understanding of the phenomena.

*simple calculations.* To R. RUFFINI for his impromptu flashing suggestions, whose number has been (unfortunately) decreasing over the years, because of the divergence between our interests. This however did not prevent him to unselfishly support my activities. To M. PETTINI and L. GALGANI, for continuous moral encouragements and many interesting discussions. To A. POLITI, for many seemingly unrelated discussions, not really so; and also for his tolerance. To V. GURZADYAN: I have profited very much, since the beginning of my study in this field, from periodic exchange of ideas with him, although often without each other agreeing with other's opinion. I remember the many repeated efforts, made together with G. PUCACCO and D. BOCCALETTI, trying to understand a little more on geometry, statistical and classical mechanics. The author is partially supported by CSS under the initiative n.2002B:CaPMeP.

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